TOPICS IN THE THEORY OF EXCITATIONS IN GRANULAR MATTER

DISSERTATION

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ABSTRACT

We use theoretical methods to study properties of excitations in various granular materials. We begin with three topics involving superconducting qubits. First, a three Josephson-junction persistent-current qubit is considered, with two junctions being identical, and the third junction differing from the other two by a factor of $\alpha$ in Josephson energy and capacitance. We show that when $\alpha > 1$ and the bias voltages are such that the total charge stored on the two gate capacitors is an odd multiple of electronic charge, the two levels of the qubit become degenerate. Secondly, energy loss of a Cooper-pair box (CPB) capacitively coupled to a nanomechanical oscillator (NMO) is studied within the rotating wave approximation (RWA). We show that the energy decay rate of the CPB can be decreased by coupling it to a high quality factor ($Q$) NMO. Finally, we extend the last study beyond the RWA.

Four topics in the theory of superlattices are considered next. First, an electronic graphene superlattice is studied. We show that if graphene is subjected to the potential from an external superlattice, a band gap develops at the Dirac point provided the superlattice potential has broken inversion symmetry. Secondly, a magnetic superlattice of periodically arranged ferromagnetic cylinders embedded in a different ferromagnetic host is considered. We show that when the two ferromagnets have different Gilbert damping factors, this superlattice acts as a waveguide for spin waves. Thirdly, a photonic superlattice of silicon (Si) dielectric cylinders in air is considered.
A simple method for calculating the effective dielectric constant $\epsilon_e$ of the superlattice is presented. Finally, we show the presence of a Dirac point in the photonic band structure of a triangular superlattice of Si cylinders in air.

The final topics presented involve inhomogeneous carbon based materials. We use an effective medium approximation (EMA) to calculate the magnetoresistance of a graphene sheet broken into $n$-type and $p$-type puddles. Finally, we use EMA to show that the effective sound speed of a suspension of carbon nanotubes in dimethyl formaldehyde (DMF) is lower than the sound speed in pure DMF.
Dedicated to my mother Mrs. Jagadamba Tiwari.
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CHAPTER 1

INTRODUCTION

This dissertation is divided into three parts. The first part (Chapter 2) on superconducting qubits is divided into three topics. The first topic is a persistent-current superconducting qubit (phase qubit) with three Josephson-junctions. When the bias voltage on the gate capacitors is such that the total charge stored on the gate capacitors is an odd multiple of an electronic charge, the two levels of the qubit become degenerate. Tunnelling between these states is suppressed due to completely destructive interference between various tunnelling paths. The second topic is the energy decay of a Cooper-pair box (CPB) qubit capacitively coupled to a nano mechanical oscillator (NMO) calculated within the rotating-wave approximation (RWA). The qubit decay rate is decreased by coupling it to a high-$Q$ NMO. The last part of this chapter extends the study of a coupled CPB and NMO to regimes where the RWA is invalid by using first a second-order perturbation theory on the coupled system and then using a first-order time-dependent perturbation to calculate the decay rates.

The second part of the dissertation (Chapter 3) on electronic, magnonic and photonic superlattices is divided into four topics. The first topic is an electronic superlattice on graphene. By breaking the inversion symmetry of the superlattice potential a tunable band gap can be opened at the Dirac point in graphene, which is otherwise
a semimetal. The second part shows that a two-dimensional magnonic superlattice acts as a waveguide for spin waves, by allowing spin waves to have a much higher dissipation in most directions but a lower dissipation in one particular direction. In the third and fourth sections, photonic superlattices are considered. The third topic is a method of finding an effective dielectric constant of photonic superlattices using an analog of $\mathbf{k} \cdot \mathbf{p}$ perturbation theory. In the last part a triangular photonic superlattice with a *Dirac point* is considered, and a tunable band gap is opened up at the Dirac point by breaking the inversion or time-reversal symmetry of the superlattice.

The last part of this dissertation (Chapter 4) describes applications of *effective medium approximation* (EMA) to explain some experimental results on magnetoresistance of graphene and sound speed in a suspension of carbon nanotubes. The first application of EMA explains the experimentally observed large magnetoresistance in graphene which has broken down into $n$ and $p$ type puddles. The second application of EMA explains the experimentally measured anomalous behavior of the speed of sound in a system of carbon nanotubes suspended in dimethyformaldehyde (DMF).

Chapter 5 summarizes the various topics considered in this dissertation, and provides further discussion of the results.
CHAPTER 2

SUPERCONDUCTING QUBITS

2.1 Introduction

A bit (0 or 1) is the fundamental concept of classical computation and information. Quantum computation and information are built upon an analogous concept, the quantum bit, or qubit for short. The difference between bits and qubits is that a qubit can be in a state other than 0 or 1. For a qubit it is possible to form linear combinations of states 0 and 1. Qubits are realized as a two-level quantum-mechanical systems[83].

There have been many proposed systems which can act as a qubit. Advances in electronics have proven that solid state devices are highly integrable and scalable. This has motivated the search for solid state qubits, and one such system is a qubit based on Josephson-junctions.

A Josephson-junction is simply two superconductors separated by a thin insulating layer. In 1962, Josephson [51, 52] predicted that even if no voltage is applied across the two superconductors a current (I) flows through the junction, because of tunneling, given by \( I = I_C \sin(\Delta \phi) \). Here \( I_C \) is the maximum current the junction can support and \( \Delta \phi \) is the difference between the phases of the two superconducting wavefunctions on either side of the junction. In addition he predicted that if a voltage
difference $V$ is applied across the junction, the phase difference $\Delta \phi$ evolves according to $\frac{d}{dt}\Delta \phi = \frac{2eV}{\hbar}$, so that the current will be an alternating current of amplitude $I_C$ and frequency $\nu = \frac{2eV}{\hbar}$ [117]. When a Cooper-pair tunnels across the junction, two sides of the junction get equal and opposite charge of magnitude $2e$, which can be modeled as a capacitor. By choosing a material such that the superconducting gap $\Delta$ is the largest energy scale in the problem, quasiparticle tunneling is suppressed, and a situation can be reached where no quasiparticle excitation is found and only Cooper-pairs tunnel. In particular attention is paid to systems where the lowest two levels of the device are well separated from higher levels such that to a good approximation the device can be modeled as a two level quantum system, or qubit.

**Cooper-Pair Box (CPB)**

Fig. 2.1 shows the simplest possible Josephson-junction device which can be modeled as a two level system. It consists of a small superconducting island (“box”) with $n$ Cooper-pair charges in excess, relative to some neutral reference state, connected by a tunnel junction with capacitance $C_J$ and Josephson coupling energy $E_J$ to a superconducting electrode. $V_g$ is the gate voltage applied via a gate capacitor $C_g$.

With present day technologies the junctions can be fabricated with capacitances in the range of femtofarad and below, $C_J \leq 10^{-15}F$ [137]. The charging energy of a single electron ($E_C$) is given by $E_C = \frac{e^2}{2(C_J+C_g)}$, and is typically in the range of 1K and above, $E_C \geq 1K$. The Josephson coupling energy is proportion to the critical current of the junction [117], and is typically in the range of 100$mK$. The gate charge is given by $C_gV_g$, this charge can be converted in units of number of Cooper-pairs on gate capacitor ($n_g$) as $n_g = \frac{C_gV_g}{2e}$.
Figure 2.1: A Cooper-pair box (CPB) qubit.

The charging energy of this system is given by \( 4E_C(n - n_g)^2 \), in addition there is Josephson coupling energy of the junction given by \( E_J \cos \phi \), where \( \phi \) is the phase of the superconducting order parameter. The quantum mechanical conjugate of \( \phi \) is \( n \), \( n = -i \hbar \frac{\partial}{\partial \phi} \). Thus the system is described the Hamiltonian, \( \mathcal{H} = 4E_C(n - n_g)^2 - E_J \cos \phi \). Considering \( E_J \ll E_C \), a convenient basis for \( \mathcal{H} \) is formed by the charge states, parametrized by the number of Cooper-pairs \( n \) on the island. In this basis the Hamiltonian is given by

\[
\mathcal{H} = \sum_n \left[ 4E_C(n - n_g)^2 |n\rangle \langle n| - \frac{1}{2}E_J (|n\rangle \langle n + 1| + |n + 1\rangle \langle n|) \right]. \tag{2.1}
\]

The energy levels are dominated by the charging part of the Hamiltonian for most values of \( n_g \), but when \( n_g \) is approximately half a integer the charging energy of two adjacent states is close to each other, while all other charge states have much higher energy. For eg. at \( n_g = \frac{1}{2} \), the charging energy of \( n = 0 \) and \( n = 1 \) states is \( E_C \),
while the charging energy of $n = 2$, $n = 3$, $n = 4 \ldots$ states is $9E_C$, $25E_C$, $49E_C \ldots$ respectively. So, in the case where $n_g \approx \frac{1}{2}$ the superconducting charge box effectively reduces to a two-state quantum system, with Hamiltonian which can be written in spin-$\frac{1}{2}$ notation as
\begin{equation}
\mathcal{H} = \frac{1}{2} B_z \hat{\sigma}_z - \frac{1}{2} B_x \hat{\sigma}_x. \tag{2.2}
\end{equation}
The charge states $n = 0$ and $n = 1$ correspond to the spin basis states $|\uparrow\rangle \equiv (1 \ 0)^T$ and $|\downarrow\rangle \equiv (0 \ 1)^T$ respectively. The charging energy splitting is controlled by the gate voltage, and in spin notation is given by the $z$ component of the magnetic field, $B_z \equiv \delta E_C \equiv -4E_C(1 - 2n_g)$, while the Josephson energy provides $x$ component of the effective magnetic field $B_x \equiv E_J$. In the limit where the charging energy of the states are very close, Josephson tunneling mixes them strongly. So by operating the device close to the degeneracy point $n_g = \frac{1}{2}$, the CPB can be prepared in the mixed state of two charge states $n = 0$ and $n = 1$.

**Josephson-junction Flux Qubit**

The two conjugate variables for the Josephson-junction Hamiltonian are $n$, the number of Cooper-pairs, and the flux $\Phi$. When $E_J \ll E_C$ the flux degree of freedom is not important and the relevant quantity is $n$, representing charge states. Consider the opposite regime $E_J \gg E_C$, where flux is the appropriate quantum degree of freedom. The simplest flux qubit is shown in Fig. 2.2. Such devices are also called Superconducting QUantum Interference Device, or SQUID. The phase difference $\phi$ across the junction is related to the total flux $\Phi$ through the loop by $\phi = 2\pi \left( \frac{\Phi}{\Phi_0} + \text{integer} \right)$, where $\Phi_0 = h/2e$ is the flux quantum. Here $h$ is the Planck’s constant. So the Josephson coupling part of the Hamiltonian is simply $-E_J \cos (2\pi \Phi/\Phi_0)$ and the charging
energy in term of charge operator \( Q = -i\hbar \partial / \partial \Phi \), is \( Q^2 / 2C_J \), where \( C_J \) is the capacitance of the junction. The circuit as shown in Fig. 2.2, will also give some magnetic contributions to the Hamiltonian of the system. If, \( L \) represents the self-inductance of the loop, \( I \) represents the induced current in the loop and \( \Phi_{\text{ext}} \) represents the external bias flux the total flux \( \Phi \) is given by \( \Phi = \Phi_{\text{ext}} + LI \). So the total Hamiltonian of the SQUID, \( \mathcal{H}^{\text{SQUID}} \) is

\[
\mathcal{H}^{\text{SQUID}} = -E_J \cos \left( 2\frac{\pi \Phi}{\Phi_0} \right) + \frac{(\Phi - \Phi_{\text{ext}})^2}{2L} + \frac{Q^2}{2C_J}.
\]  

(2.3)

If the self inductance is large, such that \( E_J / (\Phi_0^2 / 4\pi^2L) \) is larger than 1, and the external flux flux is close to half flux quantum, i.e, \( \Phi_{\text{ext}} \approx \Phi_0 / 2 \), the first two terms in the above Hamiltonian form a double well potential near \( \Phi = \Phi_0 / 2 \). At low temperatures only the lowest states in the two wells contribute. Hence the system

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Figure 2.2: Qubit based on flux degree of freedom, SQUID.
can be modeled as a two level system. These two levels are in fact Clockwise and Counterclockwise currents in the loop.

Now that we have introduced basic qubits based on Josephson-junctions, we will consider a flux qubit based on three Josephson-junctions in the next section. Section 2.2 and 2.3 will consider a CPB coupled to a nanomechanical oscillator.

2.2 Suppression of tunneling in a superconducting persistent-current qubit

2.2.1 Introduction

Surprising physical effects can be produced by quantum-mechanical interference between particles moving from one site to another along different paths[106, 14]. Examples include the Aharonov-Bohm effect[2] and the Aharonov-Casher effect[3, 99]. Many authors have considered this Aharonov-Casher effect for Josephson-junction arrays and devices[126, 129, 48, 33]. Starting from this topological effect Loss et al.[69] predicted suppression of tunneling due to interference of different tunneling paths for magnetic particles with half integer spin, and also oscillations in tunnel splitting with applied magnetic field. These oscillations were confirmed experimentally by Wernsdorfer and Sessoli [136].

Effects related to those analyzed in Ref. [69] have also been studied in systems of Josephson-junctions[48, 88, 16]. For example, a three-junction loop has been studied as a possible phase qubit[88, 16]. In its original design[88], the junctions were deliberately made asymmetric to avoid interference of different tunneling paths, and to protect the qubit from random charge fluctuations.

In this section, we analyze the same three-junction loop but in a different regime, namely, one in which the asymmetry is chosen to observe and control the interference
Figure 2.3: Schematic of the circuit for the three-junction qubit, after Ref. [88]. There are two superconducting islands, denoted 1 and 2, whose voltages are $V_1$ and $V_2$. Of tunneling paths. We show that for this chosen asymmetry, the interference is easily detected because the tunnel splitting \textit{vanishes perfectly} for certain special induced gate charges. The suppression of the tunneling splitting is closely analogous to that discussed in Ref. [69]. Although this qubit is potentially subject to random charge noise, it may be possible to minimize this noise by appropriately tuning the gate voltage[125]. The results obtained in this section were published in \textit{Physical Review B} as a rapid communication[122]
2.2.2 Overview of formalism

The circuit diagram for the three-junction qubit of Ref. [88] is shown in Fig. 2.3. The \(i\)th junction \((i = 1, 2, 3)\) has capacitance \(C_i\) and Josephson coupling energy \(E_{J_i}\). An external flux \(\Phi = f\Phi_0\), where \(\Phi_0 = h/(2e)\), is applied through the three-junction loop, which is assumed to have negligible self-inductance. The properties of the qubit can be manipulated by controlling \(\Phi\), and also the two external voltages, \(V_A\) and \(V_B\), which are applied to the circuit through two gate capacitors \(C_{gA}\) and \(C_{gB}\). The voltages across these capacitors are \(V_{gA} = V_A - V_1\) and \(V_{gB} = V_B - V_2\).

We assume, following Ref. [88], that junctions 1 and 2 have equal Josephson energies \(E_J\) and equal capacitances \(C\), while junction 3 has Josephson energy \(\alpha E_J\) and capacitance \(\alpha C\). Because of the fluxoid quantization, the three gauge-invariant phase differences \(\phi_1\), \(\phi_2\), and \(\phi_3\) satisfy the constraint \(\phi_1 - \phi_2 + \phi_3 = -2\pi f\). We choose \(\phi_1\) and \(\phi_2\) to be the independent dynamical variables, and write \(-\phi_3 = 2\pi f + \phi_1 - \phi_2\).

With these choices, the circuit Lagrangian \(\mathcal{L}\) can be written as \(\mathcal{L} = \mathcal{T} - \mathcal{U} - (\Phi_0/2\pi)\dot{\phi}^T \cdot C_g \cdot \mathbf{V}_g = \mathcal{L}_0 + \mathcal{L}_{WZ}\), where \(\mathcal{L}_0 = \mathcal{T} - \mathcal{U}\) and \(\mathcal{L}_{WZ}\) is the remaining term, which we call the Wess-Zumino term. The kinetic energy term \(\mathcal{T}\) represents the electrical energy stored in all the capacitors of the system; it can be written as \(\mathcal{T} = \frac{1}{2}(\Phi_0/2\pi)^2 \dot{\phi}^T \cdot C \cdot \dot{\phi}\). The Josephson coupling energy \(\mathcal{U} = E_J [2 + \alpha - \cos \phi_1 - \cos \phi_2 - \alpha \cos (2\pi f + \phi_1 - \phi_2)]\). Finally, \(\mathcal{L}_{WZ} = (\Phi_0/2\pi)^2 \dot{\phi}^T \cdot C_g \cdot \mathbf{V}_g\).

In the above expression for \(\mathcal{L}\), the quantity \(C\) represents the capacitance matrix for the junctions, with matrix elements \(C_{11} = C_{22} = C(1 + \alpha + \gamma)\), \(C_{12} = C_{21} = -\alpha C\). Also, \(\dot{\phi}\) represents the \((1 \times 2)\) column vector with elements \(\dot{\phi}_1\), \(\dot{\phi}_2\); \(\mathbf{V}_g\) is the \(1 \times 2\) column vector with elements \(V_A\) and \(V_B\); and the gate capacitance matrix \(C_g\) is a \(2 \times 2\)
diagonal matrix with both diagonal elements equal to $\gamma C$. All the above formalism is identical to that in [88]. However, we consider a different set of parameters: $\alpha > 1$ (rather than $\alpha < 1$) and $f \sim 1/2$. This difference has a qualitative effect on the qubit behavior.

Fig. 2.4 shows a contour plot of the potential energy $U(\phi_1, \phi_2)$ for $\alpha = 1.3$ and $f = 1/2$, represented in the repeated cell scheme. The origin $(\phi_1 = 0, \phi_2 = 0)$ is shown.

Figure 2.4: Contour plot of the potential $U(\phi_1, \phi_2)$ for the special case $\alpha = 1.3$ (see text).
at the center of the plot. The potential energy is periodic in both $\phi_1$ and $\phi_2$ with period $2\pi$. With our choice of parameters, this potential energy has two inequivalent states of the same minimum energy, indicated by boxes with horizontal and vertical lines within each unit cell. If we choose the unit cell to be $-\pi < \phi_1 < \pi$, $-\pi < \phi_2 < \pi$, then the two inequivalent minima are in the upper left and lower right quadrants of the cell. These two minima occur at $(\phi^* + 2m\pi, -\phi^* + 2n\pi)$ and $(-\phi^* + 2m\pi, \phi^* + 2n\pi)$ where $m$ and $n$ are positive or negative integers and $\phi^* = \cos^{-1}\frac{1}{2\alpha}$. These two states are degenerate, but inequivalent. Physically, they correspond to states with clockwise and counterclockwise loop currents. When $\alpha > 1$, the lowest-barrier tunneling paths between these states are different than in the $\alpha < 1$ case considered in Ref. [88].

To see this, suppose we start from the state $(\phi^*, -\phi^*)$, and suppose that this state represents a clockwise-circulating loop current, corresponding to boxes containing vertical lines in the lower right-hand corner of the central unit cell. There are three plausible tunneling directions to reach a neighboring state with counterclockwise-circulating currents, leading to states at $(2\pi - \phi^*, \phi^*)$, $(-\phi^*, -2\pi + \phi^*)$, and $(-\phi^*, \phi^*)$. If $\alpha > 1$, one can show numerically that the potential barrier is smaller for the two located at $(2\pi - \phi^*, \phi^*)$ and $(-\phi^*, -(2\pi - \phi^*))$ than that for tunneling to $(-\phi^*, \phi^*)$. By contrast, if $\alpha < 1$, the tunneling barrier is smaller for the third path than for the other two. Because there are two possible lowest-barrier paths when $\alpha > 1$, there is an interference effect in this case which is absent when $\alpha < 1$. Furthermore, the difference in barrier heights (between the two equal-barrier tunneling paths and the third, higher-barrier path) increases with increasing $\alpha$, provided $\alpha > 1$. Thus, we can easily choose $\alpha$ so that the system tunnels only through these barriers. This tunneling corresponds to the paths near the heavy line in Fig. 2.4. We will show that,
for $\alpha > 1$, there exist certain values $Q_A$ and $Q_B$ of the stored charge, for which the tunneling along these two equal barrier paths exactly cancels out.

### 2.2.3 Path integral formulation

In the absence of tunneling, the system has two degenerate minimum-energy quantum states when $f = 1/2$, one with counterclockwise (⨂) and the other with clockwise (⨁) current. In the presence of tunneling, these two states are connected by a tunneling matrix element $w$, which breaks the degeneracy.

The transition amplitude ($\mathcal{P}$) from a state ⨁ to state ⨂ can be calculated using the imaginary time coherent state path integral method. Symbolically, at temperature $T = 0$,

$$\mathcal{P} = \int_{\phi_1(0),\phi_2(0)}^{\phi_1(\infty),\phi_2(\infty)} D\Omega e^{-\frac{i}{\hbar} S_{\phi_1\phi_2}},$$

where $D\Omega$ represents an integral over all paths in imaginary time starting from the clockwise state at $(\phi_1(0), \phi_2(0)) = (\phi^*, -\phi^*)$ at $\tau = 0$ and ending at the counterclockwise state at $(\phi_1(\infty), \phi_2(\infty)) = (2\pi - \phi^*, \phi^*)$ or $(-\phi^*, -(2\pi - \phi^*))$ at $\tau = \infty$. $S_{\phi_1\phi_2}$ represents the action calculated along each of the paths. In turn, $S_{\phi_1\phi_2} = \int_{\phi_1(0),\phi_2(0)}^{\phi_1(\infty),\phi_2(\infty)} d\tau (L_0 + L_{wz})$, where the integral is over imaginary times $\tau$ (such that $t = i\tau$), and $L_0 + L_{wz}$ is the Lagrangian but with each time $t$ replaced by $i\tau$. At $T = 0$, the integrals start at $\tau = 0$ and run to $\tau = \infty$.

The key point is that, for $\alpha > 1$, there are two classes of paths going from the point ⨁ to the point ⨂ in phase space. One of these is generally in the “northeast” (NE) direction and the other in the “southwest” (SW) direction; the paths run in generally opposite directions in the vicinity of the heavy black line in Fig. 2.4. The two end-points of the paths in the NE direction are ⨁ = $(\phi^*, -\phi^*)$, and ⨂ = $(2\pi - \phi^*, \phi^*)$, while for those in the SW direction they are ⨁ = $(\phi^*, -\phi^*)$ and ⨂ = $(-\phi^*, -(2\pi - \phi^*))$. Let us consider one particular path in the NE direction,
and denote it by \((\phi_1(\tau), \phi_2(\tau))\). This path runs from \((\phi^*, -\phi^*)\) to \((2\pi - \phi^*, \phi^*)\). Then the path \(-\phi_2(\tau), -\phi_1(\tau)\) also starts from \((\phi^*, -\phi^*)\) but runs generally in the SW direction to \((-\phi^*, -(2\pi - \phi^*))\). Thus, for every path in the NE direction, we can define a corresponding path in the SW direction by this procedure.

We now show that the contributions of these two paths to the path integral exactly cancel out for special values of \(Q_A\) and \(Q_B\). We first consider the contributions of \(U\) and \(T\) to the path integral. At any point along a NE path, the potential energy \(U(\phi_1, \phi_2)\), is given above. Along any point along the corresponding SW path, the corresponding potential energy is given by \(U(-\phi_2, -\phi_1) = U(\phi_1, \phi_2)\). Thus, the contribution of \(U\) to \(S\) is exactly the same for corresponding paths in the NE and SW directions. Similarly, the contribution of \(T\) to \(S\) is the same for corresponding paths in the NE and SW directions (because \(T\) is quadratic in the derivatives \(\dot{\phi}_1\) and \(\dot{\phi}_2\), and because the diagonal elements of \(C\) are equal). Since \(S\) appears in the exponential, the exponential \(\exp(-S/\hbar)\) terms give the same multiplicative contribution to \(P\) for each of the two paths.

For \(L_{WZ}\), we have \(L_{WZ} = -i \left(\frac{\Phi_0}{2\pi}\right) \gamma C(V_A \dot{\phi}_1 + V_B \dot{\phi}_2)\), where \(\dot{\phi}_1\) and \(\dot{\phi}_2\) are derivatives with respect to \(\tau\). Since \(L_{WZ}\) is a total time derivative, its contribution to \(S_{\phi_1, \phi_2}\) depends only on the initial and final values \(i\) and \(f\) of the phases \((\phi_1\) and \(\phi_2\)). This contribution is \(-i \left(\frac{\Phi_0}{2\pi}\right) \int_i^f d\tau (\gamma C(V_A \dot{\phi}_1 + V_B \dot{\phi}_2)) = -i \left(\frac{\Phi_0}{2\pi}\right) \gamma C[V_A(\phi_1(f) - \phi_1(i)) + V_B(\phi_2(f) - \phi_2(i))]\). Thus, for any path taking the state \((\phi^*, -\phi^*)\) in the NE direction to \((2\pi - \phi^*, \phi^*)\), \(L_{WZ}\) gives a contribution to \(S\) which will be equal to \(S_{WZ}^{NE} = -i \left(\frac{\Phi_0}{2\pi}\right) \gamma C[2V_A(\pi - \phi^*) + 2V_B\phi^*]\). Similarly, a path taking the state \((\phi^*, -\phi^*)\) in the SW direction to \((-\phi^*, -(2\pi - \phi^*))\) gives a contribution \(S_{WZ}^{SW} = i \left(\frac{\Phi_0}{2\pi}\right) \gamma C[2V_A\phi^* + 2V_B(\pi - \phi^*)]\).
We now write $\Phi_0 = \frac{\phi_0}{2\pi} \gamma CV_A = h \frac{Q_A}{2e}$ and $\Phi_0 = \frac{\phi_0}{2\pi} \gamma CV_B = h \frac{Q_B}{2e}$, where $Q_A$ and $Q_B$ represent the charge stored on the gate capacitors, and $e$ represents the electronic charge. Then the sum of the contributions of $S_{NE}^{WZ}$ and $S_{SW}^{WZ}$ to $P$ is $P_{WZ} = P_0 (e^{\frac{i}{e} [Q_A(\pi - \phi^*) + Q_B \phi^*]} + e^{-\frac{i}{e} [Q_A \phi^* + Q_B (\pi - \phi^*)]})$, where $P_0$ is a constant term which is the same for the two paths. It is always possible to define a number $n$ such that $Q_B = ne - Q_A$. In terms of $n$, we can rewrite $P_{WZ}$ as $P_{WZ} = P_0 \exp \left[ \frac{i}{e} Q_A (\pi - 2\phi^*) + in\phi^* \right] [1 + e^{-in\pi}]$. Hence, $P_{WZ}$ vanishes whenever $Q_A + Q_B = ne$, where $n$ is an odd integer. Since the contributions of $U$ and $T$ to $S$ are the same for corresponding paths in NE and SW directions, the total $P$ still vanishes when this condition is satisfied, even including the contributions of $U$ and $T$ to $S$. Our calculation is analogous to that of Loss et al.[69] for a magnetic tunneling problem.

Thus, the paths taking the state $(\phi^*, -\phi^*)$ to $(2\pi - \phi^*, \phi^*)$ and to $(-\phi^*, -(2\pi - \phi^*))$ interfere completely destructively whenever the stored charges on the gate capacitors sum to an odd multiple of $e$. This destructive interference is not restricted to straight line paths, because, as we have shown, for any general path in the NE direction, there exists a path in the SW direction which interferes destructively with it. It can be shown that similar destructive interference occurs for higher order paths, such as the next order paths which take the state $(\phi^*, -\phi^*)$ to $(4\pi - \phi^*, 2\pi + \phi^*)$ and $(-(2\pi + \phi^*), -(4\pi - \phi^*))$. This implies that the two persistent-current (clockwise and counterclockwise) states remain degenerate for these values of the stored charges, provided that $f = 1/2$. 

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2.2.4 Tight-binding formulation

The same cancellation can be demonstrated using the tight-binding formulation of Ref. [88]. The classical Hamiltonian \( \mathcal{H} \) corresponding to the above Lagrangian is

\[
\mathcal{H} = p^T \cdot \dot{\phi} - \mathcal{L},
\]

where the canonical momenta \( p_i = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} \), \( i = 1, 2 \). This procedure gives\[88\]

\[
\mathcal{H} = \frac{1}{2} \left( \frac{2\pi}{\Phi_0} \right)^2 P^T \cdot C^{-1} \cdot \overline{P} + U(\phi_1, \phi_2),
\]

where \( \overline{P} = \bar{p} + \frac{\Phi_0}{2\pi} C_g \cdot \overline{V}_g \), and \( U \) is given above.

The energy eigenstates of \( \mathcal{H} \) satisfy the time-independent Schrödinger equation

\[
\mathcal{H} \psi(\phi_1, \phi_2) = E \psi(\phi_1, \phi_2),
\]

where \( p_i = -i\hbar(\partial/\partial \phi_i) \) (\( i = 1, 2 \)). The boundary conditions, obtained from the requirement that the wave function be single-valued, are

\[
\psi(\phi_1 + 2m\pi, \phi_2 + 2n\pi) = \psi(\phi_1, \phi_2),
\]

where \( m \) and \( n \) are integers.

The charge periodicity discussed above is due to the relation between the components of \( P \) and \( p \). Specifically, using the fact that the matrix \( C_g \) is diagonal, we write

\[
P_1 = p_1 + \frac{\Phi_0}{2\pi} C_g A V_{g,A} = -i\hbar \left( \frac{\partial}{\partial \phi_1} + i \frac{Q_A}{2e} \right), \quad P_2 = p_2 + \frac{\Phi_0}{2\pi} C_g B V_{g,B} = -i\hbar \left( \frac{\partial}{\partial \phi_2} + i \frac{Q_B}{2e} \right).
\]

on using the operator forms of \( p_1 \) and \( p_2 \) and using \( Q_A = C_g A V_{g,A} \) and \( Q_B = C_g B V_{g,B} \).

We now define \( \chi(\phi_1, \phi_2) = \exp(i \mathbf{k} \cdot \mathbf{\phi}) \psi(\phi_1, \phi_2) \), where the vector \( \mathbf{\phi} = \phi_1 \hat{\phi}_1 + \phi_2 \hat{\phi}_2 \), \( \mathbf{k} = \frac{Q_A}{2e} \hat{\phi}_1 + \frac{Q_B}{2e} \hat{\phi}_2 \), and \( \hat{\phi}_1 \) and \( \hat{\phi}_2 \) are unit vectors in the \( \phi_1 \) and \( \phi_2 \) directions in Fig. 2.4. Then the boundary conditions on \( \psi \) imply that \( \chi(\phi_1, \phi_2) \) is a Bloch function, i.e., that \( \chi(\phi_1 + 2\pi m, \phi_2 + 2\pi n) = \exp(i \mathbf{k} \cdot \mathbf{R}_{mn}) \chi(\phi_1, \phi_2) \), where \( \mathbf{R} = 2\pi m \hat{\phi}_1 + 2\pi n \hat{\phi}_2 \) is a lattice vector. Also, in terms of \( \chi \), the two-variable Schrödinger equation takes the form \((T + U) \chi_{\mathbf{k}} = E(\mathbf{k}) \chi_{\mathbf{k}} \). Since \( \chi_{\mathbf{k}} \) is a Bloch function and \( U \) is periodic, the eigenvalue \( E(\mathbf{k}) \) is periodic in \( \mathbf{k} \) and hence, in the charges \( Q_A \) and \( Q_B \).

This Schrödinger equation can be solved within a tight-binding approximation\[88\] to calculate the tunnel splitting, which we previously calculated using a path integral approach. Let us consider two localized “atomic” orbitals, \( u(\phi_1, \phi_2) \) and \( v(\phi_1, \phi_2) \),
which represent the ground state wavefunctions in each of the two minima of the potential $U(\phi_1, \phi_2)$ within the central unit cell. Then, at Bloch vector $k$, the tight binding wavefunction $\chi_k(\phi_1, \phi_2) = c_{k,u}u(\phi_1, \phi_2) + c_{k,v}v(\phi_1, \phi_2)$, where $c_{k,u}$ and $c_{k,v}$ are defined by $[H_{uu}(k) - E(k)]c_{k,u} + H_{uv}(k)c_{k,v} = 0$, $H_{vu}(k)c_{k,u} + [H_{vv}(k) - E(k)]c_{k,v} = 0$. In actuality, $H_{uu}$ and $H_{vv}$ are independent of $k$.

When the applied field is such that $f = 1/2$, $u$ and $v$ are exactly degenerate, with energy which we denote $\epsilon_0$. In this case, $H_{uu} = H_{vv} = \epsilon_0$. To obtain the other two elements, we denote by $t_1$ the tunneling matrix element between these two minima in the same unit cell, and $t_2$ between the state in the “southeast” corner of that cell and either of the two adjacent minima lying along the heavy line in Fig. 2.4. Then $H_{uv} = H_{vu}^* = -t_1 - t_2 [e^{ikR_1} + e^{ikR_2}]$, where $R_1 = 2\pi \hat{\phi}_1$ and $R_2 = -2\pi \hat{\phi}_2$ are the Bravais lattice vectors from the central unit cell (denoted by a white square in Fig. 2.4) to the two adjacent cells along the heavy line in Fig. 2.4.

An estimate of the $t_i$'s can be obtained using the WKB method, by calculating the action $S_i$ between the two minima and writing $t_i \approx (\hbar \omega_i/2\pi) e^{-S_i/\hbar}$. Here $\omega_i$ is the attempt frequency for the phase “particle” to escape from the potential well. Following the approach of Ref. [88], we find that for $\alpha = 1.3$ and $E_J/E_C \sim 100$, where $E_C = e^2/(2C)$, the ratio $t_1/t_2 \sim 10^{-4}$. In fact, provided $E_J/E_C \ll 1$, we can always choose an $\alpha > 1$ such that the effect of $t_1$ is very small.

Neglecting $t_1$ and using the above values of $k$, $R_1$ and $R_2$, we obtain $H_{uv} = -2t_2 \exp[i\pi(Q_A - Q_B)/(2e)] \cos[\pi(Q_A + Q_B)/(2e)]$. The eigenvalues of $H$ are then $E = \epsilon_0 \mp |H_{uv}|$, with corresponding normalized eigenvectors $(u \pm v)/\sqrt{2}$. The result for the eigenvalues shows that, when the offset charges satisfy $Q_A + Q_B = ne$, with $n$ an odd integer, the levels become degenerate. This is exactly the result we found.
by our path interference analysis. Note that the energy splitting depends only on the sum \( Q_A + Q_B \), not on the difference \( Q_A - Q_B \).

2.2.5 Deviation from \( f = 1/2 \); control parameters

As \( f \) deviates slightly from 1/2, the potential \( U \) changes such that the two minimum states of the two wells in a unit cell become unequal in energy, and the barrier heights also change. If we define the zero of energy as the average of the two lowest energy states at \( f = 1/2 \), the elements of \( H \) become \( H_{uu} = -H_{vv} = F \); \( H_{uv} = H_{vu}^* = -t \).
Here \( F \sim (\partial H_{uu}/\partial f)(f - 1/2) \) is the change in the diagonal matrix element of \( H \) with a small change in flux. Also, if we write \( Q_A + Q_B = (2n + 1)e + \delta Q \), and we assume \( |\delta Q/e| \ll 1 \), we find \( t \sim -2t_2 \exp[i\pi(Q_A - Q_B)/(2e)](-1)^n \pi \delta Q/(2e) \). Thus, to first order in \( \delta f \) and \( \delta Q \), \( F \) and \( t \) are controlled by \emph{two} different parameters: \( f - 1/2 \) and \( \delta Q/e \). The corresponding eigenvalues of \( H \) are \( E_{\pm} = \mp \sqrt{F^2 + |t|^2} \), and depend on \( f - 1/2 \) (through \( F \)) and \( Q_A + Q_B \) (through \( t \)), but not on \( Q_A - Q_B \). (The eigenvectors do depend on \( Q_A - Q_B \).) By manipulating these two control parameters independently, one could, in principle, adjust the splitting of this two-level system.

Fig. 2.5 shows a contour plot of the quantity \( 2\sqrt{F^2 + |t|^2} \), which represents the energy difference between the two lowest eigenvalues of \( H \), as a function of the quantities \( f \) and \((Q_A + Q_B)/e\). In constructing this plot, we assume the following parameters: \( E_J/E_C = 80, \gamma = 0.02, \alpha = 1.3 \), and an attempt frequency \( \hbar \omega/(2\pi) = 0.193E_J \). Except for \( \alpha \), all these quantities have the same values as in Ref. [88]. There are eight contour curves visible, equally spaced between 0 and a maximum value of \( 0.3266E_J \). These are calculated using the above parameters and the relation 
\[
[\partial H_{uu}/\partial f]_{f=1/2} = 4\pi \alpha E_J \sin(2\pi f + 2\phi^*). 
\]

The splitting vanishes when \((Q_A + Q_B)/e\) is an odd integer and \( f = 1/2 \).

The parameters \( F \) and \( |t| \) should be controllable experimentally. \( F \) can be finely adjusted by changing \( f \), the magnetic flux through the loop. For the parameters of Ref. [88], \( |t| \) should also be controllable. Taking \( E_J = 800\mu eV \), we have \( E_C = 10\mu eV \), corresponding to a junction capacitance \( C = 10fF \), and hence gate capacitances \( C_g = 0.16fF \). With this value for \( C_g \), \((Q_A + Q_B)/e = 1\) corresponds to \( V_A + V_B = C_g(Q_A + Q_B) = 1mV \), a value which should be tunable to a small tolerance. In the different regime of small junctions \((E_J \sim E_C)\), the periodicity of energies with
offset charges has been observed, e. g., in Ref. [125]. In that work, a computer-controlled method was used to accurately compensate for the random offset charges. For operation of the present system as a qubit in the regime with $\alpha > 1$, one would need a temperature $T$ low enough to avoid creation of single-electron excitations, or exciting the system above its two lowest levels. Using the parameters of Ref. [88], this would be $k_B T \ll 0.2E_J \sim 2K$. A temperature of 0.2-0.4 K should be sufficient, and is readily attainable with current cryogenics.

2.2.6 Discussion

To summarize, we have demonstrated that the three-junction persistent-current qubit can be placed in a regime such that the states are determined by the interference of tunneling paths. For certain values of the offset charges, this interference is perfectly destructive, leading to a vanishing of the tunnel splitting between the two states of the qubit for appropriate values of the gate charges and the applied magnetic field. This effect should be observable experimentally, as long as the sum of the offset charges can be controlled experimentally, as we have briefly discussed above. It would certainly be of interest to observe the cancellation suggested here.

2.3 Study of energy loss by a nanomechanical oscillator coupled to a Cooper-pair box

2.3.1 Introduction

Observing quantum effects in a mechanical object has been a long-sought goal, because such effects would represent a macroscopic manifestation of quantum mechanics[105]. Nanomechanical oscillators (NMO’s) with frequencies $\omega/(2\pi)$ as high as 1 GHz have
recently been realized in the laboratory[45]. It is possible to observe quantum ef-
fects in such objects, provided that they are cooled to temperatures $T$ such that $k_B T$
is near or slightly above $\hbar \omega[54]$. For a realistic NMO frequency of 500 MHz, this
-corresponds to a $T$ of a few mK.

In this section, we numerically analyze energy loss by a NMO capacitively cou-
−pled to a dissipative Cooper-pair box (CPB). A CPB consists of a small Josephson-
-junction whose Josephson energy is much smaller than its charging energy, and which
-is voltage-biased so that only the two lowest energy levels are experimentally acces-
sible. Naik et al.[80] have recently suggested that an NMO could be cooled by ca-
−pacitively coupling it to a CPB. Here, we numerically demonstrate an increased rate
-of energy loss by this mechanism, by solving a time-dependent Schrödinger equation
-with a stochastic term. We also relate the rate of energy loss to the coupling constant
-and the NMO and CPB damping rates. Several studies of the coupled NMO/CPB
-system have already been carried out[47, 6, 72], as have studies of the formally similar
-system consisting of a CPB coupled to a single-mode electromagnetic cavity[15]. If
-both the CPB and the cavity are dissipative, this system is closely analogous to the
-one studied here[15]. The main results of this calculation have been published in

$\text{Physical Review B}[119]$

2.3.2 Formalism

Dissipation in quantum systems was treated by Caldeira and Leggett, who studied
the suppression of quantum tunneling out of a metastable state by dissipation[21].
 Later, Leggett et al. studied the dynamics of a dissipative TLS [64]. In both of these
approaches, the dissipation is treated as arising from coupling to a bath of harmonic
oscillators. An alternative method starts from Lindblad’s quantum-mechanical master
equation for the density operator of an open system[68]. An equivalent approach is
to start from a pure-state Schrödinger equation, which contains a stochastic term to
represent the effect of dissipation[28]. Here, we use this approach to treat energy loss
by an NMO coupled to a CPB.

We assume that the Hamiltonian for the coupled NMO/CPB system is given by

\[ H = H_{CPB} + H_{NMO} + H_I + H_\kappa + H_\gamma, \]

\[ H_{CPB} = 4E_C(n_g - \frac{1}{2})\sigma_z - \frac{1}{2}E_J\sigma_x, \]

\[ H_{NMO} = \hbar\omega_0(a^\dagger a + \frac{1}{2}), \]

\[ H_I = \hbar g(a^\dagger + a)\sigma_z. \]  

(2.4)

Here \( \sigma_z \) and \( \sigma_x \) are the Pauli spin matrices, which act on the two charge states of the
CPB; \( n_g = (C_bV_b + C_gV_g)/2e \), where \( C_b \) and \( V_b \) are the bias capacitance and voltage of
the CPB; \( C_g \) and \( V_g \) are the capacitance and voltage between the NMO and the CPB;
\( E_C \) and \( E_J \) are the Coulomb and Josephson energies for the CPB; \( \omega_0 \) is the frequency
of the fundamental mode of the NMO; \( a \) and \( a^\dagger \) are the usual annihilation and creation
operator for the fundamental mode of the NMO, and \( g = -4E_C(C_gV_g)\Delta x_{zp}/(2e\hbar d) \)
represents the coupling constant for capacitive coupling between the NMO and the
CPB. The zero-point displacement of the NMO is given by \( \Delta x_{zp} = \sqrt{\hbar/2m\omega_0} \), where
\( m \) is the effective mass of the NMO and \( d \) is the distance between the NMO and the
CPB[46]. The last two terms in \( H \) represent the effects of dissipation. \( H_\kappa \) represents
the dissipation in the NMO, which is assumed to be characterized by a decay rate
\( \kappa = \omega_0/Q \), where \( Q \) is the quality factor of the NMO. \( H_\gamma \) represents the dissipation
in the CPB, which is described by a decay rate \( \gamma \). We also assume that only the
fundamental mode of the NMO is coupled to CPB. The precise forms of $H_\kappa$ and $H_\gamma$ are given below.

The Hamiltonian (Eq. (2.4)), in the absence of dissipation, has been discussed, e.g., in Refs. [47] (which shows a sketch of a typical experimental configuration), [6] and [137]. We assume that the CPB is biased to $n_g = 1/2$, where it would be degenerate in the absence of Josephson coupling, and work in the coordinate system obtained from that of eq. (2.4) by a rotation of $\pi/2$ about $y$-axis. In this coordinate system $H_{CPB} = (E_J/2)\sigma_z$ and $H_I = \hbar g(a + a^\dagger)\sigma_x$. Moreover, in this coordinate system, the two eigenstates of $H_{CPB}$ represent symmetric and antisymmetric superpositions of charge states. In addition, we will make the rotating wave approximation (RWA) to obtain the Hamiltonian used in all our calculations. This Hamiltonian is given by

$$H = \frac{\hbar \Omega}{2} \sigma_z + \hbar \omega_0 \left( a^\dagger a + \frac{1}{2} \right) + \hbar g(a^\dagger \sigma^- + \sigma^+ a) + H_\kappa + H_\gamma,$$

(2.5)

where $\Omega = E_J/\hbar$ and $\sigma^\pm = (\sigma_x \pm i\sigma_y)/2$. Thus, we neglect the counter rotating terms $\hbar g(a^\dagger \sigma^+ + a \sigma^-)$. If $\Omega \sim \omega$ and the coupling is sufficiently weak, the RWA is believed justified [46]. For this reason, we believe that the RWA is also reasonable when the two damping terms are included.

We include dissipation in both the CPB and the NMO by using a stochastic time-dependent Schrödinger equation. This approach originates in the von Neumann equation for the total density matrix $\rho$ of any system: $\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$. The Hamiltonian of eq. (2.5) consists of two parts: the CPB plus NMO, described by the first three terms, and the dissipative parts, described by $H_\kappa$ and $H_\gamma$, which represent the damping. If the evolution of $\rho$ is considered to be Markovian, and if the coupling between the open system and the baths is weak, the reduced density matrix $\rho_{sys}$ of the
CPB plus NMO can be shown to be described by the following master equation[133]:

\[
\dot{\rho}_{\text{sys}} = -\frac{i}{\hbar} [H - H_\kappa - H_\gamma, \rho_{\text{sys}}] - \frac{1}{2} \sum_{m=\{\kappa, \gamma\}} (L_m^\dagger L_m \rho_{\text{sys}} + \rho_{\text{sys}} L_m^\dagger L_m - 2 L_m \rho L_m^\dagger).
\]

Here the $L_m$ are so-called Lindblad operators, which are in general non-Hermitian and which describe dissipation in CPB plus NMO system. In the present work, we include only the two Lindblad operators $L_\kappa = \sqrt{\kappa} a$ and $L_\gamma = \sqrt{\gamma} \sigma^-$, which represent dissipation within the NMO and the CPB. The inclusion of only these two Lindblad operators is appropriate if $T$ is sufficiently low (typically $k_B T \ll \hbar \omega_0$), and if other dissipative processes can be neglected.

Eq. (2.6) is a matrix equation for the density operator $\rho_{\text{sys}}$. If we truncate the state space by including only the lowest $N$ vibrational states, then $\rho_{\text{sys}}$ is a square matrix of size $2N \times 2N$. Eq. (2.6) then leads to $(2N)^2$ coupled differential equations for the elements of $\rho_{\text{sys}}$. An alternative computational scheme is to use a stochastic pure state representation [28, 37] for the master equation. In this representation, eq. (2.6) reduces to a stochastic equation of motion for the state vector $|\psi\rangle$ given by [15, 104]

\[
|d\psi\rangle = -\frac{i}{\hbar} (H - H_\kappa - H_\gamma) |\psi\rangle \, dt + \sum_m \left( L_m - \langle L_m \rangle_{\psi} \right) |\psi\rangle \, d\xi_m

- \frac{1}{2} \sum_m \left( L_m^\dagger L_m + \langle L_m^\dagger \rangle_{\psi} \langle L_m \rangle_{\psi} - 2 \langle L_m^\dagger \rangle_{\psi} L_m \right) |\psi\rangle \, dt,
\]

where $\langle L_m \rangle_{\psi}$ is the expectation value of $L_m$ in state $|\psi\rangle$, and $|d\psi\rangle$ is the change in $|\psi\rangle$ in time $dt$. In eq. (2.7), the first sum represents random fluctuations due to the interaction of the system with the baths, while the second denotes the (non-random) drift of the state vector due to those baths. The $d\xi_m$ are independent complex differential random variables representing a complex normalized Wiener process, whose
ensemble averages satisfy

\[ \overline{d\xi_m} = \overline{d\xi_m d\xi_n} = 0, \]  
\[ \overline{d\xi_m^* d\xi_n} = \delta_{mn} dt, \]

(2.8)
(2.9)

where the overbar denotes an ensemble average over realizations of the random variables \( d\xi_n \).

Eq. (2.7) represent only 2N coupled differential equations for the components of \( |\psi\rangle \), rather than \((2N)^2\) as in the density matrix formulation. The price paid is that the differential equations are stochastic, and thus must be averaged over many realizations. But such stochastic equations can be solved very efficiently, even including this averaging. Thus, we use this stochastic approach in the following.

To see how this procedure can lead to faster energy loss by the NMO, suppose that the initial state vector is \( |\psi\rangle = |\alpha, n\rangle \), where \( \alpha (= 0 \text{ or } 1) \) indicates an eigenstate of \( H_{CPB} \) and \( n \) represents the initial number of excitations in the NMO. Thus, the NMO is assumed to be initially in a Fock (or number) state. As time progresses the NMO and CPB become entangled, and the wave function \( |\psi\rangle \) spreads out over an increasing part of the accessible 2N-dimensional Hilbert space. After some time \( t \), \( |\psi(t)\rangle \) is a superposition of many states \( |\alpha, m\rangle \), with \( m \leq n + 1 \); the weight of each component is determined by eq. (2.7). Several experimental methods for preparing an NMO in a specified Fock state have been proposed [47, 102].

2.3.3 Results

We have solved eq. (2.7) at resonance for different values of \( \kappa \) and \( \gamma \), using the value \( g = 0.1\omega_0 \), by straightforward Euler integration, using a time step \( dt = 5 \times 10^{-5} \text{ns} = 2.5 \times 10^{-5}(2\pi/\omega_0) \). From these solutions, we compute various averages of interest, such
as $\langle \sigma_z(t) \rangle$ and $\langle a^\dagger a(t) \rangle$, as functions of time $t$. The triangular brackets and overbars denote quantum-mechanical and noise averages, respectively. For conciseness, we denote these quantities simply $\sigma_z(t)$ and $\varpi(t)$. The results are averaged over 100 realizations of the noise, which appear sufficient to give reasonably smooth results. We carry out calculations assuming $\Omega/(2\pi) = \omega_0/(2\pi) = 500$ MHz, $g/(2\pi) = -50$ MHz, $\kappa = 0.0005$ (ns)$^{-1}$ and $\gamma = 0.05$ (ns)$^{-1}$. These values of $\kappa$ and $\gamma$ correspond to decay times of the uncoupled NMO and CPB of 2000 ns (corresponding to a $Q$ factor of $10^3$) and 20 ns, respectively, as used in Ref. [81]. A much larger decay time for the CPB has been achieved in some more recent experiments (see, e. g., Wallraff et al. [132], who find an energy relaxation rate of around 7$\mu$sec). However, one does not want such a long decay time for the CPB, since this will reduce the rate at which the NMO loses energy when coupled to the CPB. We have, therefore, carried out our calculations using the original parameters of Ref. [81].

We first carried out calculations of the uncoupled CPB and NMO, using the stochastic Schrödinger equation, starting from the state $|1,20\rangle$. In this case, the CPB and NMO each decay exponentially with decay rates 20 (ns)$^{-1}$ and 2000 (ns)$^{-1}$, respectively, as shown in Figs. 2.6 and 2.7. Next, we turned on the coupling $g$, so that $g/(2\pi) = -50$ MHz, with results shown in Figs. 2.6 and 2.7 for $\sigma_z(t)$ and $\varpi(t)$.

2.3.4 Discussion

We now discuss the results. In both cases, we use $\gamma \gg \kappa$ of the NMO, as in experiment[81, 47]. Fig. 2.6 shows that, in the presence of coupling, the decay rate of the CPB is substantially reduced, relative to the uncoupled CPB. The reduction in the decay rate is greatest when the damping in the NMO is smallest. Besides
Figure 2.6: Calculated $\sigma_z(t)$ versus time $t$, averaged over 100 realizations of the noise, for the case of zero coupling to the NMO ($g = 0$), and for fixed $g/(2\pi) = -(50 \text{ MHz})$, and three different values of the NMO damping parameter $\kappa$.

this reduction in decay rate, Fig. 2.6 shows the expected Rabi oscillations in $\sigma_z$ for all three calculations involving nonzero $g$. These Rabi oscillations, of frequency $\omega_R \propto \sqrt{n + 1} g[4]$, occur between the states $|1, n\rangle$ and $|0, n + 1\rangle$. They are the well-known results of solving the time-dependent Schrödinger equation for the present Hamiltonian in the absence of dissipation; our calculations show that they still occur with dissipation present.

By contrast, Fig. 2.7 shows that, when the coupling is turned on, the decay rate of the NMO is increased relative to that of the uncoupled NMO. Furthermore, the decay rate is the largest when the damping rate of the CPB is largest. Once again, we see Rabi oscillations in $\pi(t)$.
Figure 2.7: Expected number of excitations in the NMO, $n(t)$, plotted versus time. $n(t)$ is averaged over 100 noise realizations, and is shown for zero coupling ($g = 0$) and for $g/(2\pi) = -50$ MHz and three different values of the CPB damping parameter $\gamma$ as indicated.

The results of both Figs. 2.6 and 2.7 can be understood qualitatively when $\gamma \gg \kappa$. The coupling allows energy to be transferred periodically between the CPB and the NMO. Since the NMO has a much lower decay rate than that of the CPB, this new channel should reduce the effective decay rate of the CPB, as we observed numerically. Similarly, this transfer should increase the effective damping rate of the NMO, again as seen numerically. Furthermore as the damping rate $\gamma$ of the CPB increases, the effective damping rate of the NMO should also increase, again as seen numerically.

Finally, in Fig. 2.8, we show how this behavior depends on the assumed initial Fock state of the NMO. In the three cases shown, we start from state $|1, n\rangle$ with four
Figure 2.8: $-\ln[n(t)/n(0)]$ for different initial Fock states of the NMO. In all cases, $g/(2\pi) = -50$ MHz, $\gamma = 0.05(\text{ns})^{-1}$ and $\kappa = 0.0005(\text{ns})^{-1}$.

different initial Fock states, $n(0)$, of the NMO. $\overline{n}(t)/n(0)$ decays roughly exponentially with time, with superimposed Rabi oscillations. The exponential decay rate is considerably smaller for $n(0) = 1$ than for the other cases. This difference occurs, we believe, because, in the absence of damping, the coupling between the CPB and NMO is proportional $\hbar g\sqrt{n + 1}$ (this is the splitting between states $|1, n\rangle$ and $|0, n + 1\rangle$ in the RWA in the absence of damping).

We now discuss the possible relation between the present results and energy loss by a real NMO. We have considered the time-dependent NMO/CPB system, starting from the state $|1, n\rangle$. Our approach permits us to calculate the time needed for the NMO, starting from this excited state, to approach its equilibrium temperature, given
that the intrinsic damping within the NMO is very small. If the NMO is coupled to a much more heavily damped CPB, we find that the equilibration process is greatly speeded up. This result might be useful in designing ways of rapidly equilibrating an NMO, initially in an excited state, to a low ambient temperature.

We also find that the rate of equilibration of the CPB is reduced when it is coupled to an NMO. Our results are consistent with those of Trees et al.[123], who used a very different approach. These workers studied a current-biased Josephson junction capacitively coupled to an oscillator, in the presence of dissipation, using the formalism of Caldeira and Leggett[21], and found that the CPB is less damped when it is coupled to an NMO. Our results show the same behavior, using a formally quite different stochastic differential equation. We also find an additional result, not shown in Ref. [123]: for a given coupling constant, the CPB is damped most slowly when the damping of the NMO is smallest (see Fig. 2.6).

It should also be pointed out that we have included only two Lindblad operators in our calculation, namely, those involving the constants \( \kappa \) and \( \gamma \). Other Lindblad operators could readily be included, such as ones describing finite temperature and pure dephasing[15]. In the present calculation, \( \kappa \) and \( \gamma \) parametrize energy loss from the NMO and the CPB to their thermal environments. Another point is that the regime we have considered, in which the CPB is more heavily damped than the NMO, is not necessarily the regime in which a CPB is typically studied. When one wishes to use the CPB as an element in a quantum computing geometry, it is usually desirable to have a CPB with as little dissipation, and as long a decoherence time, as possible. In the present work, by contrast, we are envisioning a setup where the CPB is being used as a means of rapidly extracting energy from a high-Q NMO, so as to observe the
expected quantum effects in the NMO. As shown by our calculations, this requires a
CPB which is more heavily damped than the NMO. Finally, we should note that our
calculation is applicable, in principle, to energy loss by any harmonic oscillator mode
coupled to any two-level system, provided that the model Hamiltonian describing the
interactions and energy losses is that used in the present work.

Next, we briefly comment on the initial conditions used in these calculations. We
have assumed that the NMO begins in a Fock state. In some cases, a more appropriate
initial condition might be one in which the initial state of the oscillator is a mixture
of Fock states weighted according to a suitable temperature. If this calculation were
carried out, it might represent a study of the rate of cooling of an NMO, initially at
some temperature $T$, if it were placed in a thermal bath at a much lower temperature
and also coupled to an NMO at a similarly lower temperature. Another possible
initial state might be a coherent state of the oscillator, i.e., an eigenstate of $a$. Both
initial states may be achievable experimentally. Calculations starting from such mixed
states would be more demanding numerically, using the present approach, but will
probably lead to qualitatively similar results regarding the rate of energy loss of both
the NMO and the CPB.

Finally, we comment on our use of the RWA. The RWA is believed justified when
the coupling between the NMO and CPB is reasonably small, compared to $\hbar \omega_0$, and
also provided the NMO and CPB are in resonance. Both conditions are satisfied
in the present calculation. We have carried out similar RWA calculations off reso-
nance, with results similar to those shown in Figs. 2.6-2.8, but we believe that the
RWA approximation is less accurate in this case. To go beyond the RWA leads to
a considerably more complicated set of stochastic differential equations. To confirm
our results, we have, in fact, gone beyond the RWA for the parameters used in the calculations discussed above (NMO and CPB in resonance, relatively weak coupling), solving eq. (2.7) including all the counter rotating terms. In this case, it proves more convenient to solve numerically for $|\psi'\rangle = \exp[-i(H - H_\kappa - H_\gamma)t/\hbar]|\psi\rangle$, where $H$ is given by eq. (2.4), then transform back to get $|\psi\rangle$. The resulting time dependent averages, for these parameters, are nearly indistinguishable from those shown in Figs. 2.6-2.8, showing that the RWA is indeed an excellent approximation, as expected, for this case. For substantially stronger coupling between the NMO and the CPB, or for frequencies far off resonance, we have not yet succeeded in obtaining a converged solution for $|\psi(t)\rangle$ when the counter rotating terms are included, showing that, once again as expected, the RWA is inaccurate in this regime.

To summarize, we have demonstrated, within the RWA, and using a suitable time-dependent Schrödinger equation with stochastic terms, that the rate of equilibration of an NMO with a thermal bath can be considerably speeded up by coupling the NMO to a CPB. Using the same approach, we have demonstrated that the decay rate of the CPB can be easily reduced by coupling it to a high $Q$ factor cavity, such as a nanomechanical oscillator; this latter result is consistent with previous calculations[123] using a very different approach. Both of these effects may be very useful experimentally. In particular, the use of a CPB as a means of removing energy from an NMO may be helpful in observing macroscopic quantum effects in such oscillators.
2.4 Effective decay rates of coupled nanomechanical oscillator and Cooper-pair box: beyond rotating wave approximation

2.4.1 Introduction

With recent advances in micro-fabrication, there has been an increasing interest in observing quantum behavior in a macroscopic mechanical system[105]. In order to detect the quantum nature of such a system, known as a nanomechanical oscillator (NMO), it is necessary to carry out highly sensitive measurements at low temperatures $T$, such that $k_B T < \hbar \omega_0$, where $\omega_0$ is the angular frequency of the NMO in its lowest vibrational state. The Heisenberg uncertainty principle imposes fundamental limits on such measurements[17], because the product of the uncertainties in the displacement and momentum must exceed Planck’s constant. NMOs with frequencies $\omega_0/(2\pi)$ as high as 1 GHz have been realized experimentally[45], allowing measurements to be made at accessible temperatures.

A NMO which is capacitively coupled to a CPB is a subject of recent studies[80, 6, 47, 119]. The interaction between a dissipative NMO and a dissipative CPB was treated within the rotating wave approximation (RWA) in the previous section[119]. A regime where RWA is not valid can be easily obtained for these systems. Thus we wish to consider the regime where the NMO frequency $\omega_0/(2\pi)$ is much smaller than the CPB frequency $\Omega/(2\pi)$. The interaction between the NMO and CPB is then treated using time independent second-order perturbation theory, which is justified as long as coupling strength is around a tenth of $\omega_0$. Then, in the basis of these perturbed states we do a first-order time-dependent perturbation theory calculation to include dissipation in both the NMO and the CPB.
2.4.2 Hamiltonian without dissipation; perturbation solution

We start by considering the Hamiltonian for the coupled NMO/CPB system described in the previous section. We first discuss this system without the dissipative terms. If the interaction energy $H_I$ is sufficiently weak, the energy levels can be calculated using second-order perturbation theory in the coupling constant $g$. This second-order calculation has been carried out in Ref.[47], and for completeness we summarize the main results here. We wish to find the eigenstates of $H = H_T - H_{diss} = H_{CPB} + H_{NMO} + H_I$ using second-order perturbation theory in the interaction. The unperturbed states are eigenstates of $H_{CPB} + H_{NMO}$ and satisfy

\[
(H_{CPB} + H_{NMO}) |\psi_{\pm}, N\rangle = E_{\pm,N}^{(0)} |\psi_{\pm}, N\rangle
\]

\[
= \left( \pm \frac{1}{2} E(n_g) + \left(N + \frac{1}{2}\right) \hbar \omega_0 \right) |\psi_{\pm}, N\rangle. \tag{2.10}
\]

Here $N$ is an integer corresponding to a Fock state of the NMO. The unperturbed CPB energies are given by $E(n_g) = \sqrt{[4E_C (1 - 2n_g)]^2 + E_J^2}$, and the corresponding eigenstates expressed in the charge basis are

\[
|\psi_-\rangle = \cos \theta |0\rangle + \sin \theta |1\rangle \tag{2.11}
\]

and

\[
|\psi_+\rangle = - \sin \theta |0\rangle + \cos \theta |1\rangle, \tag{2.12}
\]

where $\tan 2\theta = E_I/[4E_C(1 - 2n_g)]$. The states $|0\rangle$ and $|1\rangle$ represent the two charge states of the CPB. It is reasonable to model the CPB as a two level system for the low temperature regime of interest, in which $k_BT \ll E_C$ and $k_BT \ll E_J$.

With $H_I$ treated as a perturbation, we readily find that the correction to the energy levels to second-order in $g$ is

\[
E_{\pm,N}^{(2)} = E_{\pm,N}^{(0)} + \Delta_{\pm,N}^{(1)} + \Delta_{\pm,N}^{(2)}. \tag{2.13}
\]
The first-order correction \( \Delta_{\pm,N}^{(1)} = \langle \psi_{\pm}, N \rangle H_I | \psi_{\pm}, N \rangle \) vanishes because \( \langle N | (a + a^\dagger) | N \rangle = 0 \). The second order term is

\[
\Delta_{\pm,N}^{(2)} = \sum_{i,M \neq \pm,N} \frac{|\langle \psi_i, M | H_I | \psi_{\pm}, N \rangle|^2}{E_{\pm,N}^0 - E_{i,M}^0}
= |g|^2 \left[ -\frac{\cos^2 2\theta}{\hbar \omega_0} + \sin^2 2\theta \left( \frac{\pm (2N + 1) E(n_g) + \hbar \omega_0}{E(n_g)^2 - (\hbar \omega_0)^2} \right) \right].
\] (2.14)

Corresponding to this second order shift in the energy levels, the perturbed eigenstates to first order in \( g \) are

\[
|\psi_{\pm}, N\rangle^{(1)} = |\psi_{\pm}, N\rangle + \sum_{i,M \neq \pm,N} |\psi_i, M\rangle \frac{\langle \psi_i, M | H_I | \psi_{\pm}, N \rangle}{E_{\pm,N}^0 - E_{i,M}^0}
= |\psi_{\pm}, N\rangle + \frac{\pm g \sqrt{N + 1} \cos 2\theta}{\hbar \omega_0} |\psi_{\pm}, N + 1\rangle - \frac{\pm g \sqrt{N} \cos 2\theta}{\hbar \omega_0} |\psi_{\pm}, N - 1\rangle
- \frac{g \sqrt{N + 1} \sin 2\theta}{\pm E(n_g) - \hbar \omega_0} |\psi_{\mp}, N + 1\rangle - \frac{g \sqrt{N} \sin 2\theta}{\pm E(n_g) + \hbar \omega_0} |\psi_{\mp}, N - 1\rangle.
\] (2.15)

These new eigenstates clearly exhibit the entanglement arising from the interaction: the perturbed eigenstates can no longer be written as products of oscillator states and Cooper-pair box states.

### 2.4.3 Inclusion of dissipation and decoherence

Next, we include dissipation by adding a randomly time-dependent perturbation \( H_{\text{diss}} \) to the time-independent Hamiltonian \( H_{\text{CPB}} + H_{\text{NMO}} + H_I \). For \( H_{\text{diss}} \), we choose the following form:

\[
H_{\text{diss}} = \hbar \sqrt{\gamma} \sigma^d \xi_\sigma(t) + \hbar \sqrt{\kappa a} \xi_\alpha(t).
\] (2.16)

The operators \( a \) and \( \sigma^d \) produce dissipation in the NMO and decoherence in the CPB, respectively. \( a \) is the annihilation for a vibrational quantum, and the operator \( \sigma^d \) induces phase relaxation processes described by the relaxation time \( T_2 \). It is
defined by

\[ \sigma^d|\psi_+\rangle \equiv |\psi_-'\rangle, \]

\[ \sigma^d|\psi_-\rangle \equiv |\psi_+'\rangle, \]  \hspace{1cm} (2.17)

where \(|\psi^\pm\rangle\) are the two eigenstates of the Cooper-pair box. In terms of the angle \(\theta\) introduced earlier, \(\sigma^d\) is written as

\[ \sigma^d = \begin{pmatrix} -\sin 2\theta & \cos 2\theta \\ \cos 2\theta & \sin 2\theta \end{pmatrix}. \]  \hspace{1cm} (2.18)

The symbols \(\xi(a)(t)\) and \(\xi(\sigma)(t)\) represent complex normalized Wiener processes, whose ensemble averages (denoted by overbars) satisfy

\[ \overline{\xi_a(t)} = \overline{\xi_\sigma(t)} = 0, \]  \hspace{1cm} (2.19)

\[ \overline{\xi_\sigma(t')\xi_\sigma^*(t'')} = \overline{\xi_a(t')\xi_a^*(t'')} = \delta(t' - t''), \]  \hspace{1cm} (2.20)

\[ \overline{\xi_\sigma(t')\xi_a^*(t'')} = \overline{\xi_a(t')\xi_\sigma^*(t'')} = 0. \]  \hspace{1cm} (2.21)

For all other pairs of variables, the ensemble averages vanish. Finally, the constants \(\gamma\) and \(\kappa\) represent decay rates associated with \(\sigma^d\) and \(a\), respectively. \(\kappa\) is related to the \(Q\) factor of the NMO by \(\kappa = \omega_0/Q\).

Given this model, we now calculate the energy relaxation time of the NMO, and the decoherence time of the CPB, taking into account the interaction between the two systems. We assume that the entangled states are adequately described by perturbation theory; the conditions for the validity of this assumption are given below.
Let us suppose that the system is in state $|i\rangle$ at time $t = 0$. The probability amplitude that it makes a transition to state $|f\rangle$ at time $t$ is, to first-order in time-dependent perturbation theory,

$$d_f(t) = -\frac{i}{\hbar} \int_0^t \langle f | H_{\text{diss}} | i \rangle e^{i\omega_{fi}t} dt,$$

(2.22)

where $\omega_{fi} = (E_f - E_i)/\hbar$. Substituting in the perturbation, and averaging $|d_f(t)|^2$ over an ensemble of realizations of the randomly time-dependent perturbation, we find that

$$|d_f(t)|^2 = \int_0^t \int_0^t dt' dt'' \left[ \frac{\gamma}{\hbar} \xi_{\sigma}(t') \xi_{\sigma}^*(t'') \langle f | \sigma^d | i \rangle|^2 + \kappa \xi_a(t') \xi_a^*(t'') \langle f | a | i \rangle|^2 \right].$$

(2.23)
Figure 2.10: Calculated $\kappa_e$ versus initial number of vibrational quanta $N$ in the NMO with $n_g = 0.5, E_J = h(1 \text{ GHz}), \omega_0 = 500 \text{ MHz} \text{ and } g = -50 \text{ MHz}$ for fixed $\kappa = 0.002 \text{ (ns)}^{-1}$ and $\gamma = 0.1 \text{ (ns)}^{-1}$.

Evaluating these correlation functions using eqs. (2.21), we find that

$$w_{if} \equiv \frac{|d_f(t)|^2}{t} = [\gamma |\langle f|\sigma^d|i\rangle|^2 + \kappa |\langle f|a|i\rangle|^2].$$

(2.24)

Next, we consider the effective decay rate for the NMO, which we denote as $\kappa_e$. We calculate this from the rate of the process where the initial state is $|i\rangle = |\psi_-, N\rangle^{(1)}$ and the final state is $|f\rangle = |\psi_-, N - 1\rangle^{(1)}$. With these initial and final states the
relevant matrix elements are

\[
\langle \psi_-, N - 1 | a | \psi_-, N \rangle^{(1)} = \sqrt{N} \left[ 1 + \frac{g^2 \cos^2 2\theta}{(\hbar\omega_0)^2} 2N + \frac{g^2 \sin^2 2\theta}{(E(n_g)^2 - (\hbar\omega_0)^2)} \left( 2N(E(n_g)^2 + (\hbar\omega_0)^2) - 4E(n_g)\hbar\omega_0 \right) \right]; \tag{2.25}
\]

\[
\langle \psi_-, N - 1 | \sigma^d | \psi_-, N \rangle^{(1)} = \frac{2gE(n_g) \sin 2\theta}{E(n_g)^2 - (\hbar\omega_0)^2} \sqrt{N}. \tag{2.26}
\]

Thus, according to eq. (2.24), \( \kappa_e \) is obtained by multiplying the square of the right hand side of eq.(2.25) with \( \kappa \) and adding to it the product of \( \gamma \) and the square of the right hand side of eq.(2.26).

To obtain the effective decay rate \( \gamma_e \) of the CPB, we consider the process where \(|i\rangle = |\psi_+, N \rangle \) and \(|f\rangle = |\psi_-, N \rangle \). The relevant matrix elements are now

\[
\langle \psi_-, N | a | \psi_+, N \rangle^{(1)} = - \frac{g \sin 2\theta}{E(n_g) - \hbar\omega_0}; \tag{2.27}
\]

\[
\langle \psi_-, N | \sigma^d | \psi_+, N \rangle^{(1)} = 1 - \frac{g^2 \cos^2 2\theta}{(\hbar\omega_0)^2} (2N + 1) - \frac{g^2 \sin^2 2\theta}{E(n_g)^2 - (\hbar\omega_0)^2} \left[ (E(n_g)^2 + (\hbar\omega_0)^2) \right] \tag{2.28}
\]

\( \gamma_e \) is obtained by multiplying the square of the right hand side of eq.(2.27) by \( \kappa \), and adding the product of \( \gamma \) and the square of the right hand side of eq.(2.28).

**2.4.4 Discussion**

Now we discuss the implication of our approximate calculation. Fig. 2.9 and 2.10 show \( \gamma_e \) and \( \kappa_e \) as a function of initial number of vibrational quanta in the NMO. In these plots \( n_g = 0.5 \) which implies that \( \theta = \frac{\pi}{4} \), \( E_J = \hbar(1 \text{ GHz}) \), \( \omega_0 = 500 \text{ MHz} \) and \( g = -50 \text{ MHz} \). The decay rates for the uncoupled NMO and CPB are fixed, and given by \( \kappa = 0.002 \text{ (ns)}^{-1} \) and \( \gamma = 0.1 \text{ (ns)}^{-1} \), respectively. Fig. 2.9 suggests that the effective decay rate for the qubit can be increased by coupling it to a high Q NMO.
This is in agreement with the conclusions made in the previous section. However, here the CPB and NMO are not in resonance and thus RWA is invalid. So within this regime the full hamiltonian predicts the same qualitative behavior for $\gamma_e$. Similarly, Fig. 2.10 suggests that as a result of this coupling the effective decay rate of the NMO increases.

To summarize, we have shown that within these energy regimes the quality of a qubit can be increase by coupling it to a high $Q$ NMO.
CHAPTER 3

ELECTRONIC, MAGNONIC AND PHOTONIC SUPERLATTICES

Superlattices have proven to be extremely successful in controlling the electronic structure of more conventional semiconducting materials (see, e. g., Ref. [124]). In these materials, the presence of the additional periodic potential gives rise to superlattice electronic[124], magnonic[127], photonic[94, 65] or acoustic[101] band structure, which has extra band gaps at high symmetry points in the superlattice Brillouin zone (SBZ).

In the following section we consider an electronic superlattice on graphene. The results of this section were published in Physical Review B [121].

3.1 Tunable band gap in graphene with a electronic superlattice potential which is non-centrosymmetric

3.1.1 Introduction

Ever since the synthesis of high-quality graphene[85], there has been tremendous interest in the properties of this single-layer form of carbon. Graphene has a honeycomb lattice structure, with two atoms per primitive cell and a hexagonal Brillouin zone (BZ). The Fermi energy $E_F$ of homogeneous, neutral graphene lies at the so-called Dirac point, which occurs at high symmetry points $K$ in the BZ. In fact, there
are two inequivalent Dirac points $K_0$ and $K'_0$ with two distinct valleys of excitations. Near the Dirac point, the density of states is linear in $|E - E_F|$ and the spectrum of quasiparticle states is well described by the Dirac equation for massless fermions. Partly as a result of this electronic structure\cite{85, 141, 10, 35}, graphene has many unusual electronic properties, such as a unique type of quantum Hall effect\cite{85, 95}, ballistic conduction by massless Dirac fermions\cite{85, 95}, size-dependent band gap\cite{43}, large magnetoresistance\cite{44, 35, 25}, and gate-tunable optical transitions\cite{134}.

A number of workers have investigated the possibility of building graphene electronic circuits without physically cutting or etching the graphene monolayer. A natural way to accomplish this is by subjecting graphene to an external potential with a suitable superlattice periodicity, e. g., by applying appropriate gate voltages.

There have been several predictions of electronic effects in graphene due to an external superlattice potential. For example, with one-dimensional (1D) and two-dimensional (2D) superlattices, the group velocity of the low-energy charge carriers is anisotropically renormalized \cite{91, 8}, while a corrugated graphene sheet is expected to show charge inhomogeneity and localized states \cite{39}. Superlattices in graphene can be realized experimentally by using periodically patterned gates. Using an electron-beam, adatoms with a superlattice patterns of periodicity as small as 5 nm have been achieved on freestanding graphene membranes \cite{77}. Superlattice patterns have also been observed for graphene on metal surfaces \cite{71, 27, 138}. In a recent theoretical study, a triangular graphene superlattice (TGS) was considered, and a new class of massless Dirac fermions was predicted to occur at the M point in the SBZ\cite{90}.

In the studies so far, the external periodic potential giving rise to the superlattice has had spatial inversion symmetry. As a result of this symmetry, the degeneracy
of the conduction and valence band at the original Dirac point (ODP) is preserved. In the present work, by contrast, we consider the potentials of an external TGS and a square graphene superlattice (SGS) without inversion symmetry. We show that, because of the absence of inversion symmetry, an energy gap opens up at both the original and the new Dirac points in the TGS and at the Dirac point in the SGS. The magnitude of these gaps can, in principle, be controlled by modifying the externally applied voltages. Thus far, we have been able to achieve a band gap as large as 65 meV extending throughout the SBZ. Because of the controllability of the band gap, this type of graphene superlattice represents a system in which the band gap can be chosen with considerable freedom by modifying the applied external potential. Such a system, and particularly the control at the ODP, might be quite useful in realizing future graphene electronic circuits.

3.1.2 Formalism

We first describe the formalism we use to calculate the superlattice band structure for a non-centrosymmetric superlattice potential, mostly following the approach of Ref. [90]. If the periodicity of the superlattice is much larger than the intercarbon distance \( a \sim 1.42 \, \text{Å} \), which is the case considered here, the intervalley scattering (between \( K_0 \) and \( K'_0 \)) can be neglected [5]. We limit our discussion to the spectrum near one of the two inequivalent Dirac points, which we denote \( K_0 \), in the presence of a periodic external potential \( V(x, y) \). In pure graphene, we use a pseudospin basis \( \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik \cdot r} \) and \( \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik \cdot r} \), where \( \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} 0 \\ 1 \end{pmatrix} \) are Bloch sums of \( \pi \) orbitals with wave vector \( K_0 \) on the sublattices A and B, respectively, and \( k \) is the wave vector relative to the \( K_0 \) point. The single valley Hamiltonian for the quasiparticles
of pure graphene is[131]

\[ H_0 = \hbar v_0 (-i\sigma_x \partial_x - i\sigma_y \partial_y), \]  
(3.1)

where \( v_0 \) is the (isotropic) group velocity at the Dirac point and the \( \sigma \)'s are Pauli matrices. The eigenstates and energy eigenvalues are

\[ \psi_{s,k}(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ se^{i\theta_k} \end{pmatrix} \]  
(3.2)

and

\[ E_{s}^0(k) = s \hbar v_0 k, \]  
(3.3)

where \( s = \pm 1 \) is the band index and \( \theta_k \) is the polar angle of the wavevector \( k \). Eq. (3.2) indicates that the pseudospin vector is parallel and antiparallel to \( k \) in the upper \((s = 1)\) and lower \((s = -1)\) bands, respectively.

We wish to consider the spectrum of elementary excitations near one of the Dirac points in the presence of \( V(x,y) \). The total Hamiltonian then takes the form \( H = H_0 + H' \), where

\[ H' = IV(x,y), \]  
(3.4)

\( I \) being the \( 2 \times 2 \) identity matrix. We consider a periodic external potential having either a triangular Bravais lattice with basis vectors \( b_1 = b\hat{x}, \ b_2 = b \left( \frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y} \right) \), or a square Bravais lattice with \( b_1 = b\hat{x}, \ b_2 = b\hat{y}. \) We also assume that \( V(x,y) \) varies slowly on the scale of a lattice constant \((b \gg a)\). Then the band structure of the elementary excitations near the \( K_0 \) point can readily be obtained by diagonalizing \( H_0 + H' \) in a plane wave spinor basis[90]. The basis states are of the form \( \chi(s) \exp[i(k + G) \cdot r] \), where \( \chi(s) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) or \( \begin{pmatrix} 0 \\ 1 \end{pmatrix} \) and \( G \) is a reciprocal lattice vector corresponding to the periodic external potential \( V(x,y) \). If we include \( N \) plane waves, we must thus diagonalize a \( 2N \times 2N \) matrix to obtain the band structure of
elementary excitations non-perturbatively near the \( K_0 \) point in the presence of the external periodic potential. We use \( N = 625 \) for both the triangular and the square graphene superlattice. In our actual calculations, we have considered an external potential produced by a periodic array of circular regions, within each of which the potential is a constant. These are easy to treat by the above approach, because the Fourier transform of the constant potential is available analytically. To break the inversion symmetry, we have added a second, smaller circular region within each primitive cell, as illustrated in Figs. 3.1 and 3.2. If the second region is not equidistant from the two adjacent larger circular regions, inversion symmetry is broken.

![Diagram of graphene plane subjected to periodic external potential](image)

Figure 3.1: Schematic of graphene plane subjected to a periodic external potential \( V(x, y) \) consisting of a periodic arrangement of circular contacts, within each of which \( V \) is a constant. The large circles are arranged on a triangular lattice of edge \( b \). The small circles are not midway between the large circles; for the case shown, they are centered at \( 0.4b\hat{x} \) relative to the centers of the large circles.
3.1.3 Results

We first review the case of a triangular array of large circles, with a constant external potential within each circle. Elsewhere in the superlattice, the external potential is zero. The resulting band structure has been computed in Ref. [90]. In the presence of the superlattice, there are several Dirac points: the ODP, which is at Γ of the SBZ, and “next generation” Dirac points, at M and K of the SBZ. Of these new Dirac points, only the ODP (with energy set to 0 eV) and the new Dirac point (NDP) at M with energy 0.196 eV) have vanishing density of states [90]. Near both of these points, the density of states goes linearly to zero with energy. However, the group velocity near the NDP is highly anisotropic.

We now consider the superlattice band structure (SBS) for graphene subject to the non-centrosymmetric potential shown in Fig. 3.1. We choose the lattice constant of the external potential to be \( b = 10 \) nm, and the radius \( r_1 \) of the large circles to be 2.5 nm, so that the filling fraction of large circles is 0.226725. We take the smaller circular gates to have radius \( r_2 = 1 \) nm, and to be centered at \( \mathbf{R} + 0.4b\hat{x} \), where \( \mathbf{R} \) is a Bravais vector of the superlattice. The resulting band structure is shown in Fig. 3.3 for the case \( V_1 = 0.5V, V_2 = -1.65V \), where \( V_1 \) and \( V_2 \) are the voltages on the larger and smaller circles. Once again \( V = 0 \) in the rest of the lattice. A substantial direct gap opens up at the ODP of magnitude \( \Delta_\Gamma = 58.15 \) meV for these parameters (between the first and second bands). Although not obvious from Fig. 3.3, there is also a gap \( \Delta_M \) which opens up at the NDP, of magnitude \( \sim 1 \) meV. For these parameters, we have checked that there is, in fact, a full band gap at ODP extending through the entire SBZ.
Although there is also a small gap also at $M$, it does not extend throughout the SBZ, as is evident from the Figure (the gap at $M$ does extend throughout the SBZ for $V_2$ positive). The inset of Fig. 3.3 shows the SBZ, with the symmetry points $\Gamma$, $K$, and $M$ indicated.

![Figure 3.2](image)

**Figure 3.2:** Same as Fig. 3.1, except that the large and small circular contacts are arranged on a square lattice, rather than a triangular one. Each small circle is now centered at $0.375b\hat{x}$ relative to the center of the nearest large circle.

In Fig. 3.4, we show the corresponding SBS for graphene subjected to the potential with square symmetry shown in Fig. 3.2. Once again, we choose the superlattice constant $b = 10$, $r_1 = 2.5$ nm, and $r_2 = 1$ nm, so that the filling fraction of circles in this case is 0.227765. We choose $V_1 = 0.5$ V and $V_2 = \ -1.4$ V, and each small circle is located at $0.375\hat{x}$ relative to the center of each large circle. There is a gap of magnitude 64.4 meV, at the ODP at $\Gamma$ which extends throughout the SBZ.
Figure 3.3: Superlattice band structure (SBS) for graphene subjected to an external potential produced by a triangular superlattice of contacts, as shown in Fig. 3.1. The calculation is carried out using $b = 10$ nm, $V_1 = 0.5$ V, $V_2 = -1.65$ V, $r_1/b = 0.25$, $r_2/b = 0.1$, and the small circles are located at $0.4\hat{x}$. The $\Gamma$ point of the superlattice corresponds to one of the $K$ point of the original graphene lattice. If only the large circular contacts were present, the SBS would have Dirac points at both $\Gamma$ and $M$ of the SBS Brillouin zone, at both of which the density of states would go linearly to zero. Inset: first Brillouin zone of a triangular lattice showing the three high-symmetry points $\Gamma$, $M$, and $K$.

In Fig. 3.5, we show how the direct gaps at the Dirac point depend on the voltage $V_2$ on the smaller circles in the triangular and square superlattices. For the square superlattice, we take $b = 10$ nm, $r_1/b = 0.25$ $r_2/b = 0.125$, $V_1$ at 0.5 V, and the small circles are located at $0.375\hat{x}$. For the triangular superlattice, $b = 10$ nm, $r_1/b = 0.25$, $r_2/b = 0.1$, $V_1 = 0.5$ V, and the small circles are located at $0.4\hat{x}$. In both cases, these gaps show clear maxima as functions of $V_2$. We have carried out similar calculations using positive values of $V_2$ in both cases and also obtain nonzero gaps.
Figure 3.4: SBS for graphene subjected to an external potential produced by a square superlattice of contacts, as in Fig. 3.2. The Γ point of the superlattice corresponds to one of the K point of the original graphene lattice. In this case, we use \( b = 10 \) nm, \( V_1 = 0.5 \) V, \( V_2 = -1.4 \) V, \( r_1/b = 0.25 \), \( r_2/b = 0.125 \) and the small circles are located at 0.375\( \hat{x} \). Inset: first Brillouin zone of a square lattice showing the three high-symmetry points Γ, X, and M.  

... extending throughout the SBZ. In the case of positive \( V_2 \), they are generally smaller than for negative voltages.)  

In Fig. 3.6, we show the dependence of the gaps at the Dirac point on the radius \( r_2 \) in both the triangular and square superlattices. For the square superlattice, we take \( b = 10 \) nm, \( V_1 = 0.5 \) V, \( V_2 = -1.4 \) V, \( r_1/b = 0.25 \) and the small circles are located at 0.375\( \hat{x} \). For the triangular case, \( b = 10 \) nm, \( V_1 = 0.5 \) V, \( V_2 = -1.65 \) V, \( r_1/b = 0.25 \), and we locate the small circular contacts at 0.4\( \hat{x} \). The direct band gaps can reach as large as \( \sim 65 \) meV for the square superlattice. Because of the special form of the Hamiltonian of eqs. (3.1) and (3.4), the superlattice band structure, and hence the
band gap at the ODP, exhibits a simple scaling relation: under the transformation $b \rightarrow \lambda b$ and $V(x, y) \rightarrow V(\lambda x, \lambda y)/\lambda$, where $\lambda$ is a dimensionless scaling factor, the eigenvalues of $H$ satisfy $E(k_x, k_y) \rightarrow E(k_x/\lambda, k_y/\lambda)/\lambda$. Thus, in particular, $\Delta_\Gamma$ is multiplied by $1/\lambda$. For example, if $b$ is halved (and all other lengths are also halved), and the potentials on all the contacts are doubled, then the band gap is also doubled. We have confirmed numerically that this scaling relation is satisfied for our bands.

Besides these calculations, we have tried some other geometries in an effort to obtain the largest possible band gap. For example, we have calculated the SBS for triangular and square superlattices with two off-center circular contacts, one along each edge of the primitive cell. This geometry does not lead to band gaps larger than we have obtained with one off-center circle.

3.1.4 Discussion

The present results show that the band gap of graphene at the Dirac point can be manipulated by subjecting it to a superlattice potential which lacks inversion symmetry. The magnitude of the band gap can be controlled by modifying the contact potentials. Thus, if such an arrangement of contacts can be created, the resulting material has a band gap which can be controlled via the applied voltages without modifying the structure.

There are several obvious challenges before this scheme could be used in practice. First, the band gaps are rather small (of order 65 meV). These can be made larger by reducing $b$, while simultaneously increasing $V_1$ and $V_2$ as implied by the above scaling relation, but this could be challenging experimentally. The gaps can also be increased by increasing the voltages at fixed geometry. Perhaps the most promising
Scheme might be to increase $b$ while simultaneously *increasing* the bias voltages. The larger $b$ would be easier to achieve experimentally, while the large voltage offsets would increase the gap. These ideas certainly do not exhaust the possibilities offered by periodic arrangements of contacts. Any 2D superlattice of gates lacking inversion symmetry would lead to a band gap at the ODP, and some which we have not tried may lead to a larger band gap than those we have found to date. A 1D superlattice potential lacking inversion symmetry will not suffice to produce a complete band gap. But such a 1D potential, when combined with a suitable non-time-reversal-invariant perturbation such as a magnetic field, might also lead to a complete band gap.

Figure 3.5: Plot of the gap at the Dirac point $\Gamma$ as a function of the voltage $V_2$ (in V) on the smaller circles. Full curve: square lattice; dashed curve: triangular lattice.
Figure 3.6: Plot of the gap at the Dirac point as a function $r_2/b$. Full curve: square lattice; dashed curve: triangular lattice.

There are, of course, many other ways to create a band gap in graphene besides the method described here. For example, one could create a non-centrosymmetric lattice of nanoscale holes in graphene. It would be difficult to use this method, however, to create a tunable band gap. In graphene nanoribbons with armchair edges, the band structure becomes insulating if the width of the sample in units of the lattice constant ($a$) is not of the form $3M+1$, with $M$ an integer[19, 112, 31, 9, 23]. But creating such a ribbon requires cutting graphene samples with very high precision, and again, once the ribbon has been created, the band gap cannot be easily tuned. Another possibility is to induce a gap by using a substrate which lacks inversion symmetry[36]. Again in this case, the gap cannot easily be controlled because the atomic spacing of the
substrate is fixed. Our proposal of a TGS (or other 2D superlattice) with a non-centrosymmetric superlattice potential is more efficient in opening up a gap at the ODP. In principle, moreover, this gap can easily be larger than the thermal energy at room temperature for modest values of potential. Thus, this method may be a viable approach to creating graphene with a readily tunable band gap.

In summary, we have calculated the superlattice band structure for graphene subjected to a non-centrosymmetric superlattice of contacts, on each of which the voltage is held constant. We find that the superlattice band structure exhibits a band gap extending throughout the SBZ, which can thus be tuned by external voltages. For some choices of the voltages and superlattice constant, the band gap can be as large as 65 meV, significantly larger than the room temperature thermal energy. Thus, this arrangement might possibly be of use in future electronic or electromagnetic devices.

3.2 Two dimensional magnetic superlattice as a waveguide for spin waves

In this section we describe a simple method of including dissipation in the spin wave band structure of a periodic ferromagnetic composite, by solving the Landau-Lifshitz equation for the magnetization with the Gilbert damping term. We use this approach to calculate the band structure for a square or triangular array of iron (Fe) nanocylinders embedded in an nickel (Ni) host. The results show that there are certain bands and special directions in the Brillouin zone where the spin wave lifetime is increased by more than an order of magnitude above its average value. Thus, it may be possible to generate spin waves in such composite which can propagate especially large distances at certain frequencies and directions.
3.2.1 Introduction

The existence of a periodic superlattice strongly affects many types of excitations in solids. For example, the electronic band structure of a conventional semiconductor or semimetal[124], and the dispersion relations of electromagnetic waves[139], elastic waves[108, 109, 59, 60], and spin waves[56, 96, 57, 84, 58] are all greatly influenced by the presence of a periodic superlattice potential. In many cases, such potentials can give rise to new, and even complete, electronic, photonic, elastic, or magnonic band gaps which may have important implications for the properties of these materials. These excitations have, by now, been extensively studied numerically and analytically, using a variety of methods, and have been probed in a vast range of experiments[24, 130, 135].

In this section, we consider a particular class of such excitations, namely, spin waves in periodic magnetic materials. We go beyond previous work by calculating the spin wave lifetimes in such materials. Our most striking finding is that these lifetimes are strongly dependent on the Bloch wave vector $k$, even though, in our model, the same spin waves would have a $k$-independent lifetime in a homogeneous magnetic material. This strong $k$-dependence shows that magnetization in periodic magnetic materials can be transported most efficiently by spin waves propagating along special directions in $k$-space. These results suggest possible experiments in which spin waves are launched in particular directions along which they can propagate most efficiently. This generation of spin waves could be accomplished by real magnetic fields, or it might be done using spin currents via a spin torque effect.
3.2.2 Formalism

Our calculations are carried out for an array of infinitely long circular cylinders made of a ferromagnetic material $A$ embedded in another infinite ferromagnetic material $B$. All the cylinders are taken to be parallel to the $\hat{z}$-axis and their intersection with the $x - y$ plane forms a two-dimensional periodic lattice. We consider two arrangements of such cylinders: a triangular and a square superlattice. An external static magnetic field $H_0$ is applied parallel to the axis of the cylinders, and both ferromagnets are assumed to be magnetized parallel to $H_0$.

The equation of motion for this periodic composite is given by the Landau-Lifshitz-Gilbert (LLG) equation\cite{127}:

$$\frac{\partial}{\partial t} M(\mathbf{r}, t) = \gamma \mu_0 M(\mathbf{r}, t) \times H_{\text{eff}}(\mathbf{r}, t) + \frac{\alpha}{M_s(\mathbf{r})} \left( M(\mathbf{r}, t) \times \frac{\partial}{\partial t} M(\mathbf{r}, t) \right) .$$  \hspace{1cm} (3.5)

Here $\gamma$ is the gyromagnetic ratio, which is assumed to be the same in both ferromagnets, $H_{\text{eff}}$ is the effective field acting on the magnetization $M(\mathbf{r}, t)$, $\mathbf{r}$ is the position vector, $\alpha$ is the Gilbert damping parameter and $M_s$ is the spontaneous magnetization.

For this inhomogeneous composite $H_{\text{eff}}$ can be written as

$$H_{\text{eff}}(\mathbf{r}, t) = H_0 \hat{z} + h(\mathbf{r}, t) + \frac{2 \mu_0 M_s}{\nabla \cdot A M_s} \nabla M(\mathbf{r}, t),$$  \hspace{1cm} (3.6)

where $h(\mathbf{r}, t)$ is the dynamic dipolar field and $A$ denotes the exchange constant. The last term on the right-hand side of eq. (2) denotes the exchange field. For the two-component composite we consider, the exchange constant, the spontaneous magnetization and the Gilbert damping parameter take the forms

$$A(\mathbf{r}) = A_B + \Theta(\mathbf{r})(A_A - A_B),$$

$$M_s(\mathbf{r}) = M_{s,B} + \Theta(\mathbf{r})(M_{s,A} - M_{s,B}),$$

$$\alpha(\mathbf{r}) = \alpha_B + \Theta(\mathbf{r})(\alpha_A - \alpha_B),$$  \hspace{1cm} (3.7)
where the step function $\Theta(\mathbf{r})$ is given by

$$
\Theta(\mathbf{r}) = \begin{cases} 
1 & \text{if } \mathbf{r} \text{ is inside ferromagnet A}, \\
0 & \text{otherwise}.
\end{cases}
$$

We separate the static and time-dependent parts of the magnetization by writing

$$
\mathbf{M}(\mathbf{r}, t) = M_s \hat{z} + \mathbf{m}(\mathbf{r}, t) \quad \text{where } \mathbf{m}(\mathbf{r}, t) = \mathbf{m}(\mathbf{r}) e^{-i\omega t}
$$

is the time-dependent part of the magnetization. The time-dependent dipolar field $\mathbf{h}(\mathbf{r}, t)$ has similar time dependence and can be written as $\mathbf{h}(\mathbf{r}, t) = \mathbf{h}(\mathbf{r}) e^{-i\omega t}$ with $\mathbf{h}(\mathbf{r}) = -\nabla \Psi(\mathbf{r})$, where $\Psi(\mathbf{r})$ is the magnetostatic potential. Since $\nabla \cdot (\mathbf{h}(\mathbf{r}) + \mathbf{m}(\mathbf{r})) = 0$, the magnetostatic potential $\Psi(\mathbf{r})$ obeys

$$
\nabla^2 \Psi(\mathbf{r}) - \nabla \cdot \mathbf{m}(\mathbf{r}) = 0.
$$

Within the linear-magnon approximation[26], the small terms of second order in $\mathbf{m}(\mathbf{r})$ and $\mathbf{h}(\mathbf{r})$ are neglected in the equation of motion. This is equivalent to setting $\mathbf{m}(\mathbf{r}) \cdot \hat{z} = 0[128]$. Substituting the above equations into eqs. (B.1), we obtain

$$
i\Omega m_x(\mathbf{r}) + \nabla \cdot [Q \nabla m_y(\mathbf{r})] - m_y(\mathbf{r}) - \frac{M_s}{H_0} \frac{\partial \Psi}{\partial y} + i\Omega \alpha m_y(\mathbf{r}) = 0,
$$

$$
i\Omega m_y(\mathbf{r}) - \nabla \cdot [Q \nabla m_x(\mathbf{r})] + m_x(\mathbf{r}) + \frac{M_s}{H_0} \frac{\partial \Psi}{\partial x} - i\Omega \alpha m_x(\mathbf{r}) = 0,
$$

where $\Omega = \omega / (|\gamma| \mu_0 H_0)$ and $Q = 2A / (M_s \mu_0 H_0)$.

Next, using the periodicity of $Q$, $M_s$ and $\alpha$ in the $x - y$ plane, we can expand these quantities in Fourier series as

$$
Q(\mathbf{x}) \equiv Q(x, y) = \sum_G Q(G) e^{i\mathbf{G} \cdot \mathbf{x}},
$$

$$
M_s(\mathbf{x}) \equiv M_s(x, y) = \sum_G M_s(G) e^{i\mathbf{G} \cdot \mathbf{x}},
$$

$$
\alpha(\mathbf{x}) = \alpha(x, y) = \sum_G \alpha(G) e^{i\mathbf{G} \cdot \mathbf{x}},
$$

(3.11)
where $x$ and $G$ are two-dimensional position and reciprocal lattice vectors in the $x−y$ plane. The inverse Fourier transforms are of the form

$$ Q(G) = \frac{1}{S} \int \int d^2X Q(X)e^{-iG \cdot X}, $$

(3.12)

where $S$ is the area of the unit cell; similar expressions hold for $M_s(G)$ and $\alpha(G)$.

Figure 3.7: (Left panel) Band structure for a square lattice of iron (Fe) cylinders in nickel (Ni), with lattice constant $a = 10$ nm and Fe filling fraction $f = 0.5$. Other parameters are given in the text. The widths of the cross-hatched regions are proportional to the figure of merit (FOM) defined as the ratio of the imaginary part to the real part of the eigenvalue, for the given band. (Right panel) Momentum dependence of FOM for the fourth band for three different values of filling fraction: $f = 0.77$ for top (black), $f = 0.5$ for red (middle) and $f = 0.1$ for blue (bottom).
To calculate the band structure for spin waves propagating in the $x - y$ plane, we consider the two-dimensional Bloch vector, $\mathbf{k}$ and use Bloch’s theorem to write

\[
\begin{align*}
    m_x(x) &= e^{ik \cdot x} \sum_G m_{x,K}(G) e^{iG \cdot x}, \\
    m_y(x) &= e^{ik \cdot x} \sum_G m_{y,K}(G) e^{iG \cdot x}, \\
    \Psi(x) &= e^{ik \cdot x} \sum_G \Psi_K(G) e^{iG \cdot x}.
\end{align*}
\]

After some straightforward algebra, the equations of motion reduce to

\[
\begin{align*}
    i\Omega \sum_{G'} \tilde{A}(G, G') \begin{bmatrix} m_{x,K}(G) \\ m_{y,K}(G) \end{bmatrix} &= \sum_{G'} \tilde{M}(G, G') \begin{bmatrix} m_{x,K}(G') \\ m_{y,K}(G') \end{bmatrix};
\end{align*}
\]

where the $2 \times 2$ matrix

\[
\tilde{A}(G, G') = \begin{bmatrix} \delta_{GG'} & \alpha(G - G') \\ -\alpha(G - G') & \delta_{GG'} \end{bmatrix}
\]

where $\delta_{GG'}$ is the Kronecker delta and the four components of the $2 \times 2$ matrix $\tilde{M}(G, G')$ are

\[
\begin{align*}
    \tilde{M}(G, G')_{xx} &= \frac{Ms(G - G')(K_x + G'_x)(K_y + G'_y)}{H_0(K + G')^2} \\
    \tilde{M}(G, G')_{xy} &= \delta_{GG'} + Q(G - G')(K + G) \cdot (K + G') + \frac{Ms(G - G')(K_y + G'_y)^2}{H_0(K + G')^2} \\
    \tilde{M}(G, G')_{yx} &= -\delta_{GG'} - Q(G - G')(K + G) \cdot (K + G') - \frac{Ms(G - G')(K_x + G'_x)^2}{H_0(K + G')^2} \\
    \tilde{M}(G, G')_{yy} &= -\frac{Ms(G - G')(K_x + G'_x)(K_y + G'_y)}{H_0(K + G')^2}.
\end{align*}
\]

On left-multiplying eq. 3.14 by the inverse of the matrix $\tilde{A}$, we reduce the band structure problem, including Gilbert damping, to that of finding the (complex) eigenvalues of $\tilde{A}^{-1}\tilde{M}$.

We used this formalism to calculate band structures for both a triangular Bravais superlattice, with basis vectors $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = a\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)$, and a square Bravais superlattice.
superlattice, with \( \mathbf{a}_1 = a\hat{x}, \mathbf{a}_2 = a\hat{y} \), where \( a \) is the edge of the superlattice unit cell. Since Fourier transforms are available analytically for cylinders of circular cross section, the band structure is easily calculated in this plane wave representation.

In order to solve Eq.3.14, we restrict the sum over \( \mathbf{G}' \) to first 625 reciprocal lattice vectors, which requires the diagonalization of a \( 1250 \times 1250 \) complex matrix. The resulting eigenvalues of the matrix \( \tilde{B}(\mathbf{G}, \mathbf{G}') \) are all complex. For a given \( \mathbf{k} \), the imaginary part of the eigenvalue for gives the spin wave frequency, while the real part represents the inverse spin wave lifetime. We have found that the frequencies and lifetimes are well converged to 0.1 % for this number of plane waves.

### 3.2.3 Results

For each eigenvalue, it is useful to define a figure of merit (FOM) as the ratio of the imaginary part to the real part of the eigenvalue. If the Gilbert damping parameters \( \alpha_A = \alpha_B \), the FOM would be same for all \( \mathbf{k} \)'s and all bands, so that the spin waves would have same inverse lifetimes in the composite for \( \mathbf{k} \)'s and all bands. By contrast, when \( \alpha_A \neq \alpha_B \) we find that the FOM varies from band to band and depends strongly on \( \mathbf{k} \). In particular, the FOM is particularly large in certain high symmetry directions. As a result spin waves will propagate longer when they are launched in special directions and with special frequencies.

Fig. 3.7, shows the band structure of a composite of Fe cylinders arranged on a square lattice and embedded in an Ni host. The inset in the right panel shows the first Brillouin zone (BZ). In calculating the band structure, we use an exchange constant and spontaneous magnetization at room temperature of \( 8.3 \text{ pJ/m} \) and \( 1.71092 \times 10^6 \text{ A/m} \) for Fe and \( 3.4 \text{ pJ/m} \) and \( 0.485423 \times 10^6 \text{ A/m} \) for Ni[110]. We use a superlattice
Figure 3.8: (Left panel) Same as Fig. 3.7 but for a triangular lattice of Fe cylinders in Ni, with lattice constant $a = 10$ and $f = 0.5$. (Right panel) Momentum dependence of FOM for the third band for three different values of filling fraction: $f=0.9$ for top (black), $f=0.5$ for red (middle) and $f=0.1$ for blue (bottom).

constant of 10 nm and filling fraction of 0.5 in our calculations. The Gilbert damping parameters are $\alpha_{Fe} = 0.0019$ and $\alpha_{Ni} = 0.064$ [87]. We plot the first nine bands, and we show the FOM as vertical lines on each band. The scales for the FOM and the real frequencies are different, as indicated. Table 3.1 lists the FOM for various bands at three high symmetry points, as also shown in Fig. 3.7. The left panel of Fig. 3.7 shows the momentum dependence of FOM for the fourth band for three different values of filling fraction: $f = 0.77$ for top (black), $f = 0.5$ for red (middle) and $f = 0.1$
Figure 3.9: The ratio of the imaginary part to the real part of the eigenvalue (FOM) as a function of filling fraction, $f$.

for blue(bottom). The right panel clearly shows that for the fourth band the FOM is roughly a factor of six times higher at the special symmetry point $M$, than it is everywhere else. Hence, if a spin wave is launched with frequency corresponding to the fourth band the composite will act as a waveguide and all momentum directions but the one corresponding to the SBZ corner will be heavily damped.

Fig. 3.8 shows the same quantities as Fig. 3.7, but for a triangular superlattice. Again the superlattice constant and filling fraction are 10nm and 0.5 respectively. Table 3.2 provides the FOM for various bands at three high symmetry points, as also shown in Fig. 3.8. Figs. 3.9 shows the dependence of FOM for these special symmetry points and bands on the filling fraction. The FOM increases with the filling fraction.
<table>
<thead>
<tr>
<th>Band Index</th>
<th>Re[Ω], FOM at Γ</th>
<th>Re[Ω], FOM at M</th>
<th>Re[Ω], FOM at X</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.7875, 14.2</td>
<td>27.847, 18.1</td>
<td>16.296, 20.9</td>
</tr>
<tr>
<td>2</td>
<td>51.883, 40.2</td>
<td>29.894, 28.2</td>
<td>20.110, 43.2</td>
</tr>
<tr>
<td>3</td>
<td>51.947, 25.0</td>
<td>29.961, 30.0</td>
<td>61.138, 38.9</td>
</tr>
<tr>
<td>4</td>
<td>55.277, 37.7</td>
<td>33.495, 180.3</td>
<td>66.262, 23.5</td>
</tr>
<tr>
<td>5</td>
<td>55.399, 37.2</td>
<td>114.13, 50.2</td>
<td>66.590, 23.3</td>
</tr>
<tr>
<td>6</td>
<td>98.795, 32.4</td>
<td>114.25, 50.5</td>
<td>66.811, 97.7</td>
</tr>
<tr>
<td>7</td>
<td>98.868, 32.7</td>
<td>119.28, 51.1</td>
<td>108.29, 38.9</td>
</tr>
<tr>
<td>8</td>
<td>100.30, 23.3</td>
<td>120.72, 106.3</td>
<td>111.96, 41.2</td>
</tr>
<tr>
<td>9</td>
<td><strong>101.11, 49.5</strong></td>
<td>127.36, 24.6</td>
<td>155.17, 39.1</td>
</tr>
</tbody>
</table>

Table 3.1: Band structure of the square lattice at high symmetry points. The columns represent, in order, the band index (from lowest to highest frequency), the real part of the frequency, and FOM at three high symmetry points Γ, M and X. Numbers in bold denote the bands with the largest FOMs for the specified symmetry point.

<table>
<thead>
<tr>
<th>Band Index</th>
<th>Re[Ω], FOM at Γ</th>
<th>Re[Ω], FOM at M</th>
<th>Re[Ω], FOM at K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.7875, 14.3</td>
<td>20.445, 22.28</td>
<td>25.780, 22.6</td>
</tr>
<tr>
<td>2</td>
<td>63.465, 51.7</td>
<td>23.996, 37.7</td>
<td>26.037, 22.7</td>
</tr>
<tr>
<td>3</td>
<td>69.260, 24.1</td>
<td>52.205, 32.3</td>
<td><strong>31.135, 84.3</strong></td>
</tr>
<tr>
<td>4</td>
<td>69.414, 24.0</td>
<td>55.247, 36.0</td>
<td>86.763, 26.0</td>
</tr>
<tr>
<td>5</td>
<td>70.173, 18.1</td>
<td>113.07, 35.9</td>
<td>90.519, 42.9</td>
</tr>
<tr>
<td>6</td>
<td><strong>71.012, 82.6</strong></td>
<td>113.41, 33.2</td>
<td>90.633, 43.0</td>
</tr>
<tr>
<td>7</td>
<td><strong>71.384, 82.2</strong></td>
<td>114.58, 29.2</td>
<td>143.29, 50.5</td>
</tr>
<tr>
<td>8</td>
<td>187.52, 31.7</td>
<td><strong>116.45, 49.5</strong></td>
<td>143.32, 50.3</td>
</tr>
<tr>
<td>9</td>
<td>187.53, 31.7</td>
<td>145.24, 27.4</td>
<td>148.39, 46.5</td>
</tr>
</tbody>
</table>

Table 3.2: Same as Table 3.1, but for the triangular lattice, at the high symmetry points Γ, M, and K.
because $\alpha_{Fe} \ll \alpha_{Ni}$, and it is maximum at the percolation threshold for both the superlattices.

### 3.2.4 Discussion

Several features of these plots are apparent. For example, in the square superlattice, the FOM is largest in the fourth band at the symmetry point M, and in the triangular superlattice, it is largest for the third band at the point K. In both cases, the FOM is large at these points because these spin waves spend most of their time in Fe, the low-damping component.

To summarize we have shown that this periodic magnetic superlattices can act as a waveguide for spin waves, transmitting spin waves only in the direction of SBZ corner.

### 3.3 “k • p” method for the effective dielectric constant of a photonic superlattice

#### 3.3.1 Introduction

The problem of calculating the effective dielectric constant $\epsilon_e$ of an inhomogeneous material dates back at least to Maxwell[63]. Among the widely used approaches is the Maxwell-Garnett approximation (MGA)[34, 13], thought to be most accurate when one of the components can be regarded as the host, and the self-consistent effective-medium approximation (SEMA)[20], thought to be most useful when none of the components can be regarded as a host[62].

Neither of these methods is designed specifically for a periodic dielectric, which has been studied using a range of approximations. One method involves expanding the electrostatic potential in a Fourier series[12]. In another Fourier approach[116, 107],
\( \epsilon_e \) is obtained from the limiting behavior of the solutions to a wave equation for an inhomogeneous medium at small wave vector. Other methods are typically limited to certain classes of such composites, such as arrays of non-overlapping spheres in a host material[97, 11, 75]. Additional approaches in this class yield \( \epsilon_e \) for square arrays of non-overlapping circular cylinders[75, 29, 74, 93], simple cubic arrays of non-overlapping spheres[92, 79], and more general, but still non-overlapping, shapes, such as a periodic array of rhombi[76] or coated cylinders[82].

In another approach, one first computes the dispersion relation for electromagnetic waves in the periodic dielectric, taking advantage of Bloch’s theorem. This band structure[50] generally has one or more branches whose frequency \( \omega \) goes to zero as the wave number \( k \) vanishes. The inverse of the derivative \( \lim_{k \to 0} [d\omega/dk] \) can be determined numerically from this band structure. This approach gives an effective product \( \epsilon_e \mu_e \) via the relation \( k = (\omega/c)\sqrt{\epsilon_e \mu_e} \), where \( \mu_e \) is an effective magnetic permeability of the composite[61]. If, however, \( \mu_e = 1 \), this approach does give \( \epsilon_e \). This procedure has been used by several groups [see, e. g., Ref. [140])] to obtain \( \epsilon_e \) numerically for both isotropic and anisotropic periodic dielectrics.

In this section, we describe a method for calculating \( \sqrt{\epsilon_e \mu} \) for an arbitrary periodic dielectric, based on the limiting \( k \to 0 \) behavior of the photonic band structure. We give a simple \textit{analytical} expression for this slope, based on the analogy between it and the effective mass of Bloch electrons. Just as in that case[7], an exact expression for \( d\omega/dk \) can be written down using \( k \cdot p \) perturbation theory. The slope can then be computed from knowledge of the photonic band structure and corresponding eigenstates at \( k = 0 \). If \( \mu_e \) can be taken as unity, the resulting expression for the slope gives \( \epsilon_e \) for any periodic system and for anisotropic as well as isotropic media.
3.3.2 Formalism

We first consider a periodic and isotropic dielectric with a position-dependent and frequency-independent dielectric function $\epsilon(x)$ and magnetic permeability $\mu = 1$ (we use Gaussian units throughout). Assuming a frequency-dependence $\exp(-i\omega t)$ for all fields, we write Maxwell’s equations as $\nabla \times E = \frac{i\omega}{c} B$ and $\nabla \times B = -\frac{i\omega}{c} \epsilon(x) E$. These may be combined to give an equation for $E$ alone or for $B$ alone. We choose to consider the latter equation:

$$\nabla \times \left( \frac{1}{\epsilon(x)} \nabla \times B \right) = \frac{\omega^2}{c^2} B.$$  \hfill (3.17)

For a periodic system, $B$ must satisfy Bloch’s theorem. We therefore write $B = B_{k,n}(x)$, and the corresponding eigenvalue as $\omega_{k,n}^2/c^2$:

$$B_{k,n}(x) = e^{i k \cdot x} u_{k,n}(x),$$ \hfill (3.18)

where $k$ is the Bloch vector, $n$ is the band index, and $u_{k,n}(x)$ is a periodic function with the same periodicity as $\epsilon(x)$. Substituting eq. (3.18) into eq. (3.17), we obtain

$$i k \times \left( \frac{1}{\epsilon(x)} \nabla \times u_{k,n}(x) \right) + \nabla \times \left( \frac{1}{\epsilon(x)} \nabla \times u_{k,n}(x) \right) + i \nabla \times \left( \frac{1}{\epsilon(x)} k \times u_{k,n}(x) \right) - k \times \left( \frac{1}{\epsilon(x)} k \times u_{k,n}(x) \right) = \frac{\omega_{k,n}^2}{c^2} u_{k,n}(x).$$ \hfill (3.19)

This equation can be rewritten schematically as

$$H_k u_{k,n} = \frac{\omega_{k,n}^2}{c^2} u_{k,n},$$ \hfill (3.20)

where $H_k$ is an effective “Hamiltonian” for electromagnetic waves of Bloch vector $k$.

To obtain $\epsilon_e$, we consider this equation for Bloch vector $k + q$, and take $|q| \ll \pi/a$, $a$ being the lattice constant. Then, just as for Bloch electrons, we can expand $H_{k+q}$...
about $H_k$, retaining terms only through second order in $q$:

$$H_{k+q}u_{k+q,n} = \frac{\omega_{k+q}^2}{c^2} u_{k+q,n},$$  \hspace{1cm} (3.21)

where

$$H_{k+q} = H_k + V_q,$$  \hspace{1cm} (3.22)

and $V_q$ satisfies

$$V_qu_{k,n} = iq \times \left( \frac{1}{\epsilon} \nabla \times u_{k,n} \right) - q \times \left( \frac{1}{\epsilon} k \times u_{k,n} \right) - k \times \left( \frac{1}{\epsilon} q \times u_{k,n} \right)$$

$$+ i\nabla \times \left( \frac{1}{\epsilon} q \times u_{k,n} \right) - q \times \left( \frac{1}{\epsilon} q \times u_{k,n} \right)$$  \hspace{1cm} (3.23)

Here we have suppressed the $x$-dependence of $\epsilon$ and $u_{k,n}$. Using perturbation theory through second order in $V_q$, we obtain

$$\frac{\omega_{k+q,n}^2}{c^2} = \frac{\omega_{k,n}^2}{c^2} + \langle kn|V_q|kn \rangle + \sum_{n' \neq n} \frac{|\langle kn|V_q|kn' \rangle|^2}{\omega_{k,n}^2/c^2 - \omega_{k,n'}^2/c^2} + \mathcal{O}(V_q^3),$$  \hspace{1cm} (3.24)

where we have introduced a bra-ket notation by $\langle kn|V_q|kn' \rangle = \int dx u_{k,n}^* (x) V_q u_{k,n'} (x)$. We can also use a Taylor expansion to write

$$\frac{\omega_{k+q,n}^2}{c^2} = \frac{\omega_{k,n}^2}{c^2} + \sum_{i=1}^3 \frac{1}{c^2} \left( \frac{\partial \omega_{k,n}^2}{\partial k_i} \right)_{q=0} q_i + \frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \frac{1}{c^2} \left( \frac{\partial^2 \omega_{k,n}^2}{\partial k_i \partial k_j} \right)_{q=0} q_i q_j + \mathcal{O}(q^3),$$  \hspace{1cm} (3.25)

where the sums run over the Cartesian components of $q$. The derivatives of frequency $(1/c^2)\partial \omega_{k,n}^2/\partial k_i$ and $[1/(2c^2)]\partial^2 \omega_{k,n}^2/\partial k_i \partial k_j$ are just the coefficients of the linear and quadratic terms in $q$ in eq. (3.24) respectively.

We obtain the inverse effective dielectric tensor $\epsilon^{-1}$ from the lowest ($n = 1$) photonic band, and assuming $\mu_e = 1$. This band satisfies $\omega_{k=0,n=1}^2 = 0$. Since it has a minimum at $k = 0$, the corresponding first derivative in eq. (A.9) vanishes. The second derivative is related to $\epsilon^{-1}$ by

$$(\epsilon^{-1})_{ij} = \frac{1}{2c^2} \left( \frac{\partial^2 \omega_{k,1}^2}{\partial k_i \partial k_j} \right)_{k=0}. \hspace{1cm} (3.26)$$
If the band is isotropic, \((\epsilon^{-1})_{ij} = \epsilon^{-1}\delta_{ij}\), where \(\delta_{ij}\) is the Kronecker delta function and \(\epsilon_e\) is a scalar.

From eq. (3.23), there are two contributions to these second derivatives: the linear term in \(q\) contributes via second-order perturbation theory, while the quadratic term contributes via first-order perturbation theory. For \(k = 0\), we may exhibit these terms as

\[
V_q u_{k,n} = V_{q,1} u_{k,n} + V_{q,2} u_{k,n},
\]

where

\[
V_{q,1} u_{k,n} = i q \times \left( \frac{1}{\epsilon} \nabla \times u_{k,n} \right) + i \nabla \times \left( \frac{1}{\epsilon} q \times u_{k,n} \right),
\]

and

\[
V_{q,2} u_{k,n} = -q \times \left( \frac{1}{\epsilon} q \times u_{k,n} \right).
\]

Using the above form for \(V_q\), we obtain

\[
\frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{1}{c^2} \left( \frac{\partial^2 \omega_{k,n}^2}{\partial k_i \partial k_j} \right) q_i q_j = \sum_{i=1}^{3} \sum_{j=1}^{3} (\epsilon^{-1})_{ij} q_i q_j = \langle k, n | V_{q,2} | k, n \rangle + \sum_{n' \neq n} \frac{|\langle k, n | V_{q,1} | k, n' \rangle|^2}{(\omega_{k=0,n}^2 - \omega_{k=0,n'}^2)/c^2}.
\]

From this expression, we can calculate the components of \(\epsilon^{-1}_e\) explicitly, given the eigenfunctions and eigenvalues of \(H_k\) at \(k = 0\), and assuming \(\mu_e = 1\). This approach can be applied to any periodic composite medium, even if \(\epsilon(x)\) varies continuously.

As another example, we obtain \(\epsilon^{-1}_e\) in a system where \(\epsilon(x)\) is independent of \(z\) and is periodic in the \(x - y\) plane\(^{[94]}\). Then \((\epsilon_e)_{zz}\) is just the spatial average of \(\epsilon(x, y)\). To obtain the in-plane part of \((\epsilon_e)^{-1}\), we consider a wave polarized with \(B \parallel \hat{z}\), so that the electric field \(E\) lies in the \(x - y\) plane. Then \(V_q\) [eq. (3.23)] is

\[
V_q(x) = -i \frac{1}{\epsilon(x)} q \cdot \nabla - i \nabla \cdot \left( \frac{q}{\epsilon(x)} \right) + \frac{1}{\epsilon(x)} q \cdot q,
\]

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where \( q \) and \( \nabla \) are 2D operators. Using the form (3.31) for \( V_q \), we obtain

\[
(\epsilon^{-1})_{ij} = \frac{1}{2c^2} \left( \frac{\partial^2 \omega_{k,n}^2}{\partial k_i \partial k_j} \right)_{k=0} = \delta_{ij} \langle k, n | \frac{1}{\epsilon(x)} | k, n \rangle + \sum_{n' \neq n} \frac{\langle k, n | (\theta_i) | k, n' \rangle \langle k, n' | (\theta_j) | k = 0, n \rangle}{(\omega_{k=0,n}^2 - \omega_{k=0,n'}^2)/c^2},
\]

(3.32)

where \( \theta_i \) is the \( i^{th} \) Cartesian component of the vector operator \( \theta = -i (1/\epsilon(x)) \nabla - i\nabla (1/\epsilon(x)) \), and all the matrix elements and frequencies are evaluated at \( k = 0 \).

The results up to Eq. (3.30) are general, Eq. (3.28) and (3.29), can be written in a more compact way as,

\[
V_{q,1} u_{k,n} = i(e_{abc} q_b \bar{\epsilon}^{-1}_{cd} e_{def} \frac{\partial}{\partial x_e} (u_{k,n}) f + e_{abc} \frac{\partial}{\partial x_b} \bar{\epsilon}^{-1}_{cd} e_{def} q_e (u_{k,n}) f),
\]

(3.33)

and

\[
V_{q,2} u_{k,n} = e_{abc} q_b \bar{\epsilon}^{-1}_{cd} e_{def} q_e (u_{k,n}) f,
\]

(3.34)

where \( a, b, c, d, e, f \) are dummy variables for coordinates, \( \bar{\epsilon}^{-1}_{cd} \) represents the inverse of the dielectric matrix, and \( e_{abc} \) represents the Levi-Civita symbol. Using these equation Eq. (3.30) can be expressed in a very compact form as follows

\[
\frac{1}{2} \sum_{b=1}^{3} \sum_{e=1}^{3} \frac{1}{c^2} \left( \frac{\partial^2 \omega_{k,n}^2}{\partial k_b \partial k_e} \right)_{q=0} q_b q_e = \sum_{b=1}^{3} \sum_{e=1}^{3} (\epsilon_e^{-1})_{be} q_b q_e = \langle k, n | \theta_1 | k, n \rangle + \sum_{n' \neq n} \frac{|\langle k, n | (\theta_2 + \theta_3) | k, n' \rangle|^2}{(\omega_{k=0,n}^2 - \omega_{k=0,n'}^2)/c^2},
\]

(3.35)

where the operators \( \theta_1, \theta_2 \) and \( \theta_3 \) are defined as follows

\[
\langle k, n | \theta_1 | k, n \rangle = \int dx (u_{k,n}^*) a e_{abc} q_b \bar{\epsilon}^{-1}_{cd} e_{def} q_e (u_{k,n}) f,
\]

\[
\langle k, n' | \theta_2 | k, n \rangle = \int dx (u_{k,n'}^*) a i (e_{abc} q_b \bar{\epsilon}^{-1}_{cd} e_{def} \frac{\partial}{\partial x_e} (u_{k,n}) f),
\]

\[
\langle k, n' | \theta_3 | k, n \rangle = \int dx (u_{k,n'}^*) a i (e_{abc} \frac{\partial}{\partial x_b} \bar{\epsilon}^{-1}_{cd} e_{def} q_e (u_{k,n}) f).
\]

(3.36)
To evaluate the above matrix elements we can expand $u_{k,n}$ and $\tilde{\epsilon}^{-1}$ in terms of Fourier coefficients as follows

$$\tilde{\epsilon}^{-1} = \sum_G [\tilde{\epsilon}^{-1}(G)] e^{iGx}, \quad (3.37)$$

and

$$u_{k,n}(r) = \sum_{G'} [u_{k,n}(G')] e^{iG'r}. \quad (3.38)$$

Substituting these expressions in Eq.3.36 we get

$$\langle k,n|\theta_1|k,n\rangle = \sum_{GG'} [u_{k,n}^*(G + G')]_{a} e_{abc} q_{b} [\tilde{\epsilon}^{-1}(G)]_{cd} e_{def} q_{e} [u_{k,n}(G')]_{f},$$

$$\langle k,n|\theta_2|k,n'\rangle = -\sum_{GG'} [u_{k,n'}^*(G + G')]_{a} e_{abe} q_{b} [\tilde{\epsilon}^{-1}(G)]_{cd} e_{def} [G']_{e} [u_{k,n}(G')]_{f},$$

$$\langle k,n|\theta_3|k,n'\rangle = -\sum_{GG'} [u_{k,n'}^*(G + G')]_{a} e_{abc} [G + G']_{b} [\tilde{\epsilon}^{-1}(G)]_{cd} e_{def} q_{e} [u_{k,n}(G')]_{f}.$$

Now, for the case of 2D array of cylinders in a host, when we consider H polarization, i.e, $H \parallel \hat{z}$, the only component of $u_{k,n}$ that survives is the $z$ component and Eq.3.32 follows.

### 3.3.3 Numerical results

We now apply this formalism to obtain $\epsilon_{e}$ for a triangular or square lattice of cylinders of dielectric constant $\epsilon_s$ embedded in a host of dielectric constant $\epsilon_h$. In this case, the in-plane part of $\epsilon_{e}^{-1}$ is isotropic in the $x-y$ plane and has non-zero components $[\epsilon_{e}^{-1}]_{xx} = [\epsilon_{e}^{-1}]_{yy} \equiv \epsilon_{e,\perp}^{-1}$; $[\epsilon_{e}^{-1}]_{zz} = \epsilon_{e,\parallel}^{-1}$. Furthermore, since the cylinders are all parallel, $\epsilon_{e,\parallel} = f\epsilon_s + (1 - f)\epsilon_h$, where $f$ is the volume fraction of cylinders.

To obtain $\epsilon_{e,\perp}$, we expand $\epsilon^{-1}(x)$ as

$$\frac{1}{\epsilon(x)} = \sum_G \epsilon^{-1}(G) e^{iGx}, \quad (3.39)$$

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where \( \mathbf{G} \) is a 2D reciprocal lattice vector. Similarly,

\[
\mathbf{u}_{k,n}(r) = \sum_{G'} \mathbf{u}_{k,n}(G') e^{iG'.r}. \tag{3.40}
\]

For a square or triangular lattice of circular cylinders,

\[
\epsilon^{-1}(G) = f\epsilon_s^{-1} + (1-f)\epsilon_h^{-1} \quad \mathbf{G} = 0;
\]

\[
2f(\epsilon_s^{-1} - \epsilon_h^{-1}) J_1(|\mathbf{Gr}|) [\mathbf{Gr}] \quad \mathbf{G} \neq 0. \tag{3.41}
\]

Given this result, the photonic band structure and corresponding eigenfunctions are readily obtained at any \( \mathbf{k} \), and hence \( \epsilon_{e,\perp} \) straightforwardly obtained.

We first consider a triangular array of Si cylinders (taking \( \epsilon_s = 14 \)) in air (\( \epsilon_h = 1 \)). The photonic band structure of this system has been computed by Plihal and Maradudin[94]. The photonic band structure for modes with \( \mathbf{B}(x)||\hat{z} \) is readily obtained using the plane wave expansion as described above and in Ref. [94]. We have calculated this band structure for various \( f \), including the 441 plane waves of lowest energy. For \( f = 0.431 \), our results agree well with those of Ref. [94]. We then used the \( \mathbf{k} = 0 \) eigenfunctions and eigenvalues to evaluate \( \epsilon_{e,\perp}^{-1} \), using eq. (3.32).

We will also compare our calculated \( \epsilon_{e,\perp} \) with the predictions of the Maxwell-Garnett approximation (MGA)[13]. For the present case, the MGA is simply given by the well-known 2D result (see, e. g., Ref. [65])

\[
\epsilon_{e,\perp}^{MGA} = \epsilon_h + 2f\epsilon_h \left( \frac{\epsilon_s - \epsilon_h}{\epsilon_s + \epsilon_h} \right) \frac{1}{1 - f + 2f\epsilon_h/(\epsilon_s + \epsilon_h)}. \tag{3.42}
\]

In Fig. 3.10, we show the resulting \( \epsilon_{e,\perp} \) for a triangular lattice of Si cylinders in an air host, as obtained using this approach (which we call the \( \mathbf{k} \cdot \mathbf{p} \) approach) versus \( f \). For comparison, we also show \( \epsilon_{e}^{MGA}(f) \). The two methods are in excellent agreement.
Figure 3.10: $\epsilon_{e,\perp}$ calculated using the $\mathbf{k} \cdot \mathbf{p}$ approach and the MG approximation for a triangular lattice of Si cylinders ($\epsilon = 14$) in air ($\epsilon = 1$), for different values of $f$. “Close packing” denotes the maximum filling fraction of cylinders for this structure, which is $f_c = \pi \sqrt{3}/6 \approx 0.9069$.

for most $f$. For triangular arrays, the highest allowable filling fraction of cylinders is the close-packed triangular array, which has $f = \frac{\pi \sqrt{3}}{6} \approx 0.9069 \equiv f_c$. The $\mathbf{k} \cdot \mathbf{p}$ approach results agrees very well with the MGA up to about $f = 0.8$, but increasingly less well for larger $f$. For $f = 0.9$, the disagreement is about 30%. The $\mathbf{k} \cdot \mathbf{p}$ approach is, in principle, exact if a sufficient number of plane waves is included, whereas the MGA is only approximate. The fact that the $\mathbf{k} \cdot \mathbf{p}$ approach gives a larger value than the MGA near $f = f_c$ is a percolation effect, discussed further below.
Figure 3.11: Same as Fig. 3.10 but for a square lattice of cylinders. Here $f_c = \pi/4 = 0.7854$.

The corresponding results for a square array of Si cylinders in air are shown in Fig. 3.11. In this case, the maximum $f$ is $f_c = \frac{\pi}{4} \approx 0.7854$. Once again, the MGA and $\mathbf{k} \cdot \mathbf{p}$ methods are in excellent agreement for most $f$, but disagree substantially when $f_c - f \leq 0.1$. As in the triangular case, $\epsilon_{e,\perp}$ is larger in the $\mathbf{k} \cdot \mathbf{p}$ method than in the MGA in this critical regime.

We have also considered a square lattice of cylinders with $\epsilon_s = 100$ embedded in an air host. The $\mathbf{k} \cdot \mathbf{p}$ and MGA results for $\epsilon_{e,\perp}$ are shown in Fig. 3.12. In this case, there is a huge difference between the two values of $\epsilon_{e,\perp}$ when $f$ is close to $f_c$. This large value of $\epsilon_{e,\perp}$ is readily understood as a percolation effect. If $\epsilon_s \to \infty$, $\epsilon_{e,\perp}$
would diverge when $f \to f_c$, because $f_c$ w is a percolation threshold for the material with the large dielectric constant[13]. This divergence must be reflected in any exact treatment of $\epsilon_{e,\perp}$, such as the present approach. Our numerical results show that, indeed, the $\mathbf{k} \cdot \mathbf{p}$ method does lead to the expected divergent behavior in $\epsilon_{e,\perp}$.

### 3.3.4 Discussion

We have developed an explicit expression for the effective product $\sqrt{\epsilon_e \mu_e}$ for an arbitrary periodic dielectric medium. If we can take $\mu_e = 1$, this approach directly gives $\epsilon_e$. Our approach can be used to treat even materials with a continuously varying $\epsilon_e(\mathbf{x})$, so long as it is periodic. The same method also work for systems with a tensor $\epsilon_e$. For a periodic square or triangular lattice of dielectric cylinders
in a host, our calculated $\epsilon_e$ agrees well with the MGA for small filling fraction, but differs strongly from that behavior and becomes structure-dependent for $f$ near close packing. Although there are already numerous methods for calculating $\epsilon_e$ of a periodic composite, the present approach, because of its connection to standard techniques in electronic band theory, may be particularly convenient.

Finally, we briefly comment on the question of when we can regard $\mu_e = 1$. Even if none of the components are intrinsically magnetic, we may have $\mu_e \neq 1$ if $\epsilon(x)$ is frequency-dependent and Re $\epsilon(x) < 0$ for some spatial regions. This situation will prevail if part of the composite is metallic, in which case the finite $\mu_e$ is due to eddy currents in the metallic portion[55]. In this case, one needs an additional calculation to determine $\mu_e$. We speculate that an expression similar to ours can be obtained for $\mu_e$ in this case, by evaluating the Poynting vector for long-wavelength modes.

### 3.4 Tunable band gap at the Dirac point in photonic superlattices

#### 3.4.1 Introduction

In this section it is shown how, in principle we can switch a photonic band gap on and off, near the “Dirac Point”, by applying a magnetic field. We will present the Band Structure for electromagnetic waves of $\mathbf{H}$ polarization in a structure consisting of long, parallel, cylindrical dielectric rods with circular cross-section, having the $3 \times 3$ dielectric tensor $\epsilon_a$, embedded in a medium with dielectric tensor $\epsilon_b$. As in Ref.[94] we assume that the dielectric rods are parallel to the $x_3$-axis and that their intersection with the $x_1x_2$ plane form a two-dimensional Bravais lattice, with lattice sites given by vectors

$$\mathbf{x}(l) = l_1 a_1 + l_2 a_2$$

(3.43)
where \( a_1 \) and \( a_2 \) are two non-collinear primitive translation vectors for the Bravais lattice and \( l_1 \) and \( l_2 \) are any two integers, which we collectively denote as \( l \). Further we assume that the rods do not touch each other. The dielectric tensor of the structure is position dependent and we will denote it by \( \epsilon(x) \), where \( x \) is a vector in the \( x_1x_2 \) plane. Also the dielectric tensor is a periodic function and thus satisfies the relation \( \epsilon(x + x(l)) = \epsilon(x) \).

### 3.4.2 Formalism

We adopt the same formalism as Zabel and Stroud[140]. The band structure is obtained by solving Maxwell’s equations for the system, which can be written as

\[
\nabla \times H = \frac{1}{c} \frac{\partial}{\partial t} (\epsilon(x)E),
\]

which is true in the absence of any free current density, and

\[
\nabla \times E = -\frac{1}{c} \frac{\partial}{\partial t} B,
\]

where \( E \) and \( B \) are the electric and magnetic fields respectively. Combining the above two equations, assuming the magnetic permeability to be unity everywhere and taking an \( e^{-i\omega t} \) time dependence, we arrive at the following equation

\[
\nabla \times [\epsilon^{-1}(x)(\nabla \times H)] = \frac{\omega^2}{c^2} H,
\]

where \( \epsilon^{-1}(x) \) denotes the inverse of the position dependent dielectric tensor. We can write the same equation in the form of components using the Levi-Civita symbol as

\[
\epsilon_{ijk}\epsilon_{lmn} \frac{\partial}{\partial x_j} [(\epsilon^{-1}(x))_{kl} \frac{\partial}{\partial x_m} H_n(x)] = \frac{\omega^2}{c^2} H_i.
\]
Since the system is periodic $H$ must be a Bloch function, and thus can be expressed as linear combinations of plane waves:

$$H_k(x) = \sum_G H_{k+G} e^{i(k+G) \cdot x}. \quad (3.48)$$

Since $\epsilon^{-1}(x)$ is also a periodic function, we expand it as

$$\epsilon^{-1}(x) = \sum_{G'} \tilde{\epsilon}^{-1}(G') e^{iG' \cdot x}. \quad (3.49)$$

Here $G$ and $G'$ are reciprocal lattice vectors, $k$ is a Bloch vector, and $\tilde{\epsilon}^{-1}(G')$ is the Fourier coefficient of $\epsilon^{-1}(x)$.

Substituting Eqs. (3.48) and (3.49) into Eq. (3.47) and Fourier transforming, we find a linear system of equations:

$$\sum_G e_{ijk} e_{lmn}(k + Q)_j(k + G)_m[H]_n = \frac{\omega^2}{c^2} [H]_i. \quad (3.50)$$

Following Plihal and Maradudin [94], we evaluate the Fourier coefficient by writing $\epsilon^{-1}(x)$ as

$$\epsilon^{-1}(x) = \epsilon_b^{-1} + [\epsilon_a^{-1} - \epsilon_b^{-1}] \sum_l S(x - x(l)), \quad (3.51)$$

where $S(x)$ is unity when $x$ is inside the dielectric cylindrical rods and vanishes everywhere else. The reciprocal lattice vector is expressed as

$$G(h) = h_1 b_1 + h_2 b_2, \quad (3.52)$$

with $h_1$ and $h_2$ representing the primitive translation vectors for the reciprocal lattice. For a triangular lattice with primitive vectors $a_1 = a(1, 0)$, $a_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $b_1 = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}), b_2 = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}})$, where $a$ is the lattice constant, we get the same expression for the Fourier coefficients as that of Ref.[94]. Thus, $\tilde{\epsilon}^{-1}(G) = f\epsilon_a^{-1} + \epsilon_b^{-1}(1 - f)$ for
$G=0$, and is $[\epsilon_a^{-1} - \epsilon_b^{-1}]f^2 \frac{J_1(GR)}{GR}$ for $G \neq 0$. Here $J_1(x)$ is a Bessel Function of order 1, $f$ is the filling fraction ($f = \frac{2\pi R^2}{\sqrt{3}a^2}$) and, and $R$ is the radius of the cylindrical rods.

We write Eq. (3.50) in matrix form as $\sum_{j,G} \tilde{M}_{ij} H_{k+G} + G = \omega^2 c^2 (H_k + Q)_i$. For some particular reciprocal lattice vectors $Q$ and $G$, the matrix $\tilde{M}$ is a $3 \times 3$ matrix with its 9 elements given by

$$[\tilde{M}(Q, G)]_{ij} = c_{lpj} c_{mkn} (k + Q)_n (k + G)_p [\epsilon^{-1}(Q - G)]_{kl}. \quad (3.53)$$

Figure 3.13: Reciprocal lattice for the system, Zone corners form the point group $C_{3v}$.

Thus, if we use $N$ plane waves in the Eqs. (3.48) and (3.49), $\tilde{M}$ is a $3N \times 3N$ matrix. The dispersion relation $\omega(k)$ is found by diagonalizing this matrix. Before calculating the band structure we expect the second and the third band to touch near the Dirac point, which occurs at the zone corners. As is mentioned by Haldane and Raghu[42], this is a non-accidental symmetry related degeneracy. The symmetry corresponding to this degeneracy is the spatial inversion and time reversal symmetry. The Brillouin zone corners for this system form the point Group $C_{3v}$ (see Fig. 3.13). If we break the time reversal symmetry, which is the case when we apply a "uniform"
magnetic field to the system, the states with momentum \( \mathbf{k} \) and \(-\mathbf{k}\) are no longer equivalent. Thus, the inversion symmetry of the reciprocal lattice is broken, which in turn lifts the degeneracy at the Dirac point.

![Figure 3.14: Band Diagram comparable to Ref. [94].](image)

We consider materials where the only non vanishing components of the dielectric tensor \( \epsilon_a \) are the diagonal elements. Further, we assume that the diagonal elements of \( \epsilon_a \) are all real and \( \epsilon_b \) is a 3×3 identity matrix. When we apply a magnetic field in \( z \)-direction which corresponds to our \( x_3 \)-axis, the dielectric tensor \( \epsilon_a \) changes. To the first order in field, the diagonal elements remain unchanged but \( [\epsilon_a]_{xy} = -[\epsilon_a]_{yx} \), which was previously zero, is now purely imaginary. In principle these components of the dielectric tensor depend upon the applied static magnetic field and the frequency.
3.4.3 Results

Fig 3.14 shows the band diagram for H polarization (i.e., magnetic field being parallel to the $x_3$-axis), and filling fraction, $f = 0.431$, where the only non vanishing elements, i.e, the diagonal elements, of $\epsilon_a$ are 14.0, and $\epsilon_b$ is the $3 \times 3$ identity matrix. A total of 441 plane waves are used for computation and the bands corresponding to H polarization are selected from all the bands. As in Ref.[94] we observe the Dirac point at the zone corners. As is mentioned in Ref.[42], we can verify that on average, two out of every three bands have the Dirac point degeneracies. Triangle XΓJ in Fig. 3.13 represent the irreducible part of the first Brillouin Zone. The band structure in Fig. 3.14 is plotted along this triangle.

![Dispersion relation with variation in x-direction near the “Dirac Point”](image)

Figure 3.15: Dispersion relation with variation in $x$-direction near the “Dirac Point”.
Figure 3.16: Dispersion relation with variation in $y$-direction near the “Dirac Point”.

Now, we present our results after we apply an external magnetic field, as was discussed above. The dielectric tensor $\epsilon_a$ now has five non-vanishing elements, three of them being the diagonal elements which are purely real, and two of them being the $xy$ and the $yx$ elements with $[\epsilon_a]_{xy} = -[\epsilon_a]_{yx}$, and both of them being purely imaginary. As a result of this perturbation, a gap opens up at the Dirac point. The magnitude of this gap depends upon the magnitude of the imaginary elements of the dielectric tensor. In principle, even if these imaginary elements are small, at the Dirac point, the second and the third bands which were previously degenerate do separate out, but the magnitude of this gap can be very small. We plot the bands after switching on this perturbation in Fig. 3.15, for $[\epsilon_a]_{xy} = -i0.02$. In addition,
in this plot the Bloch vector $\mathbf{k}$ varies in the $x$-direction about the Dirac point. In Fig.3.16 we show the similar result with Bloch vector varying along the $y$-direction, $[\epsilon_a]_{xy}$ is still $-i0.02$. These plots show that breaking time-reversal symmetry opens up a gap at the Dirac point.

3.4.4 Inclusion of inversion symmetry-breaking

According to Ref. [42], the most interesting effects will occur if we have both time-reversal and space-inversion symmetry breaking. The magnetic field perturbation previously discussed only breaks time reversal symmetry. In this section we suggest an alternate way to break the spatial inversion symmetry as compared to one discussed by Haldane and Raghu[42].

Consider a triangular lattice, but let each dielectric cylinder contain an asymmetric hole, that is, a cylindrical hole which is not concentric with the dielectric cylinder. This arrangement will break inversion symmetry. Also, the Fourier components of this perturbation are easy to calculate, since the integral involved is the same as before.

Consider the location of the asymmetric hole, i.e, the center of the cylindrical hole to be on positive $x$-axis, at $px_1$, with a radius $r_0$. The Fourier coefficients are easily calculated as

$$\tilde{\epsilon}^{-1}(\mathbf{G}) = \frac{1}{A_c} \int_{\text{unitcell}} \epsilon^{-1}(\mathbf{r}) e^{-i\mathbf{G}.\mathbf{r}} d^2\mathbf{r}.$$  \hspace{1cm} (3.54)

The Integration over the unit cell is done by first considering a unit cell consisting only of air (i.e, $\epsilon_b^{-1}$), and then subtracting from it, an integration over a cylinder of radius, $R$, with a medium whose inverse of dielectric constant is given by $\epsilon_a^{-1} - \epsilon_b^{-1}$, then subtracting from it an integration over a cylinder with radius $r_0$, and center
Figure 3.17: Same as Fig. 3.15, but with inversion symmetry breaking perturbation.

at $p \hat{x}_1$. Here medium $a$ represents air, and $b$ represents silicon. We consider the cylindrical hole to be filled with air. In this case, the Fourier coefficients are

$$
\tilde{\epsilon}^{-1}(\mathbf{G}) = \frac{1}{A_c} \left[ \epsilon_b^{-1} \int_{\text{unit cell}} e^{-i \mathbf{G} \cdot \mathbf{r}} d^2 \mathbf{r} + (\epsilon_a^{-1} - \epsilon_b^{-1}) \int_{C_{\text{Circle}}} e^{-i \mathbf{G} \cdot \mathbf{r}} d^2 \mathbf{r} + (\epsilon_b^{-1} - \epsilon_a^{-1}) \int_{C_{\text{Circle}0}} e^{-i \mathbf{G} \cdot (\mathbf{p} + \mathbf{r})} d^2 \mathbf{r} \right].
$$

(3.55)

where we have used

$$
\int_{C_{\text{Circle}}} e^{-i \mathbf{G} \cdot \mathbf{r}} d^2 \mathbf{r} = \frac{2\pi R J_1(|\mathbf{G}|R)}{|\mathbf{G}|}.
$$

Here $J_1$ represents the Bessel function of order one. Let $f$ be the filling fraction of the silicon rods (by area). Using the fact that the first integral in Eq. (3.55) vanishes, the Fourier coefficients are $\tilde{\epsilon}^{-1}(\mathbf{G}' - \mathbf{G}) = f \epsilon_a^{-1} + (1 - f) \epsilon_b^{-1}$ for $\mathbf{G}' - \mathbf{G} = 0$ and when
the reciprocal lattice vectors are not same it is

\[
\tilde{\epsilon}^{-1}(G' - G) = (\epsilon_a^{-1} - \epsilon_b^{-1}) \frac{2\pi RJ_a(|G' - G| R)}{A_c |G' - G|} + e^{-i(G' - G) \cdot p} (\epsilon_b^{-1} - \epsilon_a^{-1}) \frac{2\pi r_0 J_1(|G' - G|r_0)}{A_c |G' - G|}.
\]

(3.56)

We treat the second term in above equation as a perturbation, which is justified in the limit of small \( r_0 \).

First we show how the dispersion relation near the Dirac point changes with this perturbation. The dispersion relation as the Bloch vector varies along \( x \)-axis, i.e., along \( \Gamma \) to \( J \) direction is shown in Fig. 3.17. As we can see a gap opens up at the Dirac point. Similarly, Fig. 3.18 shows the dispersion relation near Dirac point by the Bloch vector in a direction perpendicular to \( \Gamma \) to \( J \) direction.
Figure 3.19: Band gap vs hole radii. The radii of the holes are in units of $\sqrt{\frac{f\sqrt{3}}{2\pi}}a/16$. The center of the holes is at $R/16$ from the center of silicon cylinders, along the $x$-axis.

The gap that opens up at the Dirac point is in principle tunable and depends upon the perturbation. Fig. 3.19, is a plot of gap at “Dirac Point, $J$”, for different values of hole radii. The radii of the holes are in units of $\sqrt{\frac{f\sqrt{3}}{2\pi}}a/16$. The center of the holes is at $R/16$ from the center of silicon cylinders, along the $x$-axis. The gap is linear in the square of the radius of the holes.

Another way to tune this gap is by changing the location of the holes. Fig. 3.20 shows how the gap depends upon the position of the hole. The location of the holes, $p$ is in units of $\sqrt{\frac{f\sqrt{3}}{2\pi}}a/160$. If the holes are concentric with the cylinders, the system still has inversion symmetry so the gap is zero as shown in Fig. 3.20.
the gap, at the Dirac point, \( J \), in units of \( \omega a/(2\pi c) \).

Figure 3.20: Band gap vs holes location along \( x \)-axis. The location of the holes, i.e, \( p \) (see text) is in units of \( \sqrt{L/2\pi}a/160 \).

3.4.5 Discussion

In summary, we have shown that there exists a Dirac point in triangular photonic superlattices as a consequence of spatial inversion and time-reversal symmetry. The degeneracy can be lifted by breaking these symmetries and the gap that opens up can be tuned by controlling the external magnetic field or the position and the radius of the holes.
CHAPTER 4

APPLICATIONS OF EFFECTIVE MEDIUM THEORY

In this chapter we use the effective medium approximation (EMA) to explain some experimentally measured results.

The first section uses EMA to explain the experimentally measured large magnetoresistance in graphene\cite{25}. The main results of this section were published in \textit{Physical Review B}[120].

In the second section we use EMA to explain the experimentally measured anomalous sound velocity in a suspension of carbon nanotubes in dimethyformaldehyde. The results of this section were also published in \textit{Physical Review B}[142]

4.1 Model for the magnetoresistance and Hall coefficient of inhomogeneous graphene

4.1.1 Introduction

Graphene is a two-dimensional form of carbon with a hexagonal crystal structure like that of a single layer of graphite. Because of this structure, it has the band structure of a semimetal: the Fermi energy $E_F$ of neutral graphene lies at a “Dirac point,” where the electronic density of states $n(E_F) = 0$. There are two inequivalent Dirac points located at different Bloch vectors $\mathbf{k}_0$ and $\mathbf{k}_1$. Near the Dirac points,
the bands are linear functions of the components of \( \mathbf{k} - \mathbf{k}_0 \) and \( \mathbf{k} - \mathbf{k}_1 \), and \( n(E) \) is proportional to \( |E - E_F| \). Because of this unusual band structure, the quasiparticle Hamiltonian near the Dirac points is formally identical to that of massless Dirac fermions, a feature which is responsible for part of the recent interest in graphene.

Graphene also has striking transport properties. For example, experiments have observed finite conductivity for all values of \( E_F \), whether above or below the Dirac point\[85\], with a minimum conductivity typically \( \sim 4e^2/h \). However, some workers have suggested that this minimum could have much smaller \[78\] or larger \[23\] values than \( 4e^2/h \). It has been proposed that the existence of a finite conductivity even at the charge neutrality point might be a result of local potential fluctuations, which could cause a homogeneous neutral graphene sheet to break up into “puddles” of electron-rich (n-type) and hole-rich (p-type) character\[1\]. These puddles have, in fact, been unambiguously observed in experiments using scanning tunneling microscopy\[73\].

Recently measurements of the magnetic-field-dependent longitudinal and Hall resistivity \( \rho_{xx} \) and \( \rho_{xy} \) measurements have been reported\[25\]. \( \rho_{xx} \) was found to increase by nearly tenfold with increasing magnetic field perpendicular to the graphene film, followed by an apparent saturation at sufficiently strong magnetic field. These authors found that the magnetoresistance was inconsistent with a two-fluid model of transport by n-type and p-type charge carriers in a homogeneous sheet of graphene, and suggested that it might agree better with a model describing the film as a mixture of n-type and p-type puddles. However, they were able to obtain close agreement between experiment and theory only by assuming an ad hoc empirical form for the magnetoresistance.
In this section, we present a simple model for the magnetoresistance and Hall coefficient of graphene, based on the effective-medium approximation (EMA) in a transverse magnetic field. Such a model is reasonable if the n-type and p-type puddles are distributed randomly, as appears to be the case in Ref. [25]. Our results show that when the area fractions of n-type and p-type puddles are exactly equal, $\rho_{xx}$ varies exactly linearly with field. At other puddle fractions, it saturates, in agreement with experiment. We find that we can obtain excellent agreement with the observed behavior of $\rho_{xx}(B)$ if we assume an n-type area fraction $f_n$ satisfying $|f_n - 1/2| \sim 0.07$ and reasonable values for average carrier density and transport relaxation time. We also make predictions about the Hall resistivity $\rho_{xy}(B)$.

4.1.2 Model

We consider magnetotransport in a single layer of graphene subject to a magnetic field $B = B\hat{z}$ perpendicular to the graphene layer. We assume that, because of a random potential due to charges in the substrate or some other cause, the graphene layer has broken up into a mixture of n-type and p-type puddles, having area fractions $f_n$ and $f_p = 1 - f_n$. We also assume that each of the puddles is large enough to be described by its own magnetoconductivity tensor $\sigma_n$ or $\sigma_p$. In practice, this assumption means that the paddle dimensions are larger than a typical carrier mean free path. If this condition is not satisfied, the results below would need to be modified.

4.1.3 Conductivity tensors of individual puddles

We assume that $\sigma_n$ and $\sigma_p$ are both given by the usual free-electron (or free-hole) forms, suitably modified to account for the linear dispersion relations of the electrons and holes near the Dirac point. We denote the charge carrier densities in the n-type
and p-type puddles by \( n \) and \( p \), and the corresponding relaxation times by \( \tau_n \) and \( \tau_p \).

We also initially assume that all the puddles have the same density of charge carriers, so that \( n = p \), and that the relaxation times \( \tau_n = \tau_p \equiv \tau \). With these assumptions, the zero-field conductivities \( \sigma_{n,0} \) and \( \sigma_{p,0} \) of the n-type and p-type puddles are equal (\( \sigma_{n,0} = \sigma_{p,0} \equiv \sigma_0 \)). We can also define zero-field mobilities \( \mu_n \) and \( \mu_p \) by \( \sigma_n = ne\mu_n \) and \( \sigma_p = pe\mu_p \), where \( e \) is the magnitude of the electronic charge; with the above assumptions, these mobilities are also equal (\( \mu_n = \mu_p \equiv \mu \)). Later in this section, we will consider the more general cases where \( n \neq p \) or \( \tau_n \neq \tau_p \).

With these assumptions, the \( 2 \times 2 \) conductivity tensor in the \( xy \) plane takes the form

\[
\sigma_n = \sigma_{n,0} \left[ \begin{array}{cc}
\frac{1}{1+(\omega_{c,n}/\tau_n)^2} & \frac{\omega_{c,n}/\tau_n}{1+(\omega_{c,n}/\tau_n)^2} \\
\frac{\omega_{c,n}/\tau_n}{1+(\omega_{c,n}/\tau_n)^2} & \frac{1}{1+(\omega_{c,n}/\tau_n)^2}
\end{array} \right] \quad (4.1)
\]

and

\[
\sigma_p = \sigma_{p,0} \left[ \begin{array}{cc}
\frac{1}{1+(\omega_{c,p}/\tau_p)^2} & \frac{-\omega_{c,p}/\tau_p}{1+(\omega_{c,p}/\tau_p)^2} \\
\frac{-\omega_{c,p}/\tau_p}{1+(\omega_{c,p}/\tau_p)^2} & \frac{1}{1+(\omega_{c,p}/\tau_p)^2}
\end{array} \right] . \quad (4.2)
\]

Both the zero-field conductivities \( \sigma_{n,0} \) and \( \sigma_{p,0} \) of the puddles and the cyclotron frequencies \( \omega_{c,n} \) and \( \omega_{c,p} \) are modified from their usual free-electron values because of the linear dispersion relations near the Dirac point. The result for \( \sigma_{n,0} \) and \( \sigma_{p,0} \) at temperature \( T = 0 \) (fully degenerate limit) is

\[
\sigma_{n,0} = \frac{2e^2}{h} v_F \tau_n \sqrt{\pi n} \quad (4.3)
\]

and

\[
\sigma_{p,0} = \frac{2e^2}{h} v_F \tau_p \sqrt{\pi p}, \quad (4.4)
\]

where \( v_F \) is the Fermi velocity (which is the same for both electrons and holes). This form is obtained from the usual solution of the Boltzmann equation for a degenerate
Fermi gas\[7\], which gives for electronic conductivity at zero magnetic field

\[
\sigma_{n,0} = \frac{2e^2\tau_n}{(2\pi^2)} \int d^2k'\hbar^{-2} \left( \frac{\partial E(k')}{\partial k'_x} \right)^2 \delta(E(k') - E_F). \tag{4.5}
\]

Here, \( k' \) is the two-dimensional wave vector, measured relative to one of the Dirac points, and \( E(k') = \hbar v_F|k'| \) is the energy relative to the Dirac point. The hole conductivity is given by a similar expression. We use \( k_{F,n} = \sqrt{\pi n} \), which takes into account the two valleys near the two inequivalent Dirac points in the graphene band structure, and we have included an extra factor of 2 in eq. (4.5) for the same reason. \( k_{F,p} \) is given by an analogous expression.

The cyclotron frequency \( \omega_{c,n} \) is readily obtained from the semiclassical equation of motion \( \hbar \dot{k} = e\mathbf{v}_k \times \mathbf{B} \), where \( \mathbf{v}_k = \hbar^{-1}\nabla_k E(k') \), as applied to a band with the dispersion relation \( E(k') = v_F\hbar|k'| \); the result is (in SI units),

\[
\omega_{c,n} = \frac{v_F eB}{\hbar\sqrt{\pi n}}. \tag{4.6}
\]

\( \omega_{c,p} \) is given by an analogous expression\[18\].

Transport in graphene is also affected by the dependence of \( \tau_n \) or \( \tau_p \) on physical parameters such as \( n \), \( p \), and \( B \). It has been suggested\[1\] that, \( \tau \) is proportional to \( 1/\sqrt{n} \) (or \( 1/\sqrt{p} \)) for scattering by impurities with short-range potentials, but is proportional to \( \sqrt{n} \) (or \( \sqrt{p} \)) for impurities with Coulomb potentials. If we assume the latter, then from eqs. (4.3) and (4.4) \( \sigma_{0,n} \propto n \) and \( \sigma_{0,p} \propto p \) and both \( \omega_{c,n} \tau_n \), and \( \omega_{c,p} \tau_p \) are independent of carrier density, as in conventional semiconductors. In our calculations below, we give results using both assumptions about the carrier density dependence of \( \tau_n \) and \( \tau_p \).
4.1.4 Effective conductivity of composite of n-type and p-type puddles

Next, we calculate the effective conductivity tensor $\sigma_e$ of a graphene sheet which has broken up into n-type and p-type puddles. If $f_n = 1/2$, and $n = p$, this would correspond to the case where the net charge carrier density is zero, corresponding to a neutral graphene sheet which would, if homogeneous, have its Fermi energy at the Dirac point. However, it is also possible to have a graphene sheet with $f_n \neq 1/2$, or $n \neq p$, or both, corresponding to a graphene sheet with a net doping. This situation could be produced in a graphene sheet biased by a suitable gate voltage.

A reasonable way of calculating $\sigma_e$ for tensor conductivities is provided by the effective-medium approximation (EMA)[114]. In this approach, the electric fields and currents within the inhomogeneous graphene sheet are calculated as if the n-type and p-type puddles are compact and approximately circular, and are embedded in an effective medium whose conductivity is calculated self consistently[114, 40]. For tensor conductivities, the defining equation for the EMA is

$$\sum_{i=\{n,p\}} f_i \delta \sigma_i (I - \Gamma \delta \sigma_i)^{-1} = 0.$$  \hspace{1cm} (4.7)

Here $\delta \sigma_i = \sigma_i - \sigma_e$, $I$ is the 2×2 unit matrix, and, for the planar geometry considered, $\Gamma = -I/(2\sigma_{e,xx})$ is the depolarization tensor. This matrix equation reduces to two coupled scalar algebraic equations for the two independent components of $\sigma_e$ ($\sigma_{e,xx}$ and $\sigma_{e,xy}$), which are easily solved numerically. The other two components are determined by $\sigma_{e,yy} = \sigma_{e,xx}$ and $\sigma_{e,yx} = -\sigma_{e,xy}$. The resistivity tensor is then obtained by inverting the matrix $\sigma_e$, so that $\rho_{e,xx} = \rho_{e,yy} = \sigma_{e,xx}/(\sigma_{e,xx}^2 + \sigma_{e,xy}^2)$ and $\rho_{e,xy} = -\rho_{e,yx} = -\sigma_{e,xy}/(\sigma_{e,xx}^2 + \sigma_{e,xy}^2)$.

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We briefly discuss the conditions under which the EMA is likely to be accurate. As is well known[13], the EMA is derived by assuming that, when an electric field $\mathbf{E}_0$ is applied to the composite of n and p puddles, the field $\mathbf{E}_{in}$ inside any given puddle is equal to that which would be found if the medium outside the puddle is uniform and has an effective conductivity tensor $\sigma_e$. The field inside the $i^{th}$ puddle is then found to equal

$$\mathbf{E}_{in,i} = \left( I - \Gamma \delta \sigma_i \right)^{-1} \mathbf{E}_0,$$

(4.8)

where $\Gamma$ is the depolarization tensor (given above for circular puddles). $\sigma_e$ is then determined by the self-consistency condition that the space average of the electric field $\mathbf{E}_{in,i}$ shall equal $\mathbf{E}_0$, which leads to eq. (4.7). Thus, one might expect that the EMA would be most accurate if the surroundings of a given puddle do not deviate too greatly from the average. However, it is difficult to give a more precise statement of the conditions under which the EMA can be expected to be a good approximation.

The EMA is known to be exact in two limiting cases. First, when the area fraction of n or p type puddles is small, the EMA becomes exact to first order in $f_n$ or $f_p$ for circular inclusions of n or p type conductor in a host with carriers of the opposite sign[115] (or, indeed, for a host with any conductivity tensor). Secondly, the EMA is also exact at $f_n = 1/2$, provided $\omega_{c,p} \tau_p = \omega_{c,n} \tau_n[40]$. Because the EMA becomes exact in these two regimes, it seems reasonable to suppose that it will be a good interpolation scheme at other values of $f_n$.

Next, we discuss the assumption that the puddles are circular. Clearly, this is at best a rough approximation. Still, one can imagine a “cellular” composite, made up of compact, roughly circular regions of n and p type puddles. In this case, it seems
reasonable to approximate the electric field inside a compact puddle using eq. (4.8). If so, the EMA form (4.7) is appropriate.

Does the observed puddle morphology of inhomogeneous graphene resemble a cellular composite of compact n and p type puddles? The published data, obtained using a scanning single electron transistor [73], seem to suggest extended, possibly percolating structures of n and p type regions, rather than circular regions. But this picture can be qualitatively reconciled with the random compact puddle picture, provided that the area fraction of n and p regions is nearly equal. In this case, according to standard models of percolation[98], even if the n and p type puddles are distributed randomly, they will connect up near percolation to form extended structures similar the experimental pictures. Thus, it may be reasonable to model the observed structures as a distribution of compact n and p type puddles, as done here.

4.1.5 Numerical results

We begin by evaluating the predictions of the above model for the simplest case: \( n = p, \tau_n = \tau_p \equiv \tau \), and \( \tau \) independent of \( n \). In order to compare this model to experiment[25], we need the values of \( v_F, n, \tau \) (or equivalently, \( \mu \)), and \( f_n \). From the band structure of graphene, \( v_F \sim 10^6 \text{ m/sec}[85, 10] \). In fact, a value of \( 1.1 \times 10^6 \text{ m/sec} \) has been inferred from measurements of the Landau level splitting in graphene[49], and we use this value in the calculations below. Also, the measured value of the zero-field resistivity is \( \sigma_0^{-1} = \rho_0 = 0.125h/e^2 \). Given this value, eq. 4.3 provides one condition satisfied by the two parameters \( n \) and \( \tau \). We then choose \( n, \tau \), and \( f_n \) so as to best fit the measured \( \rho_{xx}(B) \) at \( B = 8T \), and to yield \( \omega_c \tau = 3.1B \), where \( B \) is
Figure 4.1: $\rho_{xx}(B, f_n)$ as a function of $B$ (in $T$), with two different assumptions about the mobility. In both cases, we assume that the electron and hole mobilities are equal. Solid (red) line: calculated results, assuming $\mu \equiv \omega_c \tau / B = 3.1 T^{-1}$ and $f_n = 0.4287$ (or 0.571). Dashed (black) line: calculated results with $\mu = 2.3 T^{-1}$ and $f_n = 0.431$ (or 0.569). Open circles are experimental data from Ref. [25]. Lower panel is a blowup of the calculations and data from the upper panel.

The calculated results for $\rho_{xx}(B)$ are shown in Fig. 4.1, using these parameters. As can be seen, the fit to the experimental data is excellent over most of the field range, using $\omega_c \tau \sim 2.3B$, and at low fields using $\omega_c \tau \sim 3.1B$. The fit, especially at high fields, is also superior to the two-fluid model discussed (and found inadequate).

The magnetic field in T, as reported in Ref. [25]. This procedure gives $n \sim 6 \times 10^{14}$ m$^{-2}$ and $f_n \sim 0.43$. We find that the best agreement with the resistivity is given at high fields by $\omega_c \tau \sim 2.3$ B, and at low fields by $\omega_c \tau \sim 3.1$ B, indicating a weakly field-dependent $\tau$. The value of $n$ is close to measured value quoted in Ref. [25].
in Ref. [25]. The fit to this puddle model would be nearly perfect over the entire range of B studied experimentally, if \( \tau \) varied by about 30\% as a function of \( B \). The results for \( \rho_{xx} \) are independent of the sign of the charge and are thus unchanged if \( f_n \to 1 - f_n \).

In Fig. 4.2, we show the corresponding results for \( \rho_{xy}(B) \). In this case, we use a field-independent \( \tau \) (corresponding to \( \omega_c \tau = 2.3 \text{ B} \)). We show results for \( f_n = 0.43, 0.57, \) and 0.5. \( \rho_{xy}(B) \) for \( f_n = 0.43 \) is equal and opposite to that for \( f_n = 0.57 \). In both cases, \( \rho_{xy} \) varies roughly linearly with \( B \) for \( B \) greater than about 1T. At \( f_n = 0.5, \rho_{xy} = 0 \) for all \( B \). Within the present model, this latter result is exact, and not restricted to the EMA[40].

Fig. 4.3 shows \( \rho_{xx}(B, f_n) \) versus \( f_n \) for several values of \( B \). We use the EMA and the same parameters as in Figs. 4.1 and 4.2 (with \( \omega_c \tau = 2.3 \text{ B} \)). \( \rho_{xx} \) saturates for all
values of $f_n$ except $f_n = 1/2$, for which it increases linearly with $B$. Once again, this linearity is exact, and not restricted to the EMA[40]. In Fig. 4.4, we show $\rho_{xy}(B, f_n)$ versus $f_n$ for several values of $B$. As can be seen, $\rho_{xy}$ changes sign at $f_n = 1/2$, and approaches a constant as $f_n$ approaches either 1 or 0. The magnitude of the slope $[d\rho_{xy}/df_n]_{f_n=1/2}$ increases with increasing $B$, so that, at large $B$, the Hall resistivity is very close to that of the majority charge carrier.

Thus far, our numerical results have been limited to the special case where $n = p$ and $\tau_n = \tau_p$. To illustrate what happens when these assumptions are relaxed, we have carried out numerous additional calculations, using the effective medium approximation. A representative example is shown in Fig. 4.5. In this case, we assume $n \neq p$ and also $\tau_n \neq \tau_p$. We also take $\sigma_{n,0} \propto n$ and $\sigma_{p,0} \propto p$. This implies that $\tau_n \propto n^{1/2}$ and $\tau_p \propto p^{1/2}$, which is the expected behavior for relaxation times dominated by Coulomb scattering. In addition, we choose $n/p$ and $\mu_n/\mu_p$ so as to optimize the
Figure 4.4: Calculated $\rho_{xy}$ as a function of $f_n$ for several different values of $B$, using $\mu = 2.3T^{-1}$.

agreement between our calculations and experiment. The resulting parameters are $n/p = 1.376$ and $\mu_n/\mu_p = 0.7$, with $\mu_p = 2.3T^{-1}$ as in our other calculations above. The plots shown in Fig. 4.5 are drawn at the charge neutrality point, which now lies at $f_n = 0.4209$ for this choice of $n/p$. Thus, in contrast to the examples shown in Figs. 4.1-4.4, this model gives a saturating (but large) magnetoresistance at the charge neutrality point, in agreement with experiment. The calculated Hall resistivity, however, does not vanish at this value of $f_n$, as shown in Fig. 4.5(b). In fact, for all models we have considered, the Hall resistivity changes sign at $f_n = 1/2$, whatever the value of $n/p$ or $\mu_n/\mu_p$. 

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Figure 4.5: Calculated and measured $\rho_{xx}(B)$ and calculated $\rho_{xy}(B)$ with $B$ in Tesla. The calculations are carried out using different assumptions than Figs. 1 and 2. Specifically, we assume that $n/p = 1.376$, $\mu_n/\mu_p = 0.7$, and $\mu_p = 2.3T^{-1}$. We also assume that $\sigma_{n,0} \propto n$ and $\sigma_{p,0} \propto p$. The calculations are carried out at the charge neutrality point, $f_n = 0.4209$. In both panels, the full curves are the calculated values, while the circles in the top panel represent experimental data from Ref. [25].

4.1.6 Discussion

We turn now to a discussion of our results. First, what is responsible for the large magnetoresistance emerging from our calculations? This large magnetoresistance seems surprising, because because the individual $n$ and $p$ puddles have zero magnetoresistance, yet that of the composite is large. Clearly, the magnetoresistance must originate in current distortion effects. Because the conductivity tensor is inhomogeneous at finite fields, the current does not travel in a straight line through
the medium in the presence of a magnetic field, but is strongly distorted by discontinuities at the boundaries between the n and p type conductors. Since the current travels a longer path than it would in a homogeneous medium, the resistance should be larger. In a three-dimensional metal with a small concentration of macroscopic defects, this current distortion effect is known to produce a magnetoresistance linear in field\[115, 100\]. However, in 2D, we have not found a simple physical argument which would show that the magnetoresistance varies linearly with $B$ at $f_n = f_p$, and saturates at other concentrations. We can say only that the linearity is precisely true in some models, as was discussed previously in Ref. [40], and also that it emerges from our effective-medium calculations.

An intriguing question about our result is the role of the geometrical percolation threshold. In two dimensions, if one has a composite of two components (say n and p), and they are distributed in some symmetrical way, then the percolation threshold for either component occurs at an area fraction of 1/2. That is, if the area fraction $f_n > 1/2$, there is an infinite connected cluster of n, and if $f_n < 1/2$, the connected cluster of n is only finite. An analogous statement can be made about the p component. If $\sigma_{n,0} = \sigma_{p,0}$, this geometrical percolation will have no effect on transport in our model at $B = 0$, because the medium is effectively homogeneous. However, at large $B$, the two components have very different conductivities, so the percolation threshold should have a much stronger effect.

Based on the above argument, and our numerical results, we suggest that at large fields, the resistivity $\rho_{e,xx}(B)$ in our model has a singular “scaling” behavior of the form

$$
\rho_{e,xx}(B, f_n) = B^c F(|f_n - 1/2|^{-a}/B),
$$

(4.9)
where $c$ and $a$ are suitable critical exponents which can be inferred from our numerical results. First, $\rho_{e,xx} \propto B$ at $f_n = 1/2$. This implies that $B^c F(\infty) \propto B$ or $c = 1$. For $f_n \neq 1/2$, our effective-medium results show that $\rho_{e,xx}(B \to \infty, f_n) \propto |f_n - 1/2|^{-1}$ (this behavior can be seen in Fig. 4.3). This behavior, combined with $c = 1$, implies that $a = 1$. Thus, our effective-medium results are consistent with eq. (4.9) with $c = 1$ and $a = 1$.

The physical basis for this scaling behavior is presumably that there are two divergent lengths in our problem at small $|f_n - 1/2|$ and large $B$. The first is the linear dimension of the percolation cluster, $\xi_p$, which diverges near the percolation threshold. The second is a length related to the magnetic field. This length will vary as some power of $\omega_c \tau$. The ratio of these two lengths should determine the behavior of $\rho_{e,xx}(B, f_n)$ near a hypothetical high-field critical point at $f_n = 1/2$ and $B = \infty$. However, we emphasize that this scaling behavior is rather speculative, since we can verify it only within the effective-medium approximation.

### 4.1.7 Connection to experiments in graphene

The present model agrees well with the measured values of $\rho_{xx}(B)$ in graphene. However, it is based on certain assumptions whose validity for graphene we now discuss. One assumption is that graphene can be treated as a macroscopically inhomogeneous assembly of puddles, each with its own conductivity tensor. The scanning probe images shown in Ref. [73] suggest that the carrier density varies appreciably over a distance of perhaps $0.2\mu$. Using the above density estimates, the number of charge carriers in a puddle of linear dimension $0.2\mu$ would be $\sim 25$. This size is rather small to be treated macroscopically. On the other hand, a more reasonable definition
of a “puddle” might be a region where the charge carriers were all of one sign. Judg-
ing from the images, a typical linear dimension of such a region would be larger than 0.2µ - perhaps 0.5 - 1µ, and would contain \( \sim 500 \) carriers. This is probably large enough to describe each puddle by its own macroscopic conductivity, provided that the mean free path \( \Lambda \) is less than 1µ. In fact, experimentally measured \( \Lambda \) for both sus-
pended and non-suspended graphene sheets with typical carrier densities considered here \( (6 \times 10^{14} \text{ m}^{-2}) \) are less than 0.1µ for reasonable values of temperature[30]. Thus, treating the puddle mixture macroscopically is probably appropriate in the case of some disordered samples of graphene, and the results seem to agree with experiment.

Another point, as can be seen from Fig. 4.3, is that the \( \rho_{xx}(B, f_n) \) saturates only if \( f_n \neq 1/2 \). If \( n = p \), then \( f_n \neq 1/2 \) would imply a net charge imbalance produced by a suitable gate voltage. However, if \( n \neq p \), we can still have a saturating magnetoresistance and no net charge imbalance, as can be seen in Fig. 4.5. Such saturation seems to be observed in experiments[25]. As can be seen from Figs. 4.2, 4.4, and 4.5, even if there is no charge imbalance, a value of \( f_n \neq 1/2 \) would still lead to a nonzero \( \rho_{xy}(B) \). It would be of interest if \( \rho_{xy}(B) \) could be measured and compared to the values needed for the present model to agree with experiment.

Thirdly, the present model treats the electron dynamics semiclassically, and thus does not take into account the quantum Hall effect (QHE), which is seen at sufficiently high fields[86, 49, 85]. Typically, the QHE will become visible when the spacing between the Landau levels is large compared to \( k_B T \). This can occur even at room temperature in graphene[86]. If the QHE becomes important, the present semiclassical model would need to be modified.
A fourth point is that we have carried out our calculations within the EMA, which may introduce some error. In this regard, it would be of some interest if one could calculate the magnetotransport of a model of n and p puddles using a more exact procedure, such as a suitably defined network of random impedance matrices. Such a calculation has previously been carried out for a somewhat different model of n and p carriers[89], and could, in principle, be extended to the present problem.

Finally, we obtain the best fits to experiment if we assume a weakly magnetic-field dependent relaxation time, as described above. Such field-dependence could be reasonable, but it would be useful to have a model which explicitly produces a magnetic field-dependent $\tau$.

We find that our results are quite insensitive to slight changes in the parameters or other features of the model. For example Fig. 4.1 suggests that $\rho_{xx}$ changes only slightly, but not dramatically, when $\tau$ is varied by $\sim 30\%$. Also, we have recalculated $\rho_{e,xx}(B,T)$ without the assumption that the electrons and holes have equal mobilities. Even if the mobilities are different, we find that $\rho_{xx}(B)$ still varies linearly with $B$ at $f_n = 0.5$ and saturates at other values of $f$. Another change in our model is suggested by that fact that the carrier density in graphene must be a continuous function of position, rather than being simply bimodal as postulated in our model. To check the effects of a non-bimodal distribution, we have repeated our calculations assuming four types of puddles, two n-type and two p-type, with two different densities each of electrons and holes. Once again, we find that the resulting $\rho_{xx}(B, f_n)$ depends primarily on $f_n$ and $\tau$, and not on the presence of two types of n and of p puddles. Finally, we have considered the case of a three-component composite, made up of n-type, p-type, and insulating regions. Here, once again, we find that, for a small
insulating areal faction (\(\sim 0.1\)), we obtain linear magnetoresistance if \(f_n = f_p\) and saturating magnetoresistance otherwise, similar to the case of no insulating regions. Thus, our results are not much affected by small modifications in our model.

To summarize, we have calculated the magnetoresistance and Hall resistivity for a semiclassical model of graphene, on the assumption that it is a mixture of n-type and p-type puddles, and using the correct form of the band structure near the Dirac points. The resulting magnetoresistance is in good agreement with experiment, provided that the areal fractions of n and p-type puddles are slightly different and that the relaxation time is weakly magnetic-field dependent. Further confirmation of the model could be obtained if the measured Hall resistivity were compared to that computed from this model.

4.2 Effective sound speed in a suspension of carbon nanotubes in dimethyl formaldehyde

4.2.1 Introduction

In this section we examine the acoustical properties of a suspension of parallel cylinders in a liquid host. We can think of the parallel cylinders as carbon nanotubes, or, more plausibly, as bundles of carbon nanotubes. In what follows, we develop a simple effective-medium theory for the dispersion relation of sound waves in such a suspension, based on certain plausible assumptions about the materials in the suspension.

4.2.2 Formalism

Let us assume that the suspension consists of a collection of two types of cylinders, \(A\) and \(B\), each of radius \(a\). Cylinder \(A\) is assumed to be solid and \(B\) is liquid. The
volume fraction of A is denoted $f$. We are interested in sound waves propagating perpendicular to the cylinder axis, so that we are considering an effectively two-dimensional problem.

We assume that the solid cylinders have the same mass density as the liquid, but are very stiff. Eventually, we will assume that the speed of sound in the cylinders is infinite. The liquid is assumed to have a speed of sound $c_\ell$. Within the liquid, the local pressure $p(\mathbf{r})$ satisfies the 2D Helmholtz equation:

$$\nabla^2 p(\mathbf{r}) + \frac{\omega^2}{c_\ell^2} p(\mathbf{r}) = 0.$$  \hfill (4.10)

Here $\mathbf{r}$ is a two-dimensional position vector in the xy plane, and $\nabla$ is the 2D gradient operator. The boundary conditions at any surface between two different media are described, e. g., by Chen and Ye[22]:

$$p_1 = p_2$$

$$\frac{1}{\rho_1} \frac{\partial p_1}{\partial n} = \frac{1}{\rho_2} \frac{\partial p_2}{\partial n}.$$  \hfill (4.11)

Here the subscripts 1 and 2 denote the two media in contact, and the derivative with respect to $n$ means a normal derivative; $\rho_1$ and $\rho_2$ are the densities in the two media. For the special case of an infinitely stiff medium 2, the only necessary boundary condition is

$$\frac{\partial p_1}{\partial n} = 0$$  \hfill (4.12)

at the boundary between the liquid (medium 1) and the solid.

The idea of the self-consistent approximation is as follows. We replace our entire suspension by an effective medium, in which the speed of sound is $c_e$. This effective speed of sound depends on frequency, even if the original sound speed does not. $c_e$
is determined by a self-consistent embedding procedure. Namely, we embed each
type of cylinder in an effective medium of sound speed $c_e$, which is determined self-
consistently. For convenience, we assume that all three media have the same mass
density $\rho$.

The pressures in the effective medium and the interior medium $i$ ($i = A, B$) take the following forms:

\[ p = \sum_{n=-\infty}^{\infty} \left[ p_1 i^n J_n(k_e r) + D_n H_n^{(1)}(k_e r) \right] e^{in\phi}, \quad (4.13) \]

in the effective medium, and

\[ p = \sum_{n=-\infty}^{\infty} B_n^i J_n(k_i r) e^{in\phi}, \quad (4.14) \]

in the interior medium. Here $k_i = \omega/c_i$, $i = A, B$. The solutions in the interior satisfy eq. (4.10), with the additional condition that the pressure should be finite at the origin. The pressure in the exterior (effective) medium is the sum of two terms: the incident wave and the scattered wave. The incident wave is

\[ p_{inc}(r, t) = p_0 + p_1 \exp(ik_e x), \quad (4.15) \]

and can be expressed as a sum of partial waves, using suitable Bessel function identities, and gives rise to all the Bessel function terms in eq. (4.13).

The two boundary conditions give the following conditions on the unknown coeff-
ients $B_n^i$ and $D_n$:

\[ k_i B_n^i J_n'(k_i a) = k_e \left[ i^n p_1 J_n'(k_e a) + D_n H_n^{(1)}(k_e a) \right], \]

\[ B_n^i J_n(k_i a) = i^n p_1 J_n(k_e a) + D_n H_n^{(1)}(k_e a). \quad (4.16) \]
Multiplying the first equation by \( J_n(k_i a) \) and the second equation by \( k_i J'_n(k_i a) \) gives

\[
k_i B^i_n J_n(k_i a) J'_n(k_i a) = k_e J_n(k_i a) \left[ i^n p_1 J'_n(k_e a) + D_n H_n^{(1)}(k_e a) \right], \tag{4.17}
\]

\[
k_i B^i_n J'_n(k_i a) J_n(k_i a) = k_i J'_n(k_i a) \left[ i^n p_1 J_n(k_e a) + D_n H_n^{(1)}(k_e a) \right] \tag{4.18}
\]

Subtracting eq. (4.18) from eq. (4.17) gives

\[
i^n p_1 [k_e J_n(k_i a) J'_n(k_e a) - k_i J'_n(k_i a) J_n(k_e a)] + D_n [k_e J_n(k_i a) H_n^{(1),'}(k_e a) - k_i J'_n(k_i a) H_n^{(1)}(k_e a)] = 0. \tag{4.19}
\]

This equation is solved for \( D_n \), with the result

\[
D_n = -\frac{i^n p_1 [k_e J_n(k_i a) J'_n(k_e a) - k_i J'_n(k_i a) J_n(k_e a)]}{k_e J_n(k_i a) H_n^{(1),'}(k_e a) - k_i J'_n(k_i a) H_n^{(1)}(k_e a)}. \tag{4.20}
\]

To obtain a self-consistency condition, we imagine that we have a pressure wave propagating through the effective medium with frequency \( \omega \) and wave vector \( k_e = \omega/c_e \). When the wave hits the (A or B) cylinder, it is scattered. We choose the effective medium to minimize the scattering. Specifically, we choose the medium so that the forward scattering amplitude from the cylinder vanishes, on average. If we make this choice, then the effective medium is such that, on average, there is no further scattering by the inclusions.

To obtain the forward scattering amplitude, we consider the scattered wave far away from the cylinder. In this region, we use the large-argument approximation for \( H_n^{(1)}(x) \), namely,

\[
H_n^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}} \exp \left[ i \left( x - \frac{n\pi}{2} - \frac{\pi}{4} \right) \right]. \tag{4.21}
\]

Thus, the scattered wave at large distances is

\[
p_{\text{scatt}}(r, \phi) \sim \sum_{n=-\infty}^{\infty} D_n \sqrt{\frac{2}{\pi k_{\ell} r}} \exp(ik_{\ell} r - i\pi/4) \exp(-in\pi/2) \exp(in\phi). \tag{4.22}
\]
The condition that the forward scattering vanishes is obtained by setting $\phi = 0$ in the above equation, and requiring that the right-hand side vanishes. This gives

$$\sum_{n=-\infty}^{\infty} D_n e^{-in\pi/2} = 0. \quad (4.23)$$

Finally, the self-consistency condition determining $k_e$ is just the average of eq. 4.23. This is written, using the identity $\exp(-in\pi/2) = (-i)^n$, as

$$\sum_{n=-\infty}^{\infty} \langle D_n (-i)^n \rangle = 0 \quad (4.24)$$

where

$$\langle D_n \rangle = fD_{n,A} + (1-f)D_{n,B}. \quad (4.25)$$

Eq. (4.24) is a self-consistent equation which determines the one unknown quantity, $k_e$, as a function of frequency $\omega$ and the speeds of sounds in the two media, which enter through the wave vectors $k_A = \omega/c_A$ and $k_B = \omega/c_B$. Given $k_e$, we obtain $c_e$, the speed of sound in the effective medium, as a function of frequency.

For the particular case of interest here, one of the two media (the carbon nanotube (CNT) bundle) is much stiffer than the liquid. To simplify the self-consistent equation, we take the speed of sound in the CNT bundle to be infinite. This limit is obtained by letting $k_A \to 0$ in eq. (4.20), with the result

$$\sum_{n=-\infty}^{\infty} \left[ f \frac{J_n'(k_e a)}{H_n^{(1)/'}(k_e a)} + (1-f) \frac{[k_e J_n(k_l a) J_n'(k_e a) - k_l J_n'(k_l a) J_n(k_e a)]}{k_e J_n(k_l a) H_n^{(1)/'}(k_e a) - k_l J_n'(k_l a) H_n^{(1)}(k_e a)} \right] = 0. \quad (4.26)$$

We solve eq. (4.26) to obtain the effective composite wave vector $k_e$, and hence the speed of sound $c_e$ in the composite, as a function of $f$ for several choices of $a$ and $\omega$. In general we find, for all parameters we have considered, that $c_e$ is smaller in the composite than in the pure liquid. This result may appear counterintuitive, since
the suspended CNT bundles have a much higher speed of sound than the liquid. The result is, however, consistent with previous theories[101], which have demonstrated the same effect in an ordered two-dimensional array of infinitely stiff cylinders in a fluid host. In the previous work, since the array is periodic, Ref. [101] obtains a complete phononic band structure. In the present case, since we are dealing with a random composite, there is no band structure.

Along similar lines we consider a 3-dimensional effective medium approximation, where we assume solid and liquid spheres embedded in an effective medium. Using similar boundary conditions, we arrive at the following equation which can be solved similarly

$$\sum_{n=0}^{\infty} (2n+1) \left[ f \frac{j_n'(k_e a)}{h_n^{(1)}(k_e a)} + (1-f) \frac{k_e j_n'(k_e a) j_n(k_l a) - k_l j_n(k_e a) j_n'(k_l a)}{k_e j_n'(k_e a) h_n^{(1)}(k_e a) - k_l j_n(k_e a) h_n^{(1)}(k_l a)} \right] = 0. \quad (4.27)$$

The sums in eq.(4.26) and eq.(4.27) converge very fast. For eq.(4.26) only 7 terms, i.e, \( n \in \{-3, 3\} \) are needed for 0.1\% error, and for eq.(4.27) only 3 terms, i.e, \( n \in \{0, 2\} \) are needed.

In principle, our calculated speed of sound should be a function of frequency, but, for the parameters we have considered, this dependence is very weak. Likewise, the calculated wave vector, \( k_e \), as obtained in the EMA, has a small imaginary part, suggesting a finite damping of the wave through the composite, even if the individual components have no dissipation. For the cases we have considered, however, the damping is very small.
4.2.3 Results

Fig. 4.6 shows the effective speed of sound versus volume fraction \( f \) of carbon nanotube bundles calculated using 2D EMA (Eq. (4.26)), for some suitable frequency given by the single parameter in the calculation, namely the dimensionless parameter \( \omega a / c_1 \), where \( \omega \) is the frequency, \( a \) is the radius of the CNT bundle, and \( c_1 \) is the speed of sound in the liquid. The speed of sound in the liquid is assumed to be 1200 m/s and the radius of the bundles is assumed to be 20 nm. Fig. 4.7 shows the results for the 3D EMA (Eq. (4.26)).
In general, the speed of sound $c_e$ in the effective medium, as predicted by this model, is described by the order of magnitude relation $c_e(f) = [1 - Kf]c_e(0)$, where $f$ is the volume fraction of carbon nanotube bundles and $K$ is a constant of order unity. Thus, a volume fraction of 1% CNT bundles will reduce the speed of sound only by around 1%.

### 4.2.4 Discussion

One might ask if there is an intuitive explanation for why the speed of sound is reduced even though the impurities have a much higher speed of sound than the pure
fluid. We speculate that this might occur because the sound waves are scattered by
the suspended CNT bundles, thereby slowing down the sound propagation.

Recently [142], it was shown that in fact the measured speed of sound in a suspen-
sion of CNT bundles in DMF is less than the speed of sound in pure DMF. However,
the measured reduction was much higher than one predicted by this theory. But once
the agglomeration of CNT bundles on exposure to laser beams is taken into account
[142], and an effective filling fraction is calculated, this theory agrees well with the
experiments.
CHAPTER 5

CONCLUSIONS AND DISCUSSION

In this dissertation we studied three topics in superconducting qubits, four topics in superlattices and two topics in the application of effective medium theory.

In the second chapter we first studied a superconducting persistent-current qubit consisting of a three-junction superconducting loop in an applied magnetic field. It was shown that by choosing the field, Josephson couplings, and offset charges suitably, we can perfectly suppress the tunneling between the two oppositely directed states of circulating current, leading to a vanishing of the splitting between the two qubit states. This suppression arises from interference between tunneling along different paths and is analogous to that predicted previously for magnetic particles with half-integer spin. Then we calculated the dynamics of a nanomechanical oscillator (NMO) coupled capacitively to a Cooper-pair box (CPB) by solving a stochastic Schrödinger equation with two Lindblad operators[68]. Both the NMO and the CPB were dissipative, and the coupling was treated within the rotating wave approximation. It was shown numerically that, if the CPB decay time is smaller than the NMO decay time, the coupled NMO will lose energy faster and the coupled CPB more slowly than the uncoupled NMO and CPB do. These results show that the efficiency of energy loss by an NMO can be substantially increased if the NMO is coupled to a CPB. Finally
the coupled system of CPB and NMO was studied beyond RWA. It was shown that in this case the effective decay rate of the system is strongly dependent on the initial number of vibrational quanta \((N)\) in the NMO. In particular we used perturbation theory which is valid only for small \(N\). Also the results indicate that the decay time for the CPB can be decreased by coupling it to a high \(Q\) NMO, provided we can prepare the NMO in desired initial vibrational state.

In the third chapter various superlattices were studied. It was shown that, if graphene is subjected to the potential from an external superlattice, a band gap develops at the Dirac point provided the superlattice potential has broken inversion symmetry. As numerical example, the band structure of graphene in the presence of an external potential due to periodically patterned gates arranged in a triangular graphene superlattice (TGS) or a square graphene superlattice with broken inversion symmetry was calculated, and we found that a band gap is created at the original Dirac point. This gap, which extends throughout the superlattice Brillouin zone, can be controlled, in principle, by changing the external potential and the lattice constant of the superlattice. For a square superlattice of lattice-constant 10 nm, we obtained a gap as large as 65 meV, for gate voltages no larger than 1.5 V. Then we studied magnonic superlattices with two ferromagnets having different Gilbert damping parameter. As a numerical example Fe cylinders in Ni were considered and we found that the figure of merit was a factor of six bigger at the Brillouin zone corner than it is at other points in the Brillouin zone. These superlattices can be thought of as ferromagnetic nanowires in another ferromagnetic matrix (For statistical properties of a single magnetic nanowire, see Appendix A). Finally we discussed photonic superlattices. We first provided a simple method for calculating the effective
dielectric constant $\epsilon_e$ of a periodic composite. In the method, we first calculated the photonic band structure, then obtained an explicit expression for the small $k$ slope $d\omega/dk$, using the analog of $k \cdot p$ perturbation theory. If the effective magnetic permeability $\mu_e = 1$, this approach gives $\epsilon_e$ explicitly for any periodic solid. We illustrated the method for a lattice of infinitely long circular cylinders in a triangular or a square array. The results agreed well with the Maxwell-Garnett approximation (MGA), except near close packing. In this regime, $k \cdot p$ correctly gives an $\epsilon_e$ which is much larger than the MGA and depends on the composite structure. In the last topic of this chapter we discussed the presence of Dirac point in a triangular superlattice of Si cylinders in air. The degeneracy at the Dirac point was shown to be removed by breaking the time reversal and inversion symmetry of the superlattice.

In the fourth chapter, first it was shown that when bulk graphene breaks into n-type and p-type puddles, the in-plane resistivity becomes strongly field dependent in the presence of a perpendicular magnetic field, even if homogeneous graphene has a field-independent resistivity. We calculated the longitudinal resistivity $\rho_{xx}$ and Hall resistivity $\rho_{xy}$ as a function of field for this system using the effective-medium approximation. The conductivity tensors of the individual puddles were calculated using a Boltzmann approach suitable for the band structure of graphene near the Dirac points. The resulting resistivity agrees well with experiment provided that the relaxation time is weakly field dependent. The calculated Hall resistivity has the sign of the carriers in the puddles occupying the greater area of the composite and vanishes when there are equal areas of n- and p-type puddles. Finally, we calculated the sound velocity in a porous medium, using a self-consistent effective-medium approximation. The results of this calculation agrees qualitatively with experiment. This observed
sound wave would be the analog of the slow compressional mode of porous solids at a structural length scale of order of 100 nm.

It is worth mentioning that some of the ideas discussed in this thesis can be extended to other systems. For example, one can actually consider a magnetic super-lattice of spin torque oscillators and calculate the band structure for spin waves. In this case it will be of great interest to find complete band gaps, which would mean that spin waves with frequencies in the gap cannot propagate through the device. Also if we want to use spin torque oscillators as a microwave source, an array of them will have much more power compared to a single spin torque oscillator (for details see Appendix B). As another example the presence of a Dirac point can be extended in triangular magnonic superlattices. In this case there is no time reversal symmetry so there would be no degeneracy (in fact we speculate a small gap) at the Dirac point, but there will be a region with zero density of states around this Dirac point frequency (for details see Appendix C). One can further increase the gap at the Dirac point by breaking the spatial inversion symmetry.
A.1 Introduction

Scalapino, Sears and Ferrell [103] used the technique of replacing a functional integration by an eigenvalue problem to study the statistical mechanics of one dimensional real or complex scalar fields. Later, Stoeckly and Scalapino [113] extended this for weakly coupled one dimensional systems. In general the functional integrals are difficult to evaluate while straightforward numerical methods can be used to obtain an essentially exact solution for the corresponding eigenvalue problem. Here we follow the same philosophy and map the Ginzburg-Landau free energy for a magnetic order parameter, which is a 3 component vector, to an equivalent Schrödinger equation.

A.2 Formalism

We consider a one-dimensional magnetic wire aligned along z-axis. At each point along the wire, we have a 3 component magnetization vector (\( \mathbf{M} \)). Although this mapping of functional integration to a quantum mechanical problem is well established, for the sake of completeness, we do it explicitly here. In this appendix we
closely follow the work of Scalapino, Sears and Ferrell [103]. The only difference is that our order parameter is now a vector quantity.

The Ginzburg-Landau free energy functional per unit length for one dimensional magnetic wire in the presence of an external field \(H_{ext}\) is

\[
F[M] = \int_0^L dz \left( a |M|^2 + b |M|^4 + c \sum_{i=1}^3 \left| \frac{dM_i}{dz} \right|^2 - \mu_0 H_{ext} \cdot M - gM_z^2 \right). \tag{A.1}
\]

Note that the effect of a depolarizing field can be easily taken care of, since it just changes the magnitude of \(H_{ext}\). The coefficient \(a\) vanishes linearly as the reduced temperature \(t = T/T_c\) approaches unity;

\[
a = \alpha (t - 1), \tag{A.2}
\]

\(\alpha, b, c\) are positive constants. The constant \(g\) represents anisotropy, \(g > 0\) implies uniaxial or easy axis system and \(g < 0\) implies biaxial or easy plane system while \(g = 0\) implies isotropic system. The magnetization vector \(M\) is measured in units of constant magnetization \(M_0\) chosen to be saturated magnetization at room temperature [110], such that the magnetization vector \(M\), and \(M_z\) are dimensionless.

Using \(F[M]\) as the energy associated with an order-parameter configuration \(M\), the partition function for a canonical ensemble is expressed as a functional integral

\[
Z = \int \delta M e^{-\beta F[M]}, \tag{A.3}
\]

As is well known, the transfer-matrix technique allows one to replace the functional integration by an eigenvalue problem. In this one dimensional case, the eigenvalue problem is reduced to a one-particle quantum mechanical problem. This approach has been studied by several authors[38] and is simply related to Feynman’s path integral formulation of quantum mechanics [32]. Now we will give a brief summary of the
ideas as they apply to the vector order parameter case. It is convenient to consider boundary conditions appropriate to a ring of length \( L \). Dividing \( L \) into \( N \) segments of length \( \Delta z \), the explicit expression for the partition function Eq.(A.3) is

\[
Z = \prod_{i=1}^{N} \int d\tilde{M}_i e^{-\beta \Delta z f(M_{i+1}, M_i)}, \tag{A.4}
\]

with

\[
f(M_{i+1}, M_i) = a |M_{i+1}|^2 + b |M_{i+1}|^4 + c \left| \frac{M_{i+1} - M_i}{\Delta z} \right|^2 - \mu_0 H_{\text{ext}} \cdot M_{i+1} - g(M_{i+1})^2. \tag{A.5}
\]

The boundary conditions corresponding to a ring imply, \( M_{N+1} \) equals \( M_1 \). The integration elements \( d\tilde{M}_i \) in terms of the 3 components of the vector element are

\[
d\tilde{M}_i = \left( \frac{\beta c}{\pi \Delta z} \right)^{\frac{3}{2}} d(M_x)_i d(M_y)_i d(M_z)_i. \tag{A.6}
\]

Now we formally introduce an additional variable \( \tilde{M}_1' \), so that

\[
Z = \int d\tilde{M}_1' d\tilde{M}_1 d\tilde{M}_2 \ldots d\tilde{M}_N \delta(\tilde{M}_1 - \tilde{M}_1') e^{-\beta \Delta z f(M_1', M_N)} e^{-\beta \Delta z f(M_{i+1}, M_i)} \ldots e^{-\beta \Delta z f(M_2, M_1)}. \tag{A.7}
\]

Now, the \( \delta \) function is expanded in terms of a complete set of normalized eigenstates

\[
\delta(\tilde{M}_1 - \tilde{M}_1') = \sum_n \Psi^*_n(\tilde{M}_1') \Psi_n(\tilde{M}_1), \tag{A.8}
\]

so that

\[
Z = \sum_n \int d\tilde{M}_1' \ldots d\tilde{M}_N \Psi^*_n(\tilde{M}_1') e^{-\beta \Delta z f(M_1', M_N)} \ldots e^{-\beta \Delta z f(M_2, M_1)} \Psi_n(\tilde{M}_1). \tag{A.9}
\]

This expression is readily evaluated if \( \Psi_n \) are the eigenfunctions of the transfer operator

\[
\int d\tilde{M}_i e^{-\beta \Delta z f(M_{i+1}, M_i)} \Psi_n(\tilde{M}_i) = e^{-\beta \Delta z \epsilon_n} \Psi_n(\tilde{M}_{i+1}). \tag{A.10}
\]
implying

\[ Z = \sum_n e^{-\beta L \epsilon_n}. \]  

(A.11)

Note that for a thermodynamical system in which \( L \to \infty \), only the ground state contributes and the free energy per unit length is

\[ f = -\frac{kT}{L} \ln Z = \epsilon_0, \]  

(A.12)

where \( k \) is the Boltzmann constant.

The transfer-matrix-eigenvalue equation Eq. (A.10) is reduced to a one-particle eigenvalue problem by expanding \( \Psi_n(\vec{M}_i) \) about \( \Psi_n(\vec{M}_{i+1}) \), and carrying out the \( d\vec{M}_i \) integral. Expanding \( \Psi_n(\vec{M}_i) \) about \( \Psi_n(\vec{M}_{i+1}) \) we get

\[ \Psi_n(\vec{M}_i) = \Psi_n(\vec{M}_{i+1}) + \left[ (\vec{M}_i - \vec{M}_{i+1}) \cdot \nabla_{\vec{M}} \Psi_n(\vec{M}') \right]_{\vec{M}'=\vec{M}_{i+1}} \]
\[ + \frac{1}{2} (\vec{M}_i - \vec{M}_{i+1}) \cdot \left[ (\vec{M}_i - \vec{M}_{i+1}) \cdot \nabla_{\vec{M}} \left( \nabla_{\vec{M}} \Psi_n(\vec{M}') \right) \right]_{\vec{M}'=\vec{M}_{i+1}} \]  

(A.13)

Using the definition of \( d\vec{M}_i \), i.e, Eq.(A.6), and the properties of a Gaussian integral, we see that linear order term in the above Taylor expansion gives a vanishing integral. Therefore, the only terms that contribute are the zeroth and the second order term.

The integral for the zeroth order term gives

\[ \int \int \int \left( \frac{\beta c}{\pi \Delta z} \right)^n d(M_i)_x d(M_i)_y d(M_i)_z e^{-\frac{\beta \Delta z f(M_{i+1}, M_i)}{\pi \Delta z}} \Psi_n(\vec{M}_{i+1}) \]
\[ = e^{-\beta \Delta z (a|\vec{M}_{i+1}|^2 + b|\vec{M}_{i+1}|^4 - \mu_0 H_{ext} \cdot \vec{M}_{i+1} - g(|\vec{M}_{i+1}|^2)^2)} \Psi_n(\vec{M}_{i+1}). \]  

(A.14)
In the second order term, all the terms involving linear order in \((\tilde{M}_i - \tilde{M}_{i+1})_x\) or similar terms for \(y\) and \(z\) give vanishing contribution, and the remaining terms give

\[
\int \int \int \left( \frac{\beta c}{\Delta z} \right)^2 d(M_i)_x d(M_i)_y d(M_i)_z e^{-\beta \Delta z f(M_{i+1}, M_i)}
\]

\[
\frac{1}{2} \left[ \left( \sum_s (\tilde{M}_i - \tilde{M}_{i+1})^2_s \frac{\partial^2}{\partial (\tilde{M}')^2_s} \right) \Psi_n(\tilde{M}') \right]_{\tilde{M}'=M_{i+1}}
\]

\[
e^{-\beta \Delta z (a |M_{i+1}|^2 + b |M_{i+1}|^4) - \mu_0 H_{ext} \cdot M_{i+1} - g(M_{i+1})^2 \frac{\Delta z}{4 \beta c} \nabla^2_{M_{i+1}} \Psi_n(\tilde{M}_{i+1}).
\]

(A.15)

Now we add Eq.(A.14) and Eq.(A.15) to get

\[
\int d\tilde{M}_i e^{-\beta \Delta z f(M_{i+1}, M_i)} \Psi_n(\tilde{M}_i) = e^{-\beta \Delta z (a |M_{i+1}|^2 + b |M_{i+1}|^4 - \mu_0 H_{ext} \cdot M_{i+1} - g(M_{i+1})^2)} \left( 1 + \frac{1}{4 \beta c} \frac{\Delta z}{\nabla^2_{M_{i+1}}} \right) \Psi_n(\tilde{M}_{i+1}).
\]

(A.16)

Formally the derivative term in the above equation can be exponentiated and combined with the potential to order \(\Delta z\), so that the transfer eigenvalue equation Eq.(A.10) becomes

\[
e^{-\beta \Delta z \mathcal{H}} \psi_n = e^{-\beta \Delta z \epsilon_n} \psi_n,
\]

(A.17)

with the Hamiltonian \((\mathcal{H})\) defined as

\[
\mathcal{H} = -\frac{1}{4 \beta c} \nabla^2_M + a |M|^2 + b |M|^4 - \mu_0 H_{ext} \cdot M - g(M)^2.
\]

(A.18)

### A.3 Choice of parameters

In order to get the parameters \(c\) and \(g\), we take the values of these parameters from [110], and multiply them with the cross section to get these parameters representing free energy per unit length. We consider a single wire made of Cobalt (Co), having a circular cross section with diameter of 2 nm (i.e, radius, \(r_0 = 10^{-9}\) m). So, \(g = \)
\[6.8(10)^5 \pi r_0^2 \text{ J/m} = 2.136(10)^{-12} \text{ J/m} \text{ and } c = 1.3(10)^{-11} \pi r_0^2 \text{ Jm} = 4.084(10)^{-29} \text{ Jm.}

To get the values of \(a\) and \(b\), we consider a homogeneous free energy of type \(F[M/M_0] = a \left( \frac{M}{M_0} \right)^2 + b \left( \frac{M}{M_0} \right)^4 - g \left( \frac{M}{M_0} \right)^2\). Minimizing the free energy gives the relation \(\frac{M}{M_0} = \sqrt{-\frac{(a-g)^2}{2b}}\). The minimum free energy for this value of \(\frac{M}{M_0}\) is \(-\frac{(a-g)^2}{4b}\), where \(a = \alpha(t-1)\) and for low temperatures \(a \approx -\alpha\). The free energy can be computed by approximating \(kT_c\) as the energy per atom and multiplying this by atomic density.

This gives the free energy per unit volume, which is then multiplied by cross section to get free energy per unit length. \(T_c = 1388\text{K}, \text{ for Co, and the atomic density is } 9.1(10)^{22} \text{atoms/cm}^3[41]. \text{ The free energy per unit length is } 5.47595(10)^{-9} \text{ J/m. So, } \alpha \sim 5.5(10)^{-9} \text{ J/m and } b = a/2. \text{ Now we know all the parameters needed to cast the Schrödinger equation corresponding to Hamiltonian Eq.(A.18) in dimensionless form.}

The time independent Schrödinger equation we wish to solve is

\[
\left[ -\frac{1}{4\beta^2c} \left( \frac{\partial^2}{\partial M_x^2} + \frac{\partial^2}{\partial M_y^2} + \frac{\partial^2}{\partial M_z^2} \right) + aM^2 + bM^4 - gM_z^2 - \mu_0 \mathbf{H} \cdot \mathbf{M} \right] \Psi = \epsilon \Psi. \tag{A.19}
\]

Define dimensionless variables \(M_1 = M_x \sqrt{2\beta \sigma c}, M_2 = M_y \sqrt{2\beta \sigma c}\) and \(M_3 = M_z \sqrt{2\beta \sigma c}\), where \(\sigma = \sqrt{ag}\). In terms of these variables Eq.(A.19) reduces to

\[
\left( \frac{1}{\beta \sqrt{c}} \right) \left[ -\frac{1}{2} \left( \frac{\partial^2}{\partial M_1^2} + \frac{\partial^2}{\partial M_2^2} + \frac{\partial^2}{\partial M_3^2} \right) - \frac{\alpha \left( 1 - \frac{T}{T_c} \right)}{2\sigma} (M_1^2 + M_2^2 + M_3^2) \right.
\]

\[
\left. - \frac{g}{2\sigma} M_3^2 + \frac{b}{4\beta \sigma \sqrt{c}} (M_1^2 + M_2^2 + M_3^2) - \mu_0 \sqrt{\frac{\beta \sqrt{c}}{2\sigma \sqrt{\sigma}}} H_{ext} M_3 \right] \Psi = \epsilon \Psi. \tag{A.20}
\]

where in the last term, the external magnetic field is assumed to be along \(z\)-axis, i.e, \(\mathbf{H} = H_{ext} \hat{z}\). The above equation is easily reduced to a matrix eigenvalue problem by expanding the wavefunction in the basis set of harmonic oscillators[118]. Then we find the ground state of the system.
A.4 The coercivity

Consider the potential energy $\mathcal{V}[M_z] = -\gamma_1 (M_z)^2 + \gamma_2 (M_z)^4 + \gamma_3 (M_z)$. When $\gamma_1 > 0$, $\gamma_2 > 0$ and $\gamma_3 = 0$, this represents a symmetric double well potential. When $\gamma_3$ is non zero the symmetry breaks and we get an asymmetric double well potential. One well is deeper than the other and the two states of the hysteresis loop are actually the two states located in these 2 wells. If we increase the magnitude of $\gamma_3$, we arrive at the case where one well is very deep while the other well has disappeared. The value of $\gamma_3$ for this case actually represents the coercivity. There is a very simple way to find the coercivity in this case. The critical points for the above potential are given by the following cubic equation.

\[-2\gamma_1 (M_z)^2 + 4\gamma_2 (M_z)^3 + \gamma_3 = 0. \quad (A.21)\]

For a cubic equation of type $ax^3 + bx^2 + cx + d = 0$, the discriminant is defined by $\Delta = 4b^3d - b^2c^2 + 4ac3 - 18abcd + 27a^2d^2$, and whenever $\Delta = 0$ then at least 2 roots must coincide, which corresponds to disappearance of one well. For our case $\Delta = 16(27\gamma_2^2\gamma_3^2 - 8\gamma_2\gamma_1^3)$, thus the condition for vanishing of the discriminant gives us

$$\gamma_3 = \sqrt{\frac{8\gamma_1^3}{27\gamma_2}}. \quad (A.22)$$

A.5 Many wires

Consider a lattice of $N$ parallel magnetic wires with lattice constant $a_0$. Let $z$ be the number of nearest neighbors ($nn$). The Hamiltonian of the system is

$$\mathcal{H} = \sum_i^N \left( -\frac{1}{4} \beta^2 c \nabla^2_{M_i} + a |M_i|^2 + b |M_i|^4 - \mu_0 \mathbf{H}_{ext} \cdot \mathbf{M}_i - g(M_i)^2 \right)$$

$$+ \frac{1}{2} \sum_{i=1}^N \lambda \sum_{j \in nn} M_i \cdot M_j. \quad (A.23)$$
Here $\lambda$ is the coupling constant, which depends upon the lattice constant $a_0$. We solve this problem using mean field theory. For the case when $\lambda = 0$, we compute $\langle M \rangle$. The last term of the equation is then replaced by $\frac{1}{2} N z \lambda \langle M_i \rangle M_j$. So the Hamiltonian for a single wire reduces to

$$\mathcal{H} = \left( -\frac{1}{4} \frac{1}{\beta^2} \nabla^2_M + a |M|^2 + b |M|^4 - \mu_0 H_{ext} \cdot M - g(M)^2 \right) + \frac{1}{2} z \lambda \langle M_i \rangle M. \quad (A.24)$$

Alternately, we can approximate $M_j$ by its expectation value to get

$$\mathcal{H} = \left( -\frac{1}{4} \frac{1}{\beta^2} \nabla^2_M + a |M|^2 + b |M|^4 - \mu_0 H_{ext} \cdot M - g(M)^2 \right) + \frac{1}{2} z \lambda \langle M_j \rangle M. \quad (A.25)$$

The expectation value in any of the above two proposed equation is first given a value calculated for $\lambda = 0$, the Schrödinger equation for one wire is solved using this expectation value. From the solution of this equation the expectation value is calculated again and this new value is used for solving the Schrödinger equation in step two. This process is continued till the expectation value calculated for two consecutive steps is below some predefined threshold (say around 0.1 percent of the initial expectation value). In general the coupling between many wires $\lambda$ can be a complicated function of $M$ itself. As a first approximation we choose a constant coupling.
APPENDIX B

PERIODIC ARRAY OF SPIN TORQUE OSCILLATORS

Recently there has been a plethora of interest in spin torque oscillators. Spin torque oscillators can be used as a memory element, or microwave sources.

Mutual phase locking of two spin torque oscillators has already been shown [53, 70]. We propose a device which consists of an array of spin torque oscillators. A schematic of such a device is shown in Fig. 1. The top and the bottom cuboids connected by a current source are ferromagnets and the various cylinders connecting them are paramagnets. In particular we consider a triangular and square lattice arrangement of such cylinders. The bigger (bottom) ferromagnet has fixed magnetization ($M_1$) and the smaller (top) one has free magnetization ($M_2$). Through the cylinders a spin polarized current flows between the ferromagnets and this exerts a torque on the free magnetization.

Due to the periodic nature of the spin polarized current we expect a band structure effect on the magnetization of the free layer.

The equation of motion for the free ferromagnet is given by the Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation[111]:

$$\frac{\partial}{\partial t} M_2 = \gamma \mu_0 M_2 \times H_{\text{eff}} + \frac{\alpha}{M_{2s}} \left( M_2 \times \frac{\partial}{\partial t} M_2 \right) + \frac{I_e(r)}{e} \hat{M}_2 \times \left( \hat{M}_1 \times \hat{M}_2 \right).$$  (B.1)
Here $\gamma$ is the gyromagnetic ratio for the free ferromagnet, $H_{\text{eff}}$ is the effective field acting on the free magnetization $M_2(r,t)$ which includes the external field ($H_{\text{ext}}$), the demagnetization field ($H_{\text{dm}}$), the exchange field ($H_{\text{ex}}$) and the effects of anisotropy which contributes $(H_K M^z_2/M_2)\hat{x}$ to $H_{\text{eff}}$ for an easy plane anisotropy [66, 67]. $r$ is the two-dimensional position vector in the $x-y$ plane (where we have assumed that the magnetization is uniform along the direction of spin polarized current), $\alpha$ is the Gilbert damping parameter and $M_{2s}$ is the spontaneous magnetization for the free ferromagnet. The function $g$ is

$$g = \left( -4 + \frac{(1+P)^3(3 + \hat{M}_1 \cdot \hat{M}_2)}{4P^{3/2}} \right)^{-1},$$

with $P$ being the polarizing factor of the fixed ferromagnet. Let the external field applied on the free ferromagnet be parallel to its plane, so $H_{\text{ext}} = H_{\text{ext}}\hat{x}$. The free ferromagnetic layer can be considered as a thin film so the demagnetization field can be simply written as $H_{\text{dm}} = -4\pi M^z_2\hat{z}$. Finally, the exchange field is given by $H_{\text{ex}} = (2A/M^z_2)\nabla^2 M_2$, with $A$ being the exchange constant for the free ferromagnet.

Figure B.1: Schematic of the spin torque oscillator device.
Thus
\[ H_{\text{eff}} = H_{\text{ext}} \hat{x} - 4\pi M_2^z \hat{z} + \frac{2A}{M_{2s}^2} \nabla^2 M_2 + \frac{H_K M_2^z}{M_{2s}} \hat{x}. \] (B.3)

For the present system the current density \( I_e \) take the form
\[ I_e(\mathbf{r}) = \Theta(\mathbf{r}) I_e, \] (B.4)
where the step function \( \Theta(\mathbf{r}) \) is
\[ \Theta(\mathbf{r}) = \begin{cases} 
1 & \text{if } \mathbf{r} \text{ is inside circular regions,} \\
0 & \text{otherwise.} 
\end{cases} \] (B.5)

We separate the static and time-dependent parts of the free magnetization by writing \( M_2(\mathbf{r}, t) = M_{2s} \hat{x} + m(\mathbf{r}, t) \), where \( m(\mathbf{r}, t) = [m^x(\mathbf{r}), m^y(\mathbf{r}), m^z(\mathbf{r})] T e^{-i\omega t} \). The magnetization of the fixed layer is written as \( M_1 = M_1 \hat{x} \).

With above prescription the left hand side of eq. (B.1) is \( -i\omega [m^x(\mathbf{r}), m^y(\mathbf{r}), m^z(\mathbf{r})]^T e^{-i\omega t} \). Let us evaluate each of the terms on the right hand side one by one.

The \( x \) component of the term first term \( \gamma \mu_0 M_2 \times H_{\text{eff}} \) is \( \gamma \mu_0 ( -4\pi m^y(\mathbf{r}) m^z(\mathbf{r}) + \frac{2A}{M_{2s}^2} m^y(\mathbf{r}) \nabla^2 m^z(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^z(\mathbf{r}) \nabla^2 m^y(\mathbf{r}) ) e^{-2i\omega t} \). The \( y \) component is \( (4\pi M_{2s} m^z(\mathbf{r}) - \frac{2A}{M_{2s}^2} \nabla^2 m^z(\mathbf{r}) + H_{\text{ext}} m^z(\mathbf{r}) + H_K m^z(\mathbf{r}) + (4\pi m^x(\mathbf{r}) m^z(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^z(\mathbf{r}) \nabla^2 m^z(\mathbf{r}) + \frac{2A}{M_{2s}^2} m^z(\mathbf{r}) \nabla^2 m^z(\mathbf{r}) + H_{\text{ext}} m^y(\mathbf{r}) + H_K m^y(\mathbf{r}) + \frac{2A}{M_{2s}^2} m^y(\mathbf{r}) \nabla^2 m^y(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^y(\mathbf{r}) \nabla^2 m^y(\mathbf{r}) - H_{\text{ext}} m^y(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^z(\mathbf{r}) \nabla^2 m^z(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^z(\mathbf{r}) \nabla^2 m^z(\mathbf{r}) - \frac{2A}{M_{2s}^2} m^y(\mathbf{r}) ) e^{-i\omega t} \) \( e^{-i\omega t} \) \( e^{-i\omega t} \).

The components of the second term on the right hand side of eq. (B.1) i.e, \( \frac{\alpha}{M_{2s}} (M_2 \times \frac{\partial}{\partial t} M_2) \) are written as \([0, i\omega m^z(\mathbf{r}), -i\omega m^y(\mathbf{r})]^T e^{-i\omega t} \).

Now we simplify the spin torque term. Also, we calculate the properties of the device within the linear magnon approximation which means \( \{m^x(\mathbf{r}), m^y(\mathbf{r}), m^z(\mathbf{r})\} \ll M_{2s} \). This greatly simplifies the first term also, and we get rid of all the terms oscillating with \( 2\omega \).
Within the linear magnon approximation \( \hat{\mathbf{M}}_2 \approx 1 + m^x(r) + m^y(r) + m^z(r) \). So, \( \hat{\mathbf{M}}_1 \cdot \hat{\mathbf{M}}_2 = 1 + \frac{m^x(r)}{M_{2s}} e^{-i\omega t} \). Thus

\[
g = -\frac{1}{4} \left[ 1 - \frac{(1 + P)^3}{16P^{3/2}} \left( 4 + \frac{m^x(r)}{M_{2s}} e^{-i\omega t} \right) \right]^{-1}
\approx -\frac{1}{4} + \frac{(1 + P)^3}{16P^{3/2}} - \frac{(1 + P)^3}{64P^{3/2}} \frac{m^x(r)}{M_{2s}} e^{-i\omega t}.
\] (B.6)

Now \( \hat{\mathbf{M}}_2 \times \hat{\mathbf{M}}_1 \times \hat{\mathbf{M}}_2 \)

\[
= \hat{x} - \frac{m^x(r)}{M_{2s}} e^{-i\omega t} \left[ (1 + \frac{m^x(r)}{M_{2s}} e^{-i\omega t}) \hat{x} + \frac{m^y(r)}{M_{2s}} e^{-i\omega t} \hat{y} + \frac{m^z(r)}{M_{2s}} e^{-i\omega t} \hat{z} \right]
\]

\[
= -\frac{2m^x(r)}{M_{2s}} e^{-i\omega t} \hat{x} - \frac{m^y(r)}{M_{2s}} e^{-i\omega t} \hat{y} - \frac{m^z(r)}{M_{2s}} e^{-i\omega t}.
\] (B.7)

So,

\[
\frac{I_e(r)g}{e} \hat{\mathbf{M}}_2 \times \hat{\mathbf{M}}_1 \times \hat{\mathbf{M}}_2 \approx \begin{bmatrix} 2C I_e(r) m^x(r) \\ C I_e(r) m^y(r) \\ C I_e(r) m^z(r) \end{bmatrix}
\] (B.8)

with \( C = \frac{1}{e} \left( \frac{1}{4} - \frac{(1 + P)^3}{16P^{3/2}} \right) \).

Thus the left-hand side of the equation of motion within the linear magnon approximation is

\[
\text{LHS} = -i\omega \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \alpha \\ 0 & -\alpha & 1 \end{bmatrix} \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix}.
\] (B.9)

The right hand side is

\[
\text{RHS} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \gamma \mu_0 (4\pi M_{2s} + H_{ext} + H_K) \\ 0 & \gamma \mu_0 (H_{ext} + H_K) & 0 \end{bmatrix} \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix}
\]

\[+ \begin{bmatrix} 2C I_e(r) & 0 & 0 \\ 0 & C I_e(r) & -\frac{2A}{M_{2s}} \nabla^2 \\ 0 & \frac{2A}{M_{2s}} \nabla^2 & C I_e(r) \end{bmatrix} \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix}.\] (B.10)

The above equation is written as

\[-i\omega Q \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix} = R \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix} + S \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix},\] (B.11)

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with

\[
Q = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & \alpha \\
0 & -\alpha & 1
\end{bmatrix}
\]

\[
R = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & \gamma \mu_0(4\pi M_2s + H_{\text{ext}} + H_K) \\
0 & -\gamma \mu_0(H_{\text{ext}} + H_K) & 0
\end{bmatrix}
\]

\[
S = \begin{bmatrix}
2CI_e(r) & 0 & 0 \\
0 & CI_e(r) & \frac{2A}{M_2s} \nabla^2 \\
0 & \frac{2A}{M_2s} \nabla^2 & CI_e(r)
\end{bmatrix}.
\]

Eq. (B.11) is rewritten as

\[
-i[\omega I - iQ^{-1}R] \begin{bmatrix}
m^x(r) \\
m^y(r) \\
m^z(r)
\end{bmatrix} = Q^{-1}S \begin{bmatrix}
m^x(r) \\
m^y(r) \\
m^z(r)
\end{bmatrix}.
\]

Thus,

\[
-i[\omega I - iQ^{-1}R] = -i \begin{bmatrix}
\omega & 0 & 0 \\
0 & \omega - i\alpha \gamma \mu_0(H_{\text{ext}} + H_K) & 0 \\
0 & \frac{i\gamma \mu_0(H_{\text{ext}} + H_K)}{1+\alpha^2} & \omega - i\frac{\alpha \gamma \mu_0(4\pi M_2s + H_{\text{ext}} + H_K)}{1+\alpha^2}
\end{bmatrix}.
\]

Now we expand the spin polarized current in a Fourier series as

\[
I_e(r) = \sum_G I_e(G)e^{iG\cdot r}.
\]

(B.15)

Because of the periodic potential, \(m^x(r)\), \(m^y(r)\) and \(m^z(r)\) obey Bloch’s theorem and are written as

\[
m^x(r) = \sum_{G'} m^x(G')e^{i(k+G')\cdot r}
\]

\[
m^y(r) = \sum_{G'} m^y(G')e^{i(k+G')\cdot r}
\]

\[
m^z(r) = \sum_{G'} m^z(G')e^{i(k+G')\cdot r}.
\]

(B.16)
Using the above two equations we get
$$S \begin{bmatrix} m^x(r) \\ m^y(r) \\ m^z(r) \end{bmatrix} = T,$$
with the elements of the vector $T$ being

$$T_1 = \sum_{G,G'} e^{i k r} 2 C I_e(G) m^x(G') e^{i (G+G') \cdot r},$$
$$T_2 = T_{22} + T_{23}, T_3 = T_{32} + T_{33},$$
$$T_{22} = \sum_{G,G'} e^{i k r} C I_e(G) m^y(G') e^{i (G+G') \cdot r},$$
$$T_{33} = \sum_{G,G'} e^{i k r} C I_e(G) m^z(G') e^{i (G+G') \cdot r},$$
$$T_{23} = \sum_{G,G'} e^{i k r} \delta_{G,G'} \frac{2 A}{M_{2s}} (k + G')^2 m^z(G') e^{i (G') \cdot r},$$
$$T_{32} = -\sum_{G,G'} e^{i k r} \delta_{G,G'} \frac{2 A}{M_{2s}} (k + G')^2 m^y(G') e^{i (G') \cdot r}.$$  (B.17)

Now we multiply both the left and right hand side of eq. (B.13) by $e^{-i (G'' \cdot r)}$ and integrate over the unit cell to get

$$-i [\omega I - i Q^{-1} R] \sum_G \begin{bmatrix} m^x(G) \\ m^y(G) \\ m^z(G) \end{bmatrix} = \sum_{G'G} V(G',G) \begin{bmatrix} m^x(G') \\ m^y(G') \\ m^z(G') \end{bmatrix},$$  (B.18)

where the elements of matrix $V(G',G)$ are

$$V_{11} = 2 C I_e(G - G'),$$
$$V_{12} = V_{13} = V_{21} = V_{31} = 0,$$
$$V_{22} = V_{33} = \left( C I_e(G - G') + \frac{\delta_{GG'} 2 \alpha A (k + G')^2}{(1 + \alpha^2) M_{2s}} \right),$$
$$V_{23} = -V_{32} = \left( \frac{\delta_{GG'} 2 A (k + G')^2}{(1 + \alpha^2) M_{2s}} - \frac{\alpha C I_e(G - G')}{1 + \alpha^2} \right).$$  (B.19)

Finally we move the matrix $Q^{-1} R$ on the right hand side to get an eigenvalue equation:

$$-i \omega \sum_G \begin{bmatrix} m^x(G) \\ m^y(G) \\ m^z(G) \end{bmatrix} = \sum_{G'G} W(G',G) \begin{bmatrix} m^x(G') \\ m^y(G') \\ m^z(G') \end{bmatrix}.$$  With the matrix
elements of $W(G', G)$ being

\[
W_{11} = 2C\ell_e(G - G'),
\]

\[
W_{12} = W_{13} = W_{21} = W_{31} = 0,
\]

\[
W_{22} = \delta_{GG'} \frac{\alpha \gamma \mu_0 (H_{ext} + H_K)}{1 + \alpha^2} + \frac{C\ell_e(G - G')}{1 + \alpha^2} + \frac{\delta_{GG'} 2\alpha A(k + G')^2}{(1 + \alpha^2)M_{2s}},
\]

\[
W_{33} = \delta_{GG'} \frac{\alpha \gamma \mu_0 (4\pi M_{2s} + H_{ext} + H_K)}{1 + \alpha^2} + \frac{C\ell_e(G - G')}{1 + \alpha^2} + \frac{\delta_{GG'} 2\alpha A(k + G')^2}{(1 + \alpha^2)M_{2s}},
\]

\[
W_{23} = \delta_{GG'} \frac{\gamma \mu_0 (4\pi M_{2s} + H_{ext} + H_K)}{1 + \alpha^2} + \frac{\delta_{GG'} 2A(k + G')^2}{(1 + \alpha^2)M_{2s}} - \frac{\alpha C\ell_e(G - G')}{1 + \alpha^2},
\]

\[
W_{32} = -\delta_{GG'} \frac{\gamma \mu_0 (H_{ext} + H_K)}{1 + \alpha^2} - \frac{\delta_{GG'} 2A(k + G')^2}{(1 + \alpha^2)M_{2s}} + \frac{\alpha C\ell_e(G - G')}{1 + \alpha^2}.
\]  

(B.20)

Restricting the sum over reciprocal lattice vectors to $N$, we diagonalize $3N \times 3N$ matrix to get the eigenvalues. Using this procedure we obtain a band structure for this device. In particular it is interesting to note that as a result we might get band gaps, and also this device will have much higher power as a microwave source compared to a single spin torque oscillator.
APPENDIX C

DIRAC POINT IN MAGNONIC SUPERLATTICE

In this appendix we discuss the presence of a Dirac point in a triangular magnonic superlattice. We consider a triangular superlattice of iron (Fe) cylinders in europium oxide (EuO). The equation of motion for this system is given by Eq. 3.5. We ignore the Gilbert damping term for this calculation since it is small for both the components. We solve Eq. 3.5 by using a plane wave expansion. The calculation is almost identical to one presented in section 3.2.

The band structure obtained by this method is shown in Fig. C.1. The filling fraction for Fe is chosen to be 0.431. The Dirac point exists between the seventh and eight band at the Brillouin zone corner. Because the time reversal symmetry is inherently broken in a ferromagnetic system, the two bands are no longer degenerate at the Dirac point (although not clearly visible there is a small gap at the Dirac point). The density of states vanishes for the Dirac point frequency, and this small gap can be increased by breaking the inversion symmetry of the superlattice.
Figure C.1: Magnonic band structure for triangular lattice of Fe cylinders in EuO. The Dirac point is between the seventh and eighth bands at the Brillouin zone corner.


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