Summary of SI2600 Condensed Matter Theory

Yashar Honarmandi
yasharh@kth.se

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Abstract

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1 Solid-State Systems and Effects

This section concerns systems that can be studied with more familiar solid-state theory.

The Bloch Theorem The full Hamiltonian for a set of electrons in a crystal lattice is impossible to solve. Bloch's theorem is the statement that by simplifying the theory such that the electrons are moving in some effective potential, the states are given by

$$\psi_{n,\mathbf{k}} = \langle \mathbf{r}|n,\mathbf{k}\rangle = u_{n,\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}},$$

where u has the same periodicity as the potential. The wavevector $\mathbf{k}$ is confined to the first Brillouin zone and the index n labels which band the state is in. One useful property of these states is that

$$\begin{aligned}\langle \mathbf{r}|\mathcal{H}|n,\mathbf{k}\rangle =& \left(\frac{1}{2m}\mathbf{p}^2 + V(\mathbf{r})\right) u_{n,\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \\ =& e^{i\mathbf{k}\cdot\mathbf{r}}\left(\frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V(\mathbf{r})\right) u_{n,\mathbf{k}}(\mathbf{r}),\end{aligned}$$

hence we may change the wavefunction basis to only include the Bloch functions and let the parameter $\mathbf{k}$ enter as a parameter in the Hamiltonian. The Feynman-Hellman theorem then states that

$$\langle n,\mathbf{k}|\mathbf{v}|n,\mathbf{k}\rangle = \frac{1}{m}\langle u_{n,\mathbf{k}}|\mathbf{p}+\hbar\mathbf{k}|u_{n,\mathbf{k}}\rangle = \frac{1}{\hbar}\vec{\boldsymbol{\nabla}}_{\mathbf{k}}E_{\mathbf{k}},$$

where $E_{\mathbf{k}}$ is the energy eigenvalue associated with a given Bloch state.

The Tight Binding Approximation The tight binding approximation is an approximative solution of the Schrödinger equation in a periodic potential. It states that, given some solution of one element of the periodic potential, the eigenbasis for the full Hamiltonian is a set of states localized at each element in the periodic array. More specifically, it is the approximation

$$|\psi_{\mathbf{q}}\rangle = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}\,|j\rangle\,,$$

with the corresponding Bloch function

$$u_{\mathbf{q}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_j e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_j)}\phi_0(\mathbf{r}-\mathbf{R}_j),$$

where

$$\phi_0(\mathbf{r}-\mathbf{R}_j) = \langle \mathbf{r}|j\rangle\,.$$

To compute the energy of such states we will need inner products of these states. First we have

$$\langle\psi_{\mathbf{q}}|\psi_{\mathbf{q}}\rangle = \frac{1}{N}\sum_{j,l} e^{i\mathbf{q}\cdot(\mathbf{R}_j-\mathbf{R}_l)}\,\langle l|j\rangle = \sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}\,\langle 0|j\rangle\,,$$

which we dub $\eta(\mathbf{q})$. Now, because these states are eigenstates of the translation operator one can show that

$$\langle\psi_{\mathbf{q}}|\psi_{\mathbf{k}}\rangle = \eta(\mathbf{q})\delta^3(\mathbf{q}-\mathbf{k})_{\mathbf{G}},$$

where the Dirac delta is up to a reciprocal lattice vector. Next, let us consider matrix elements of the Hamiltonian. Writing

$$\mathcal{H} = \frac{p^2}{2m} + \sum_j V(\mathbf{r}-\mathbf{R}_j)$$

we have

$$\mathcal{H}\,|i\rangle = E_0\,|i\rangle + \left(\sum_{j\neq i} V(\mathbf{r}-\mathbf{R}_j)\right)|i\rangle\,.$$

Denoting the operator in the last term as ΔV_i we note that it does not have $|i\rangle$ as an eigenvector. For a Bloch state we then find

$$\langle\psi_{\mathbf{q}}|\mathcal{H}|\psi_{\mathbf{q}}\rangle = E_0\eta(\mathbf{q}) + \frac{1}{N}\sum_{j,k} e^{i\mathbf{q}\cdot(\mathbf{R}_k-\mathbf{R}_j)}\langle j|\Delta V_k|k\rangle\,.$$

Defining the right term as $\Lambda(\mathbf{q})$ we find

$$E_{\mathbf{q}} = E_0 + \frac{\Lambda(\mathbf{q})}{\eta(\mathbf{q})}.$$

Approximating the atoms to be far apart we can neglect most contributions to η by setting it to 1. In this approximation we introduce a first non-trivial correction by first setting

$$\langle j|k\rangle = \zeta$$

and

$$\langle k|\Delta V_k|k\rangle = \Delta E,\ \ \langle j|\Delta V_k|k\rangle = t_0,$$

where the off-diagonal expressions only hold for nearest neighbors. t_0 is called the transfer integral. We then have

$$\Lambda(\mathbf{q}) = \Delta E + t_0\sum_{\boldsymbol{\delta}} e^{-i\mathbf{q}\cdot\boldsymbol{\delta}},$$

where the sum is over nearest-neighbor lattice vectors. A similar result holds for the overlap. We often normalize the term by extracting a factor z from the sum, which is the coordination number, and write what is left as $\gamma(\mathbf{q})$. We then finally have

$$E_{\mathbf{q}} = E_0 + \frac{\Delta E + t_0 z\gamma(\mathbf{q})}{1 + z\zeta\gamma(\mathbf{q})}.$$

Evidently, then, the band width is $2t_0z$. Furthermore, we can use this to determine the curvature and thus an effective mass by expanding

$$E_{\mathbf{q}} \approx E_0 + \frac{\hbar^2}{2m}\mathbf{q}^2$$

close to the minimum.

Wannier Functions Wannier functions are constructions of states that are orthogonal. For band n, the Wannier function centered around atom j is

$$|\chi_{n,j}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}_j}\,|\psi_{n,\mathbf{q}}\rangle\,.$$

The $|\psi_{n,\mathbf{q}}\rangle$ are the normalized Bloch states from the tight binding approximation. These distinguish themselves in being useful even if the tight binding approximation breaks down. They are also orthogonal, as

$$\begin{aligned}\langle\chi_{n,i}|\chi_{m,j}\rangle =& \frac{1}{N}\sum_{\mathbf{k},\mathbf{q}} e^{i(\mathbf{k}\cdot\mathbf{R}_i-\mathbf{q}\cdot\mathbf{R}_j)}\langle\psi_{m,\mathbf{k}}|\psi_{n,\mathbf{q}}\rangle\\ =& \frac{1}{N}\sum_{\mathbf{k},\mathbf{q}} e^{-i(\mathbf{k}\cdot\mathbf{R}_i-\mathbf{q}\cdot\mathbf{R}_j)}\delta_{mn}\delta_{\mathbf{kq}}\\ =& \frac{1}{N}\delta_{mn}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}.\end{aligned}$$

Because each unit cell contributes one state and the complex exponential is rapidly oscillatory we have

$$\langle\chi_{n,i}|\chi_{m,j}\rangle = \delta_{mn}\delta_{ij}.$$

Graphene Graphene is a phase of carbon where the atoms arrange in a honeycomb lattice in a single atomic layer. This can be represented as a triangular lattice with two atoms in the basis. We choose the lattice vectors $a\left(\frac{3}{2}, \pm\frac{\sqrt{3}}{2}\right)$ and the basis displacement vector $a(1,0)$. Employing the tight-binding approximation with $E_0 = 0$ we write the Hamiltonian as

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} |i\rangle\langle j| + |j\rangle\langle i| \,,$$

which is a sum over nearest neighbors. The fact that there are two atoms in the basis divides the lattice into two sublattices A and B. The Bloch states are then

$$|\mathbf{q}, A\rangle = \frac{1}{\sqrt{N}} \sum_{j \in A} e^{i\mathbf{q}\cdot\mathbf{R}_j} |j\rangle \,,$$

with a similar state for the other sublattice. Neglecting overlap between neighboring wavefunctions we find

$$\begin{aligned}
\mathcal{H}|\mathbf{q}, A\rangle =& -\frac{t}{\sqrt{N}} \left(\sum_{\langle i,j \rangle} |i\rangle\langle j| + |j\rangle\langle i| \right) \sum_{k \in A} e^{i\mathbf{q}\cdot\mathbf{R}_k} |k\rangle \\
=& -\frac{t}{\sqrt{N}} \sum_{k \in A} \sum_{j = \mathrm{nn}(k)} e^{i\mathbf{q}\cdot\mathbf{R}_k} |j\rangle \\
=& -\frac{t}{\sqrt{N}} \sum_{k \in A} \sum_{j = \mathrm{nn}(k)} e^{i\mathbf{q}\cdot(\mathbf{R}_j - \boldsymbol{\delta}_{k\to j})} |j\rangle \\
=& -t \sum_{\boldsymbol{\delta}} e^{-i\mathbf{q}\cdot\boldsymbol{\delta}} |\mathbf{q}, B\rangle \,,
\end{aligned}$$

and similarly

$$\mathcal{H}|\mathbf{q}, B\rangle = -t \sum_{\boldsymbol{\delta}} e^{i\mathbf{q}\cdot\boldsymbol{\delta}} |\mathbf{q}, A\rangle \,.$$

We denote the prefactor as $-tf(\mathbf{q})$, and find that the Hamiltonian has eigenvalues $\pm t|f(\mathbf{q})|$.

Of note about the Brillouin zone of the triangular lattice, which is a hexagon, is that it only has one unique corner (and its opposite), as the others are related to these by a reciprocal lattice vector. Choosing, say, $\mathbf{K} = \frac{4\pi}{3\sqrt{3}a}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$ and its opposite we have

$$f(\mathbf{K}) = e^{i\frac{4\pi}{3\sqrt{3}}\frac{\sqrt{3}}{2}} + e^{i\frac{4\pi}{3\sqrt{3}}\left(-\frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4}\right)} + e^{i\frac{4\pi}{3\sqrt{3}}\left(-\frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4}\right)} = 2\cos\left(\frac{2\pi}{3}\right) + 1 = 0.$$

Thus there is no band gap. Next we have

$$\vec{\boldsymbol{\nabla}}_{\mathbf{q}} f(\mathbf{q}) = i \sum_{\boldsymbol{\delta}} \boldsymbol{\delta} e^{i\mathbf{q}\cdot\boldsymbol{\delta}},$$

and close to the corner we have

$$\begin{aligned}
f(\mathbf{q}) \approx& (\mathbf{q} - \mathbf{K}) \cdot ia \left((1,0)e^{i\frac{2\pi}{3}} + \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right) e^{-i\frac{2\pi}{3}} + \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \right) \\
=& ia \left(k_x e^{i\frac{2\pi}{3}} + \left(-\frac{1}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) e^{-i\frac{2\pi}{3}} - \frac{1}{2}k_x + \frac{\sqrt{3}}{2}k_y \right) \\
=& ia \left(k_x \left(e^{i\frac{2\pi}{3}} - \frac{1}{2}e^{-i\frac{2\pi}{3}} - \frac{1}{2} \right) + k_y \left(-\frac{\sqrt{3}}{2}e^{-i\frac{2\pi}{3}} + \frac{\sqrt{3}}{2} \right) \right).
\end{aligned}$$

This means that the dispersion is linear, a characteristic of solutions of the Dirac equation. This relation must be investigated further.

To do this we must remedy the fact that f does not share the periodicity of the reciprocal lattice due to the $\boldsymbol{\delta}$ not being lattice vectors. However, by introducing

$$\left|\mathbf{q}, \tilde{B}\right\rangle = ie^{-i\mathbf{q}\cdot\boldsymbol{\delta}_1} |\mathbf{q}, B\rangle \,,$$

the same treatment results in the Hamiltonian containing a new function $\tilde{f}(\mathbf{q}) = ie^{-i\mathbf{q}\cdot\boldsymbol{\delta}_1} f(\mathbf{q})$. This function has the periodicity of the reciprocal lattice. Writing

$$\tilde{f}(\mathbf{q}) = i\left(1 + e^{i\mathbf{q}\cdot\sqrt{3}a\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)} + e^{i\mathbf{q}\cdot\sqrt{3}a\left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)}\right),$$

we have

$$\vec{\boldsymbol{\nabla}}_{\mathbf{q}}\tilde{f} = -\sqrt{3}a\left(\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)e^{i\mathbf{q}\cdot\sqrt{3}a\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)} + \left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)e^{i\mathbf{q}\cdot\sqrt{3}a\left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)}\right).$$

As $\tilde{f}(\mathbf{K}) = 0$ we have

$$\begin{aligned}
\tilde{f}(\mathbf{K}+\mathbf{k}) \approx& -\sqrt{3}a\left(\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)e^{i\frac{4\pi}{3}\left(-\frac{3}{4}+\frac{1}{4}\right)} + \left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)e^{i\frac{4\pi}{3}\left(-\frac{3}{4}-\frac{1}{4}\right)}\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)e^{-i\frac{2\pi}{3}} + \left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)e^{-i\frac{4\pi}{3}}\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(-\frac{\sqrt{3}}{2}\left(e^{-i\frac{2\pi}{3}} + e^{-i\frac{4\pi}{3}}\right), \frac{1}{2}\left(e^{-i\frac{2\pi}{3}} - e^{-i\frac{4\pi}{3}}\right)\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(-\sqrt{3}\cos\left(-\frac{2\pi}{3}\right), i\sin\left(-\frac{2\pi}{3}\right)\right)\cdot\mathbf{k}\\
=& -\frac{3}{2}a\,(1,-i)\cdot\mathbf{k}.
\end{aligned}$$

In the matrix form we can represent the Hamiltonian in this basis as

$$\tilde{\mathcal{H}} = \frac{3}{2}at\begin{bmatrix}0 & k_x - ik_y\\ k_x + ik_y & 0\end{bmatrix} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\mathbf{k}.$$

This is an effective Hamiltonian for states close to the Brillouin zone boundary which is exactly the Dirac Hamiltonian in two dimensions. A similar analysis about the other corner reveals

$$\begin{aligned}
\tilde{f}(\mathbf{K}+\mathbf{k}) \approx& -\sqrt{3}a\left(\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)e^{i\frac{4\pi}{3}\left(\frac{3}{4}-\frac{1}{4}\right)} + \left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)e^{i\frac{4\pi}{3}\left(\frac{3}{4}+\frac{1}{4}\right)}\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right)e^{i\frac{2\pi}{3}} + \left(-\frac{\sqrt{3}}{2},-\frac{1}{2}\right)e^{i\frac{4\pi}{3}}\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(-\frac{\sqrt{3}}{2}\left(e^{i\frac{2\pi}{3}} + e^{i\frac{4\pi}{3}}\right), \frac{1}{2}\left(e^{i\frac{2\pi}{3}} - e^{i\frac{4\pi}{3}}\right)\right)\cdot\mathbf{k}\\
=& -\sqrt{3}a\left(-\sqrt{3}\cos\left(\frac{2\pi}{3}\right), i\sin\left(\frac{2\pi}{3}\right)\right)\cdot\mathbf{k}\\
=& -\frac{3}{2}a\,(1,i)\cdot\mathbf{k}.
\end{aligned}$$

Thus the Hamiltonian is $\tilde{\mathcal{H}} = v_{\mathrm{F}}(-\sigma_x k_x + \sigma_y k_y)$. We can write this in a unified way by introducing a so-called valley degree-of-freedom index $\tau_z = \pm 1$.

Polyacetylene Consider a one-dimensional chain with two atoms in the basis separated by a distance a, for which

$$\gamma(q) = 2\cos(qa).$$

By approximating $\zeta = 0$ and setting $E_0 = 0$ we then find

$$E_q = 2t\cos(qa).$$

In the localized basis for the two atoms we have

$$\mathcal{H} = \begin{bmatrix} 0 & -2t\cos(qa) \\ -2t\cos(qa) & 0 \end{bmatrix}.$$

There exists one unique Dirac point at $k_0 = \frac{\pi}{2a}$, and close to this point we have $E_q \approx 2taq$, hence the Hamiltonian in terms of a small displacement k from the Dirac point becomes $\mathcal{H} \approx 2ta\sigma_x k$. This is the Dirac Hamiltonian in one dimension.

Because only one Pauli matrix has been used, more possible non-trivial terms can be included by incorporating the Pauli matrices. The σ_z term might represent some site difference. To obtain the other kind of term we suppose the hopping elements to have some directionality - that is, $t = t_0 \pm \delta t$. The Hamiltonian then becomes

$$\mathcal{H} = \begin{bmatrix} 0 & -2t\cos(qa) - 2i\delta t\sin(qa) \\ -2t\cos(qa) + 2i\delta t\sin(qa) & 0 \end{bmatrix},$$

and close to the Dirac point we have

$$\mathcal{H} \approx 2ta\sigma_x k + 2\delta t\sigma_y.$$

This has the consequence of reducing the energy of the valence band - more specificallye we have

$$\begin{aligned}
\Delta E =& \frac{L}{2\pi}\int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} \mathrm{d}k\, v_\mathrm{F}|k| - \sqrt{v_\mathrm{F}^2k^2 + m_y^2 + m_z^2} \\
=& \frac{L}{\pi}\int_{0}^{\frac{\pi}{2a}} \mathrm{d}k\, v_\mathrm{F}k - \sqrt{v_\mathrm{F}^2k^2 + m_y^2 + m_z^2} \\
=& \frac{L}{2v_\mathrm{F}\pi}\left(\left(\frac{v_\mathrm{F}\pi}{2a}\right)^2 - \frac{v_\mathrm{F}\pi}{2a}\sqrt{\left(\frac{v_\mathrm{F}\pi}{2a}\right)^2 + m_y^2 + m_z^2} - (m_y^2 + m_z^2)\ln\left(\frac{\sqrt{m_y^2 + m_z^2 + \left(\frac{v_\mathrm{F}\pi}{2a}\right)^2} + \frac{v_\mathrm{F}\pi}{2a}}{\sqrt{m_y^2 + m_z^2}}\right)\right),
\end{aligned}$$

where we have introduced the Fermi velocity $v_\mathrm{F} = 2ta$. Defining $m^2 = m_y^2 + m_z^2$ we find in the limit that m becomes small that

$$\Delta E \approx -\frac{Lm^2}{2v_\mathrm{F}\pi}\ln\left(\frac{\sqrt{m_y^2 + m_z^2 + \left(\frac{v_\mathrm{F}\pi}{2a}\right)^2} + \frac{v_\mathrm{F}\pi}{2a}}{\sqrt{m_y^2 + m_z^2}}\right) \approx -\frac{Lm^2}{2v_\mathrm{F}\pi}\ln\left(\frac{v_\mathrm{F}\pi}{|m|a}\right),$$

meaning there is a spontaneous tendency for the system to arrange itself such that this happens. This has the consequence of deforming the lattice, however, and a proper attempt will need to account for both of these effects at the same time.

The Su-Schrieffer-Heeger Model The Su-Schrieffer-Heeger model is an attempt to account for the balance between lattice distortion and dimerization energy minimization. Its Hamiltonian is

$$\mathcal{H} = \sum_j -t(u_{j+1} - u_j)(|j\rangle\langle j+1| + |j+1\rangle\langle j|) + \frac{\lambda}{2}(u_{j+1} - u_j)^2,$$

where the degrees of freedom are the u_j for the lattice points and the electronic states represented by kets. The hopping element t now depends on the lattice structure. We can approximate

$$t(u_{j+1} - u_j) \approx t - \frac{\alpha}{2}(u_{j+1} - u_j)$$

for small displacements. For the dimeric case we may choose coordinates such that $u_j = (-1)^j u$, hence $\delta t = \alpha u$. The total energy change for dimerization is then

$$\Delta E \approx -\frac{Lm^2}{2v_\mathrm{F}\pi}\ln\left(\frac{v_\mathrm{F}\pi}{a\alpha|u|}\right) + 2\lambda N u^2.$$

At small displacements the logarithmic term dominates, meaning dimerization still occurs spontaneously. This is known as Peierls instability.

There was an implicit degeneracy in the above argument with respect to the directionality of the hopping term (or, equivalently, the sign of δt). This corresponds to the dimerization being possible in one of two ways. In excited states, these dimerized variants can be found in different domains of the polymer. Between two such regions is a so-called domain wall, called a soliton. To describe it we will need an energy functional describing the process of dimerization. By introducing the staggered displacement

$$\phi_j = (-1)^j u_j,$$

which is just $\pm u$ in the ground states, we make the anzats

$$E(\phi) = \int \mathrm{d}x \, \frac{1}{2} A \left(\frac{\mathrm{d}\phi}{\mathrm{d}x} \right)^2 - B\phi^2 + C\phi^4.$$

We make the anzats such that there is a non-zero displacement in the ground state and such there is a degeneracy with respect to the sign of ϕ. There must be ϕ-dependent terms because the case of ϕ being constant does not correspond to a constant displacement of the chain. The Euler-Lagrange equation for this theory is

$$-2B\phi + 4C\phi^3 - A\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = 0.$$

Notable is the existence of the ground state

$$\phi = \pm\sqrt{\frac{B}{2C}}.$$

To understand the behavior of such a system we can consider x as a time parameter and ϕ as a coordinate for a particle in a potential $V(q) = Bq^2 - Cq^4$. This potential has two maxima in the ground-state values of ϕ and there exists a solution which moves from one to the other asymptotically with respect to x. This solution is

$$\phi = \sqrt{\frac{B}{2C}} \tanh\left(\sqrt{\frac{B}{A}} x \right).$$

Looking back to the Dirac equation which emerged before dimerization, we see that we will have to extend it according to

$$\mathcal{H} = -i\sigma_x \frac{\mathrm{d}}{\mathrm{d}x} + m(x)\sigma_y,$$

where $m(x) = \alpha\phi(x)$ according to the Hamiltonian, assuming the ground-state energy to be zero. These then decouple, and the solutions in position space are

$$\psi_1 = c_1 e^{\int_0^x \mathrm{d}y m(x)\phi(x)}, \; \psi_2 = c_2 e^{-\int_0^x \mathrm{d}y m(x)\phi(x)}.$$

For a soliton we must enforce $c_1 = 0$, and similarly for an antisolition we enforce $c_2 = 0$. It also turns out that there are no normalizable ground states unless m changes sign somewhere. We define the topological charge

$$Q = \frac{1}{2}\left(\mathrm{sgn}(\infty) - \mathrm{sgn}(-\infty)\right).$$

It turns out that

$$Q = N_2 - N_1,$$

where $N_{1,2}$ is the number of zero modes of each kind.

Note that the Hamiltonian anticommutes with σ_z. This leads to σ_z generating a so-called chiral symmetry. Its eigenstates thus come in pairs with opposite eigenvalues, except in the case where the eigenvalue is zero. This case thus applies to the unpaired bound state.

Fractionalization in the Su-Schrieffer-Heeger Model At the domain wall there exists an atom not bonded to either side. The state localized here has zero energy. Because the number of electrons is fixed, the electron occupying this state must come from somewhere. However, due to the chiral symmetry, this state must come equally from the valence and conduction bands, meaning that half a state is removed from either. How can this be, and what does it mean?

The answer turns out to depend on the particulars of the boundary conditions. Let us first consider periodic boundary conditions with an even number of atoms. This system only permits solitons and antisolitons in pairs. Because there now is one zero mode associated with each member of the pair, the total number of removed states is $2\frac{1}{2} = 1$.

Next, consider periodic boundary conditions with an odd number of atoms. The total number of solitons and antisolitons must be odd. The number of unit cells in this system is a half-integer, so if each unit cell contributes one state, then this final half state must be absorbed by the extra soliton.

Similar, though much more vague, arguments can be made for systems with open boundary conditions.

2 The Hall Effect

The Classical Hall Effect Consider a slab of some conducting material. In the simple kinetic theory of electrons in a conductor the equation of motion is

$$\left\langle \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \right\rangle + \frac{1}{\tau} \langle \mathbf{v} \rangle = \frac{1}{m}\mathbf{F}.$$

Suppose now that the slab were to be immersed in an electric field $E\mathbf{e}_x$ and a magnetic field $B\mathbf{e}_z$. In the steady state we have

$$\frac{1}{\tau} \langle \mathbf{v} \rangle = -\frac{e}{m} \left((E + v_y B)\, \mathbf{e}_x + (E_y - v_x B)\, \mathbf{e}_y \right).$$

We impose boundary conditions such that there is no net current flow in the y direction. In the case of $B = 0$ we then find the conductivity $\sigma = \frac{ne^2\tau}{m}$. This will naturally also be the case for non-zero B as $v_y = 0$ in the steady state. This also means that $v_x = -\frac{e\tau}{m}E$, and we find

$$E_y = -\frac{e\tau}{m}EB.$$

The steady-state current is now

$$\mathbf{J} = -ne \langle \mathbf{v} \rangle = \frac{ne^2\tau}{m}\mathbf{E}.$$

On tensor form we have

$$E_i = \rho_i{}^j J_j.$$

Evidently the resistivity tensor has diagonal components $\frac{1}{\sigma} = \frac{m}{ne^2\tau}$, but the addition of the magnetic field also provides an off-diagonal component

$$\rho_y{}^x = -\frac{B}{ne}.$$

This phenomenon is termed Hall resistance or the Hall effect. From this we define the Hall coefficient

$$R_{\mathrm{H}} = \frac{\rho_y{}^x}{B} = -\frac{1}{ne}.$$

Failures of the Hall Effect The predictions based on these calculations turned out to give correct predictions for many materials, but some materials exhibited a reverse Hall effect in having a positive Hall coefficient, a property unexplainable by these purely classical arguments. The key point here is the assumption that the charge carriers have negative charge, an assumption which turns out to not be true in all materials.

Charged Particles in Magnetic Fields For studying the quantum Hall effect we will need to study the physics of classical particles in magnetic fields. We recall that the Lagrangian is

$$\mathcal{L} = \frac{1}{2}m\dot{x}^i x_i - q\left(\phi(x) - \dot{x}^i A_i\right).$$

The canonical momenta are

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i} = m\dot{x}_i + qA_i,$$

hence the Hamiltonian is

$$\begin{aligned}\mathcal{H} =& p_i\dot{x}^i - \mathcal{L} \\ =& \frac{1}{m}p_i(p^i - qA^i) - \frac{1}{2m}(p^i - qA^i)(p_i - qA_i) + q\left(\phi(x) - \frac{1}{m}(p^i - qA^i)A_i\right) \\ =& \frac{1}{2m}(p^i - qA^i)(p_i - qA_i) + q\phi(x).\end{aligned}$$

Note that the canonical momenta are not the physical momenta.

Consider now a two-dimensional system with $\mathbf{B} = B\mathbf{e}_z$. A choice of $\mathbf{A}$ is then $\mathbf{A} = -xB\mathbf{e}_y$. For this case we find that p_x is a component of the physical momentum and

$$\mathcal{H} = \frac{1}{2m}\left(p_x^2 + (p_y + qBx)^2\right) + q\phi(x).$$

For $\phi = 0$ this problem is separable and we can construct eigenstates of the Hamiltonian by starting with eigenstates of p_y. In x we may then introduce

$$\frac{1}{2}m\omega_c^2 = \frac{1}{2m}\cdot q^2B^2,\ x' = x + \frac{p_y}{qB} = x \pm k_y\ell^2,$$

where we in the last step introduced the magnetic length $\ell = \sqrt{\frac{\hbar}{|q|B}}$. The choice of sign depends on the charge of q, which we will take to be positive. The resulting Hamiltonian is then that of a shifted harmonic oscillator. Its energy levels are

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_c.$$

Note that each level is highly degenerate due to the k_y freedom.

We can now try to confine the problem by imposing periodic boundary conditions. This can only be done in the y direction due to the phase difference at either end in the x direction, but because the solutions with respect to x are Gaussian, the states can be considered to be confined. The set of states that are localized within the sample are then those with $0 < k_y < \frac{L_x}{\ell^2}$. With the k_y spread evenly out at distances of $\frac{L_y}{2\pi}$ between neighboring values, the degeneracy of each energy level is then

$$N \approx \frac{L_y}{2\pi}\cdot\frac{L_x}{\ell^2} = \frac{A}{2\pi\ell^2},$$

which is the number of quanta of flux $2\pi\ell^2 B = \frac{h}{e}$ contained in the sample. That is, each state in every Landau level is paired with one flux quantum. Thus, introducing the filling factor

$$\nu = \frac{N_e}{N_\Phi},$$

which is the ratio of electrons in the sample to flux quanta, is an integer, the ground state of the system has the ν lowest Landau levels filled and all higher levels are empty, producing a band gap in the bulk.

Evidently there is no current in the x-direction, but what about the y direction? The solutions contain a factor $e^{ik_y y}$, so there might be some. We compute this by only considering the lowest Landau level, equivalent

to assuming the energy separation to be large. The physical momentum being $P_i = p_i - qA_i$ we have

$$\begin{aligned}
I_y =& \int \mathrm{d}^2\mathbf{r}\, \langle J_y \rangle \\
=& \frac{qL_y}{m} \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{1}{L_y} \sqrt{\frac{m\omega_\mathrm{c}}{\pi\hbar}} e^{-ik_y y} e^{-\frac{m\omega_\mathrm{c}}{2\hbar}(x+k_y\ell^2)^2} (-i\hbar\partial_y + qBx) e^{ik_y y} e^{-\frac{m\omega_\mathrm{c}}{2\hbar}(x+k_y\ell^2)^2} \\
=& q\sqrt{\frac{\omega_\mathrm{c}}{\pi m\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x\, (\hbar k_y + qBx) e^{-\frac{m\omega_\mathrm{c}}{\hbar}(x+k_y\ell^2)^2},
\end{aligned}$$

which vanishes identically. This is not surprising as k_y only determines the center of the harmonic oscillator.

Reobtaining the Classical Hall Effect Let us now add an electric field using $\phi = -Ex$. The choice of $\mathbf{A}$ is still appropriate, and the Hamiltonian is

$$\begin{aligned}
\mathcal{H} &= \frac{1}{2m}\left(p_x^2 + (p_y + qBx)^2\right) - qEx \\
&= \frac{1}{2m}\left(p_x^2 + p_y^2 + 2qBxp_y + q^2B^2x^2 - 2mqEx\right).
\end{aligned}$$

This is still separable in the y direction, so we reintroduce the magnetic length to find

$$\begin{aligned}
\mathcal{H} =& \frac{1}{2m}\left(p_x^2 + \left(qBx + p_y - \frac{mE}{B}\right)^2 - \left(p_y - \frac{mE}{B}\right)^2 + p_y^2\right) \\
=& \frac{1}{2m}p_x^2 + \frac{1}{2}m\omega_\mathrm{c}^2\left(x + k_y\ell^2 - \frac{mE}{qB^2}\right)^2 - \frac{1}{2m}\left(\frac{m^2E^2}{B^2} - \frac{2mEp_y}{B}\right) \\
=& \frac{1}{2m}p_x^2 + \frac{1}{2}m\omega_\mathrm{c}^2(x - X)^2 + \frac{1}{2}m\left(\frac{E}{B}\right)^2 - qEX,
\end{aligned}$$

which is an oscillator Hamiltonian in the new peak position

$$X = \frac{mE}{qB^2} - k_y\ell^2.$$

Next there is a term that looks like a kinetic energy, which we will return to, and a linear term in the peak position. This term actually produces a non-trivial group velocity, as it depends on k_y, and we have

$$v_\mathrm{g} = \frac{1}{\hbar}\partial_{k_y}\epsilon_{k_y,n} = -\frac{qE}{\hbar}\cdot -\ell^2 = \frac{E}{B}.$$

Note that this implies the presence of a current in the y direction. The kinetic energy term can thus be associated with the drift owed to the electric field. Thus we have recaptured the essential features of the classical Hall effect.

Note that the electric field lifts the degeneracy of the individual levels but introduces degeneracy between levels. States cannot decay between levels unless there exists disorder or phonons on which the states can scatter.

The Integer Quantum Hall Effect Suppose you were to make the sample finite by introducing a potential $V(x)$ that screens off a region of space. We can surmise that

$$\psi = \frac{1}{\sqrt{L_y}} e^{ik_y y} f_{k_y}(x)$$

for some set of functions f_{k_y}. The group velocity

$$v_y = \frac{1}{\hbar}\partial_{k_y}E \approx \frac{\ell^2}{\hbar}\frac{\mathrm{d}V}{\mathrm{d}x}.$$

By the confining nature of the potential the group velocity thus has different directions in either end of the sample. The semiclassical interpretation of this is that states in the bulk move in cyclotron motion and states on the edge bounce on the potential so as to move along the edge.

The net current per Landau level is approximately

$$I = \frac{q}{L_y}\frac{L_y}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k_y \, \frac{1}{\hbar}\partial_{k_y} E n_{k_y},$$

where n_{k_y} is the probability of a given state being occupied. In the limit of zero temperature we find

$$I = \frac{q}{h}\Delta\mu,$$

where $\Delta\mu$ is the change in chemical potential between either edge. Defining the Hall voltage according to $V_{\mathrm{H}} = \frac{\Delta\mu}{q}$ we find $I = \frac{\nu q^2}{h} V_{\mathrm{H}}$. This implies a quantized Hall resistivity.

The Role of Disorder The above is almost sufficient to explain the quantum Hall effect. While we have seen that the periodic vanishing of the band gap causes it, a perfect sample would only exhibit this effect momentarily. Instead the existence of defects creates states between the Landau levels that are occupied before the band gap vanishes again, causing the Hall resistance to persist across a range of magnetic fields.

Quantum Hall Effect - a Percolation Picture Using a semiclassical argument, we can also arrive at the quantum hall effect using a semiclassical argument. The idea is the following: Consider a semiconductor in a strong magnetic field and suppose there are some small impurities creating a randomly varying electric field. This will cause the semiconductor to have some potential landscape, and the states will be localized about contours of constant field. The filling of states will thus act as if the potential landscape is filled with water. At low filling most of the landscape is "dry land", and no current can propagate. As the filling factor increases, a first phase transition arises when the shoreline percolates to the other side. Successive increases in filling causes further phase transition, implying a quantized conductivity.

3 Topology in Condensed Matter

Berry Phase Consider a Hamiltonian described by some set of parameters R, which may be time dependent. For each value of R we have a set of eigenstates

$$\mathcal{H}(R)\left|n(R)\right\rangle = E_n(R)\left|n(R)\right\rangle.$$

If the spectrum is discrete and non-degenerate for all R, the adiabatic theorem tells us that if R is varied such that the Hamiltonian changes sufficiently slowly, a state which is initialized to an eigenstate at $t = 0$ will evolve to a corresponding eigenstate at a later time. In the general case we have

$$\left|\psi_n(t)\right\rangle = e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_0^t \mathrm{d}\tau E_n(\tau)} \left|n(R(t))\right\rangle.$$

If the Hamiltonian has explicit time dependence, the former factor is different from unity. Its exponent is the so-called Berry phase. Inserting this into the Schrödinger equation we find

$$\begin{aligned}\mathcal{H}\left|\psi_n(t)\right\rangle =& E_n\left|\psi_n(t)\right\rangle \\ =& i\hbar e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_0^t \mathrm{d}\tau E_n(\tau)} \left(i\frac{\mathrm{d}\gamma_n}{\mathrm{d}t}\left|n(R(t))\right\rangle - \frac{i}{\hbar}E_n\left|n(R(t))\right\rangle + \frac{\partial}{\partial t}\left|n(R(t))\right\rangle\right),\end{aligned}$$

and taking the inner product with $\left|\psi_n(t)\right\rangle$ we have

$$\frac{\mathrm{d}\gamma_n}{\mathrm{d}t}\left|n(R(t))\right\rangle = i\left\langle n(R(t))\right|\frac{\partial}{\partial t}\left|n(R(t))\right\rangle.$$

The solution is

$$\gamma_n = i\int_0^t \mathrm{d}\tau \, \left\langle n(R(\tau))\right|\frac{\partial}{\partial \tau}\left|n(R(\tau))\right\rangle.$$

Noting that

$$\frac{\partial}{\partial\tau}\left|n(R(\tau))\right\rangle = \frac{\mathrm{d}R}{\mathrm{d}\tau}\cdot\vec{\boldsymbol{\nabla}}_R\left|n(R)\right\rangle$$

we can define the Berry connection

$$A_n = i\left\langle n(R)\right|\vec{\boldsymbol{\nabla}}_R\left|n(R)\right\rangle$$

and find

$$\gamma_n = i\int_C \mathrm{d}R\cdot A_n.$$

C is now the orbit in parameter space traversed during the time evolution.

Is the Berry phase really of interest? It might not seem so. Making a phase change

$$\left|n(R)\right\rangle \to e^{i\zeta(R)}\left|n(R)\right\rangle$$

we have

$$A_n \to A_n - \vec{\boldsymbol{\nabla}}_R\zeta.$$

Thus we can apparently remove the Berry phase entirely. For closed orbits in parameter space, however, the Berry phase is independent of this transformation. Thus it might be of physical importance.

Due to Stokes' theorem the line integral of the Berry connection about some closed path is related to the surface integral of the differential of some antisymmetric tensor. That is, we can define the Berry curvature

$$\omega_{n,\mu\nu} = \partial_\mu A_{n,\nu} - \partial_\nu A_{n,\mu},$$

which satisfies

$$\int_{\partial S}\mathrm{d}R\cdot A_n = \frac{1}{2}\int_S \mathrm{d}R_\mu\wedge\mathrm{d}R_\nu\,\omega_{n,\mu\nu}.$$

In the particular case of three dimensions the Berry curvature can be expressed in terms of a pseudomagnetic field

$$\mathbf{b}_n = i\left(\vec{\boldsymbol{\nabla}}_{\mathbf{R}}\left|n(\mathbf{r})\right\rangle\right)^\dagger\times\vec{\boldsymbol{\nabla}}_{\mathbf{R}}\left|n(\mathbf{r})\right\rangle.$$

The Aharanov-Bohm Effect Consider two wires passing a region with a very localized magnetic field, one wire being wrapped around this region. This will turn out to be a case where the Berry phase has a physical consequence, as one can measure a quantum phase difference between electrons passing through either wire.

To study this, we will consider a charged particle confined to some box with one corner at $\mathbf{R}_0$ by a potential $V(\mathbf{r}-\mathbf{R}_0)$. We will study this by adiabatically moving the box around in space. If the box never enters the region with magnetic field, we may take

$$\mathbf{A} = \frac{\Phi_0}{2\pi}\vec{\boldsymbol{\nabla}}\chi.$$

Supposing the ground state of the electron in the box is $\xi(\mathbf{r}-\mathbf{R}_0)$ in the absence of the magnetic field, we can find a normalized eigenfunction $e^{i\phi}\xi(\mathbf{r}-\mathbf{R}_0)$ by the gauge transformation anzats

$$(\mathbf{p}-q\mathbf{A})e^{i\phi}\xi(\mathbf{r}-\mathbf{R}_0) = e^{i\phi}\mathbf{p}\xi(\mathbf{r}-\mathbf{R}_0).$$

We find

$$(\mathbf{p}-q\mathbf{A})e^{i\phi}\xi(\mathbf{r}-\mathbf{R}_0) = e^{i\phi}\mathbf{p}\xi(\mathbf{r}-\mathbf{R}_0) - \left(i\hbar\vec{\boldsymbol{\nabla}}\phi + q\mathbf{A}\right)\xi(\mathbf{r}-\mathbf{R}_0),$$

hence

$$\phi = -\frac{q}{\hbar}\int_{\mathbf{R}_0}^{\mathbf{r}}\mathrm{d}\mathbf{r}'\cdot\mathbf{A} = -\frac{2\pi}{\Phi_0}\int_{\mathbf{R}_0}^{\mathbf{r}}\mathrm{d}\mathbf{r}'\cdot\mathbf{A} = \chi(\mathbf{R}_0)-\chi(\mathbf{r}).$$

There is still an ambiguity in the choice of χ, as well as the possibility to add an $\mathbf{R}_0$-dependent phase θ to the wavefunction. We now fix them by imposing that

$$\psi(\mathbf{r}) = e^{i(\theta+\chi(\mathbf{R}_0)-\chi(\mathbf{r}))}\xi(\mathbf{r}-\mathbf{R}_0)$$

be real at some point $\boldsymbol{\Delta}$ as measured within the box. Assuming ξ to be real and positive at $\boldsymbol{\Delta}$, we require

$$\theta = \chi(\mathbf{R}_0+\boldsymbol{\Delta}) - \chi(\mathbf{R}_0),$$

hence

$$\psi(\mathbf{r}) = e^{i(\chi(\mathbf{R}_0+\boldsymbol{\Delta})-\chi(\mathbf{r}))}\xi(\mathbf{r}-\mathbf{R}_0).$$

How does this tie in to the Berry phase? $\mathbf{R}_0$ now plays the role of the parameters in the Hamiltonian. For the ground state we then have

$$\begin{aligned}
\mathbf{A} =& i\int \mathrm{d}^3\mathbf{r}\,\psi^\star\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\psi \\
=& i\int \mathrm{d}^3\mathbf{r}\,e^{-i\chi(\mathbf{R}_0+\boldsymbol{\Delta})}\xi(\mathbf{r}-\mathbf{R}_0)\left(ie^{i\chi(\mathbf{R}_0+\boldsymbol{\Delta})}\xi(\mathbf{r}-\mathbf{R}_0)\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\chi(\mathbf{R}_0+\boldsymbol{\Delta}) + e^{i\chi(\mathbf{R}_0+\boldsymbol{\Delta})}\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\xi(\mathbf{r}-\mathbf{R}_0)\right) \\
=& i\int \mathrm{d}^3\mathbf{r}\,i\xi^2(\mathbf{r}-\mathbf{R}_0)\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\chi(\mathbf{R}_0+\boldsymbol{\Delta}) + \xi(\mathbf{r}-\mathbf{R}_0)\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\xi(\mathbf{r}-\mathbf{R}_0) \\
=& -\frac{2\pi}{\Phi_0}\mathbf{A}(\mathbf{R}_0+\boldsymbol{\Delta}) + \frac{1}{2}i\int \mathrm{d}^3\mathbf{r}\,\vec{\boldsymbol{\nabla}}_{\mathbf{R}_0}\xi^2(\mathbf{r}-\mathbf{R}_0),
\end{aligned}$$

having used the fact that the state is normalized. The latter term is the integral of a total derivative, which yields no contribution as the wavefunction vanishes at infinity. Thus, by slowly moving the electron we have

$$\gamma = -\int \mathrm{d}\mathbf{R}_0 \cdot \frac{2\pi}{\Phi_0}\mathbf{A}(\mathbf{R}_0+\boldsymbol{\Delta}).$$

Taking the displacement $\boldsymbol{\Delta}$ to be small, the phase difference between two wires is thus

$$\delta\phi = -2\pi\frac{\Phi}{\Phi_0},$$

where Φ is the total enclosed flux. Note that at no point along the path of the electron did it have to interact with the magnetic field, and yet this phase difference arises. This effect is thus a pure quantum effect, and is termed the Aharanov-Bohm effect.

Spin-$\frac{1}{2}$ Berry Phase Consider a single spin $\frac{1}{2}$ in an external field. The Hamiltonian is

$$\mathcal{H} = h^i\sigma_i.$$

Writing $\mathbf{h} = h(\sin(\theta)\cos(\phi),\ \sin(\theta)\sin(\phi), \cos(\theta))$, we note that the eigenstates are simultaneous eigenstates of the spin projection along the direction of $\mathbf{h}$. In the σ_3 basis they thus solve

$$\begin{bmatrix} \cos(\theta)\mp 1 & \sin(\theta)\cos(\phi) - i\sin(\theta)\sin(\phi) \\ \sin(\theta)\cos(\phi) + i\sin(\theta)\sin(\phi) & -\cos(\theta)\mp 1 \end{bmatrix}\mathbf{x}_\pm = \mathbf{0}.$$

The matrix can be simplified to

$$\begin{bmatrix} \cos(\theta)\mp 1 & \sin(\theta)e^{-i\phi} \\ \sin(\theta)e^{i\phi} & -\cos(\theta)\mp 1 \end{bmatrix}.$$

The components then satisfy

$$(\cos(\theta)\mp 1)x_{\pm,1} = -\sin(\theta)e^{-i\phi}x_{\pm,2}.$$

The eigenstates in this representation are then

$$|-\rangle = \begin{bmatrix} -\sin\left(\frac{\theta}{2}\right)e^{-i\phi} \\ \cos\left(\frac{\theta}{2}\right) \end{bmatrix},\ |+\rangle = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right)e^{-i\phi} \\ \sin\left(\frac{\theta}{2}\right) \end{bmatrix}.$$

While the eigenvalues depend on h, the structure of the states depend on θ and ϕ, which parametrize S^2. For the ground state we then have

$$\begin{aligned} A_{-,\theta} &= i\langle -|\partial_\theta|-\rangle = 0, \\ A_{-,\phi} &= i\langle -|\partial_\phi|-\rangle = i\left(-i\sin^2\left(\frac{\theta}{2}\right)\right) = \sin^2\left(\frac{\theta}{2}\right). \end{aligned}$$

The Berry curvature is then

$$\omega_{+,\theta\phi} = \frac{1}{2}\sin(\theta),$$

and the Berry flux through a small surface is half the subtended solid angle.

Berry Phase and Bloch Bands A slight generalization of Bloch states can be made for systems in a uniform magnetic field. In a periodic potential the Hamiltonian is invariant under translations by lattice vectors. Generally, in a magnetic field, we have

$$T_{\mathbf{a}}\mathcal{H}T_{\mathbf{a}}^\dagger = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{r}+\mathbf{a})\right)^2 + V(\mathbf{r}).$$

In a uniform field we have

$$\mathbf{A}(\mathbf{r}+\mathbf{a}) - \mathbf{A}(\mathbf{r}) = \vec{\boldsymbol{\nabla}} f_{\mathbf{a}}(\mathbf{r}).$$

An extra gauge transformation $e^{i\phi_{\mathbf{a}}(\mathbf{r})}$ will certainly leave the potential invariant. We find

$$\left(\mathbf{p} - q\mathbf{A}(\mathbf{r}+\mathbf{a})\right)e^{-i\phi_{\mathbf{a}}(\mathbf{r})} = e^{-i\phi_{\mathbf{a}}(\mathbf{r})}\left(\mathbf{p} - \vec{\boldsymbol{\nabla}}\phi_{\mathbf{a}}(\mathbf{r}) - q\mathbf{A}(\mathbf{r}+\mathbf{a})\right),$$

so we require

$$\vec{\boldsymbol{\nabla}}\phi_{\mathbf{a}}(\mathbf{r}) + q\mathbf{A}(\mathbf{r}+\mathbf{a}) = q\mathbf{A}(\mathbf{r}),$$

with the solution

$$\phi_{\mathbf{a}} = -qf_{\mathbf{a}}.$$

The operator

$$T_{\mathbf{a}} = e^{-iqf_{\mathbf{a}}(\mathbf{r})}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{a}}$$

thus leaves the Hamiltonian invariant. The Bloch basis is still applicable due to the translation symmetry of the system. Having established this we can now take $\mathbf{k}$ to be a parameter of the Hamiltonian in the Bloch basis.

Consider now such a system in a weak uniform magnetic field. This gives rise to a perturbation term $-q\mathbf{E}\cdot\mathbf{r}$ in the Hamiltonian. The first-order change in the state is then

$$\delta|n,\mathbf{k}\rangle = -q\mathbf{E}\cdot\sum_{m,\mathbf{q}}|m,\mathbf{q}\rangle\frac{\langle m,\mathbf{q}|\mathbf{r}|n,\mathbf{k}\rangle}{E_{n,\mathbf{k}} - E_{m,\mathbf{q}}}.$$

As the involved states are eigenstates of the Hamiltonian we have

$$\langle m,\mathbf{q}|\mathbf{r}\mathcal{H}|n,\mathbf{k}\rangle - \langle m,\mathbf{q}|\mathcal{H}\mathbf{r}|n,\mathbf{k}\rangle = \left(E_{n,\mathbf{k}} - E_{m,\mathbf{q}}\right)\langle m,\mathbf{q}|\mathbf{r}|n,\mathbf{k}\rangle.$$

Because $\mathbf{A}$ is a function of position and $[\mathbf{r},\mathbf{p}]$ is a multiple of identity we have

$$[\mathbf{r},\mathcal{H}] = \frac{1}{2m}\left[\mathbf{r},\mathbf{p}^2\right] = \frac{1}{2m}\left(\mathbf{p}\cdot[\mathbf{r},\mathbf{p}] + [\mathbf{r},\mathbf{p}]\cdot\mathbf{p}\right) = \frac{i\hbar}{m}\mathbf{p}.$$

We then find

$$\delta\left|n,\mathbf{k}\right\rangle = -i\hbar q\mathbf{E}\cdot\sum_{m,\mathbf{q}}\left|m,\mathbf{q}\right\rangle\frac{\langle m,\mathbf{q}|\mathbf{v}|n,\mathbf{k}\rangle}{(E_{n,\mathbf{k}}-E_{m,\mathbf{q}})^2}.$$

When computing the matrix element, the contributions from different unit cells differ by a factor $e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}}$. Thus they vanish unless $\mathbf{q}=\mathbf{k}$. We then have

$$\delta\left|u_{n,\mathbf{k}}\right\rangle = -iq\mathbf{E}\cdot\sum_{m\neq n}\left|u_{m,\mathbf{k}}\right\rangle\frac{\langle u_{m,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle}{(E_{n,\mathbf{k}}-E_{m,\mathbf{k}})^2}.$$

We then have to first order

$$\begin{aligned}\langle\mathbf{v}\rangle =&\frac{1}{\hbar}\left(\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle+\frac{2}{\hbar}\,\mathrm{Re}(\,\langle\delta u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle)\right)\\ =&\frac{1}{\hbar}\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\epsilon_{n,\mathbf{k}}+\mathbf{v}_{\mathrm{a}}(n,\mathbf{k}).\end{aligned}$$

The new term is called the anomalous velocity. We have

$$\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|\delta u_{n,\mathbf{k}}\rangle = -\,iq\sum_{m\neq n}\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{m,\mathbf{k}}\rangle\,\mathbf{E}\cdot\frac{\langle u_{m,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle}{(E_{n,\mathbf{k}}-E_{m,\mathbf{k}})^2}.$$

Its complex conjugate is

$$\langle\delta u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle = iq\sum_{m\neq n}\langle u_{m,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle\,\mathbf{E}\cdot\frac{\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{m,\mathbf{k}}\rangle}{(E_{n,\mathbf{k}}-E_{m,\mathbf{k}})^2}.$$

Thus

$$\mathbf{v}_{\mathrm{a}}(n,\mathbf{k}) = \frac{iq}{\hbar}\mathbf{E}\cdot\sum_{m\neq n}\frac{\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{m,\mathbf{k}}\rangle\,\langle u_{m,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle-\langle u_{m,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{n,\mathbf{k}}\rangle\,\langle u_{n,\mathbf{k}}|\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\mathcal{H}|u_{m,\mathbf{k}}\rangle}{(E_{n,\mathbf{k}}-E_{m,\mathbf{k}})^2}.$$

It can be shown that the sum is equal to the Berry curvature, hence

$$v_{\mathrm{a},i}(n,\mathbf{k}) = \frac{iq}{\hbar}E^j\omega_{n,ji} = \frac{iq}{\hbar}\varepsilon_{ijk}E^j b_n^k.$$

Noting that perturbation theory creates semiclassical motion, we can write

$$\mathbf{v}_{\mathrm{a}}(n,\mathbf{k}) = -\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\times\mathbf{b}_n.$$

For a wave packet we can then show that

$$\hbar\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t} = \vec{\boldsymbol{\nabla}}_{\mathbf{k}}\epsilon_{n,\mathbf{k}}-\hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\times\mathbf{b}_n,\ \ \hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = -\vec{\boldsymbol{\nabla}}_{\mathbf{R}}V+q\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\times\mathbf{B}.$$

Using this, we can consider the effect of time reversal. Evidently it reverses $\mathbf{v}$ and $\mathbf{k}$, which must imply $\mathbf{b}_n(\mathbf{k}) = -\mathbf{b}_n(-\mathbf{k})$. Under parity we instead have that $\mathbf{v}$, $\mathbf{k}$ and $\mathbf{E}$ are reversed, implying $\mathbf{b}_n(\mathbf{k}) = \mathbf{b}_n(-\mathbf{k})$. For a Hamiltonian with both symmetries, the Berry curvature must therefore be zero, and so must the anomalous velocity be.

Quantization of Hall Conductance In the presence of a magnetic field, time reversal symmetry in a semiconductor is broken. We have for a filled band

$$\mathbf{J}_n = -\frac{e}{A}\sum_{\mathbf{k}}\mathbf{v}_{\mathrm{a}}(n,\mathbf{k}) = \sigma_{xy}^n\mathbf{e}_z\times\mathbf{E},$$

allowing us to identify

$$\sigma_{xy}^n = \frac{e^2}{\hbar A}\sum_{\mathbf{k}}\mathbf{b}_n(\mathbf{k}) \approx \frac{e^2}{h}\int\mathrm{d}^2\mathbf{k}\,b_n(\mathbf{k}),$$

as the Berry curvature in this case always points in the z-direction. This is proportional to the total Berry curvature.

To discuss the implications of this, we first introduce the result

$$\frac{1}{2\pi}\int_M \mathrm{d}A\, K = 2 - 2g_M$$

for a closed two-dimensional surface. K is the curvature of the surface and g_M is its genus. In the case of the Berry curvature, the point $\mathbf{k} = \mathbf{0}$ may not be included in the parameter domain as the Hamiltonian is not gapped there, thus there are only two topologically distinct classes of parameter surfaces allowed. We have

$$\frac{1}{2\pi}\int \mathrm{d}^2\mathbf{k}\,\omega_n(\mathbf{k}) = \frac{1}{2\pi}\int \mathrm{d}\mathbf{k}\cdot\mathbf{A}_n(\mathbf{k}) = \frac{i}{2\pi}\int \mathrm{d}\mathbf{k}\cdot\int \mathrm{d}^2\mathbf{r}\, u^\star_{n,\mathbf{k}}\vec{\boldsymbol{\nabla}}_{\mathbf{k}} u_{n,\mathbf{k}}.$$

Note that in two dimensions we can use the Berry curvature directly. The $\mathbf{k}$ integral is about the boundary of the first Brillouin zone. Now, because we consider a general system, it may be the case that opposite edges of the Brillouin zone differ by a phase factor. The Bloch function is generally modified according to

$$u_{n,\mathbf{k}} = e^{-i(\theta_n(\mathbf{k})+\mathbf{G}\cdot\mathbf{r})}u_{n,\mathbf{k}+\mathbf{G}}.$$

If θ_n is independent of $\mathbf{k}$, the gradients at opposite edges are the same, meaning their contributions cancel. Assuming the Bloch functions to be normalized we find in the general case that

$$\frac{1}{2\pi}\int \mathrm{d}^2\mathbf{k}\,\omega_n(\mathbf{k}) = \frac{1}{2\pi}\int \mathrm{d}\mathbf{k}\cdot\vec{\boldsymbol{\nabla}}_{\mathbf{k}}\theta_n.$$

Because we are integrating about a loop, this must be a multiple of 2π - in other words,

$$\frac{1}{2\pi}\int \mathrm{d}^2\mathbf{k}\,\omega_n(\mathbf{k})$$

is an integer known as the first Chern number c_n. This leads to the conductivity being quantized.

The Haldane Model The Haldane model is a simple model of two bands with non-zero Chern number. This is obtained by starting with a two-level model for the honeycomb lattice and opening a band gap and breaking time reversal symmetry. The Hamiltonian we use is

$$\mathcal{H} = \begin{bmatrix} m & -tf(\mathbf{k}) \\ -tf^\star(\mathbf{k}) & -m \end{bmatrix}.$$

The eigenvalues are $\pm\sqrt{m^2 + t^2|f(\mathbf{k})|^2}$, using the same f as for the honeycomb lattice. This opens up a band gap of size $2m$ at the corners of the Brillouin zone.

To study the model, assume m to be small. The Hamiltonian is

$$\mathcal{H} = v_\mathrm{F}(\tau_z\sigma_x k_x + \sigma_y k_y) + m\sigma_z.$$

This doesn't break time reversal symmetry, however, and cannot produce topologically non-trivial bands. To achieve this we add the τ_z to the mass term as well. This can be achieved by using a purely imaginary hopping amplitude internally in the sublattice.

Weird Unexplained Stuff Consider a two-dimensional electron gas on a cylindrical shell. Suppose that we add a magnetic flux through the pipe which is zero at $t = 0$ and Φ_0 at $t = T$. The field along the original y-coordinate will then be

$$E_y = \frac{1}{L_y}\frac{\mathrm{d}\Phi}{\mathrm{d}t}.$$

The charge drift is

$$-e\int_0^T \mathrm{d}t\int_0^{L_y}\mathrm{d}y\, J_x = \sigma_{n,xy}\Phi_0 = C_n e.$$

This means that the Hamiltonian is approximately flux independent.

4 Superconductors

Superconductors Superconductors distinguish themselves from ideal conductors in that they repel magnetic flux. This is their defining trait

The first non-phenomenological theory of superconductivity was a Ginzburg-Landau theory of the form

$$F = \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2} n(\vec{\boldsymbol{\nabla}}\theta + q\mathbf{A})^2 + \frac{1}{2}(\vec{\boldsymbol{\nabla}} \times \mathbf{A})^2.$$

The field θ is the phase of some complex field. An important feature of this model was exactly that the magnitude of the complex field did not enter. It was thought by Ginzburg and Landau that this field was related to the wavefunction somehow. By introducing a current

$$\mathbf{J} = \frac{iq\gamma}{2}(\psi^\star \vec{\boldsymbol{\nabla}}\psi - \psi \vec{\boldsymbol{\nabla}}\psi^\star) - \gamma q^2 |\psi|^2 \mathbf{A}$$

and combining it with Maxwell's equation $\vec{\boldsymbol{\nabla}} \times \mathbf{B} = \mathbf{J}$ and the requirement that $|\psi|^2 = n_S$ we find

$$\vec{\boldsymbol{\nabla}} \times \mathbf{B} = -n_S q \left(\vec{\boldsymbol{\nabla}}\theta + \gamma q \mathbf{A} \right),$$

and inserting this into the free energy we find

$$F = \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2} \frac{n}{n_S} \frac{1}{q n_S} (\vec{\boldsymbol{\nabla}} \times \mathbf{B})^2 + \frac{1}{2}\mathbf{B}^2.$$

In the limit of $n \to n_S$ the field describing the minimum is given by the London equation

$$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}} \times \mathbf{B} + \frac{1}{\lambda^2}\mathbf{B} = \mathbf{0},$$

with the London penetration depth $\lambda = \frac{1}{\sqrt{q n_S}}$. The solutions of this equation generally vanish quickly in the bulk, as do the corresponding currents. Thus the Meissner effect is reproduced.

The next attempt used a full variation of ψ with a free energy

$$F = \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2} \left| (\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi \right|^2 - a|\psi|^2 + \frac{1}{2} b |\psi|^4 + \frac{1}{2}(\vec{\boldsymbol{\nabla}} \times \mathbf{A})^2.$$

In the absence of external fields, the constant field that minimizes the free energy is

$$|\psi| = \sqrt{\frac{a}{b}}.$$

In this state the system is superconducting. The condensation energy (density) of the superconductor is

$$\Delta F = F(|\psi| = 0) - F\left(\sqrt{\frac{a}{b}} \right) = \frac{1}{2}\frac{a^2}{b}.$$

This can be expressed in terms of a critical magnetic field $H_\mathrm{c} = \frac{a}{\sqrt{b}}$.

Let us now study the configurations that minimize the free energy. Varying with respect to $\psi^\star$ we have

$$\delta F = \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2} (\vec{\boldsymbol{\nabla}} - iq\mathbf{A})\, \delta\psi^\star \cdot (\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi + \left(b|\psi|^2\psi - a\psi \right) \delta\psi^\star .$$

To shorten this slightly we define $\mathbf{v} = (\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi$, and find

$$\delta F = \int \mathrm{d}^3\mathbf{r}\, \frac{1}{2} \mathbf{v} \cdot \vec{\boldsymbol{\nabla}}(\delta\psi^\star) + \left(b|\psi|^2\psi - a\psi - \frac{1}{2} iq \mathbf{v} \cdot \mathbf{A} \right) \delta\psi^\star .$$

Integrating by parts we find

$$\delta F = \int \mathrm{d}^3\mathbf{r} \left(b|\psi|^2\psi - a\psi - \frac{1}{2}iq\mathbf{v}\cdot\mathbf{A} - \frac{1}{2}\vec{\boldsymbol{\nabla}}\cdot\mathbf{v} \right) \delta\psi^\star + \frac{1}{2}\int \mathrm{d}\mathbf{S}\cdot\delta\psi^\star\,\mathbf{v}.$$

The surface term is zero if

$$(\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi\cdot\mathbf{n} = 0$$

on the surface of the superconductor. The remaining term is zero if

$$b|\psi|^2\psi - a\psi - \frac{1}{2}iq\mathbf{A}\cdot(\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi - \frac{1}{2}\vec{\boldsymbol{\nabla}}\cdot(\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi = 0.$$

A slight rearrangement yields

$$\frac{1}{2}(-i\vec{\boldsymbol{\nabla}} + q\mathbf{A})^2\psi + b|\psi|^2\psi - a\psi = 0.$$

Next, to vary with respect to the magnetic field we write

$$(\vec{\boldsymbol{\nabla}}\times\mathbf{A})^2 = T^{ijkm}\partial_i A_j \partial_k A_m$$

and

$$F = \int \mathrm{d}^3\mathbf{r}\,\frac{1}{2}g^{ij}(\partial_i - iqA_i)\psi^\star(\partial_j + iqA_j)\psi + \frac{1}{2}T^{ijkm}\partial_i A_j\partial_k A_m.$$

We then have

$$F = \int \mathrm{d}^3\mathbf{r}\,\frac{1}{2}g^{ij}\left(-iq\delta_i^k\psi^\star(\partial_j + iqA_j)\psi + (\partial_i - iqA_i)\psi^\star\cdot iq\delta_j^k\psi\right)\delta A_k + \frac{1}{2}T^{ijkm}\left(\delta_i^n\delta_j^p\partial_k A_m + \delta_k^n\delta_m^p\partial_i A_j\right)\partial_n\,\delta A_p$$

$$= \int \mathrm{d}^3\mathbf{r}\,\frac{1}{2}g^{ij}\left(-iq\psi^\star(\partial_j + iqA_j)\psi\,\delta A_i + (\partial_i - iqA_i)\psi^\star\cdot iq\psi\,\delta A_j\right) + T^{ijkm}\partial_k A_m\partial_i\,\delta A_j$$

$$= \int \mathrm{d}^3\mathbf{r}\,\frac{1}{2}\left(-iq\psi^\star\,\delta\mathbf{A}\cdot(\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi + iq\psi\,\delta\mathbf{A}\cdot(\vec{\boldsymbol{\nabla}} - iq\mathbf{A})\psi^\star\right) + \vec{\boldsymbol{\nabla}}\times\mathbf{A}\cdot\vec{\boldsymbol{\nabla}}\times\delta\mathbf{A}$$

$$= \int \mathrm{d}^3\mathbf{r}\,\frac{1}{2}\left(iq(\psi\vec{\boldsymbol{\nabla}}\psi^\star - \psi^\star\vec{\boldsymbol{\nabla}}\psi) + 2q^2|\psi|^2\mathbf{A} + 2\vec{\boldsymbol{\nabla}}\times\vec{\boldsymbol{\nabla}}\times\mathbf{A}\right)\cdot\delta\mathbf{A} - \vec{\boldsymbol{\nabla}}\cdot(\mathbf{A}\cdot\delta\mathbf{A}).$$

When integrating the last term by parts, we take the variations to arise solely due to the superconductor. By moving the boundaries of integration to outside the superconductor, we should automatically have $\delta\mathbf{A} = \mathbf{0}$ there, leaving boundary conditions for the magnetic field free. The equation of motion is then

$$\frac{1}{2}iq(\psi\vec{\boldsymbol{\nabla}}\psi^\star - \psi^\star\vec{\boldsymbol{\nabla}}\psi) + q^2|\psi|^2\mathbf{A} + \vec{\boldsymbol{\nabla}}\times\vec{\boldsymbol{\nabla}}\times\mathbf{A} = \mathbf{0}.$$

Combined with Maxwell's equation $\vec{\boldsymbol{\nabla}}\times\mathbf{B} = \mathbf{J}$ we see that our previous identification of the current was justified.

Allowing $|\psi|$ to vary is in fact a fundamental aspect of the theory. To examine this, let us consider a superconductor in the region $x > 0$ with $\psi(0) = 0$ and $\psi \to \sqrt{\frac{a}{b}}$ at infinity. Inside the superconductor, the Meissner effect dictates $B = 0$. By choosing the gauge $\mathbf{A} = \mathbf{0}$ and rescaling in terms of $\tilde{\psi} = \sqrt{\frac{b}{a}}\psi$, we find

$$a\sqrt{\frac{a}{b}}\tilde{\psi}^3 - a\sqrt{\frac{a}{b}}\psi - \frac{1}{2}\sqrt{\frac{a}{b}}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = 0.$$

Introducing the new length scale $\xi = \frac{1}{2\sqrt{a}}$ we find

$$-2\xi^2\frac{\mathrm{d}^2\tilde{\psi}}{\mathrm{d}x^2} - \tilde{\psi} + \tilde{\psi}^3 = 0,$$

with solution

$$\tilde{\psi} = \tanh\left(-\frac{x}{2\xi}\right).$$

Thus a completely new length scale enters the theory. Having identified the two relevant length scales, we note that $\frac{1}{\xi\lambda} = \frac{a^2}{b}$, hence we write the critical field as $H_\mathrm{c} = \frac{\Phi_0}{4\pi\xi\lambda}$.

Type 1 and 2 Superconductors If $B = H_c$ outside the superconductor, the density of Gibbs free energy there is then

$$G \to F_n - \frac{1}{2}H_c^2.$$

We have here introduced F_n, which is the free energy in the absence of any fields. The positive term from the free energy is added to the negative one from the Legendre transform to produce this result. Inside the superconductor, where $B = 0$, we also have

$$G \to F_n - \frac{1}{2}H_c^2.$$

We then define the interface energy density as

$$\sigma = \int_{-\infty}^{\infty} \mathrm{d}x\, G(x) - F(\psi = 0) + \frac{1}{2}H_c^2 = \int_{-\infty}^{\infty} \mathrm{d}x - a|\psi|^2 + \frac{1}{2}b|\psi|^4 + \frac{1}{2}\left|(\vec{\boldsymbol{\nabla}} + iq\mathbf{A})\psi\right|^2 + \frac{1}{2}\mathbf{B}^2 - \mathbf{B}\cdot\mathbf{H}_c + \frac{1}{2}\mathbf{H}_c^2.$$

We will have to analyze this in length scale limits by introducing $\kappa = \frac{\lambda}{\xi}$. In the case of $\kappa \gg 1$, $|\psi|$ recovers its equilibrium value quickly on relevant length scales. We can then neglect gradient terms to find

$$\sigma \approx -\frac{1}{2}\lambda H_c^2.$$

In the limit $\kappa \ll 1$, the field is instead what is screened on a small time scale, and the gradient terms dominate. We then have

$$\sigma \approx \frac{a^2}{2b}\int_{-\infty}^{\infty} \mathrm{d}x \left(1 - \tilde{\psi}\right)^2 + 4\xi^2 \left(\frac{\mathrm{d}\tilde{\psi}}{\mathrm{d}x}\right)^2,$$

which can be estimated to be $\frac{1}{2}\xi H_c^2$. More specifically, substituting the solutions we find

$$\sigma = \frac{4}{3}\xi H_c^2.$$

The two differ in signs, and this is a defining line between superconductors of types 1 and 2.

What is the significance of this difference? For the latter case, which is type-1, large flux-expelling domains are formed as the temperature is lowered in order to minimize the interface area. The other case, which is type-2, corresponds to the formation of small domains. The argument is that slightly below the critical field, free energy is increased by creating domains of the normal state, but decreased by creating more interface area. Being below the critical field, it must be favorable to keep at least some of the material superconducting, but at some point the energy reduction of making everything superconducting starts to dominate. This happens at the first critical field. Similarly, slightly above the critical field the energy loss of creating interface area outweighs the gain from keeping superconducting domains, up to some second critical field where the normal state becomes stable.

Vortices in Superconductors The superconducting domains in type-2 superconductors are shielded from the surrounding material by strong cylindrical currents called vortices. Let us now consider a single vortex in a superconductor. We make the anzats

$$\psi = \psi_\infty f(\rho) e^{i\phi}$$

in cylindrical coordinates. Taking $B = 0$ and choosing $A = 0$, we have

$$\int \mathrm{d}^3\mathbf{r} \left|\vec{\boldsymbol{\nabla}}\psi\right|^2 = \psi_\infty^2 L_z \int_0^d \mathrm{d}\rho\, \frac{2\pi f^2(\rho)}{\rho},$$

which diverges logarithmically at infinity. This indicates that there is an infinite energy cost to creating such a vortex. The system can cancel this by introducing its own field to cancel currents at infinity. We find

$$\mathbf{A} = -\frac{\Phi_S}{2\pi\rho}\boldsymbol{\phi},$$

where Φ_{S} is the superconducting flux quantum. It follows from this that the magnetic flux is quantized.

Consider now a vortex that carries N quanta of flux ϕ_0. With axial symmetry we have

$$\mathbf{A} = \frac{A(r)}{r}\mathbf{r} \times \mathbf{e}_z.$$

The current is

$$\mathbf{J} = -\frac{1}{\lambda^2}\left(\frac{1}{q}\vec{\boldsymbol{\nabla}}\theta + \mathbf{A}\right),$$

and because currents decay rapidly in the bulk, we must have

$$A(r) \to -\frac{N}{qr}$$

to ensure this. We then have

$$\mathbf{B} + \lambda^2 \vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}} \times \mathbf{B} = \frac{\Phi_0}{2\pi}\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}}\theta.$$

The right-hand side is in fact a distribution. We can show that

$$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}}\theta = 2\pi N \delta(\mathbf{r})\mathbf{e}_z.$$

This will correspond to a divergent solution for $\mathbf{B}$ at the origin. Imposing a cutoff of $|\psi|$ at $r = \xi$, however, we can estimate

$$B(0) = \frac{\Phi}{2\pi\lambda^2}\ln\left(\frac{\lambda}{\xi}\right).$$

This will lead us to the vortex energy

$$E_{\mathrm{v}} = \frac{1}{4\pi}\left(\frac{\Phi}{\lambda}\right)^2 \ln\left(\frac{\lambda}{\xi}\right).$$

We can from this estimate the lower critical field as

$$H_{\mathrm{c},1} = \frac{E_{\mathrm{v}}}{\Phi_0}.$$

BCS Theory BCS theory is a microscopic theory of superconductivity. It is defined by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow},$$

with $\epsilon_{\mathbf{k}}$ being electron energies relative to the Fermi energy and $V_{\mathbf{k},\mathbf{k}'}$ having the simple form

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -V_0, & |\epsilon_{\mathbf{k}}| < \hbar\omega_{\mathrm{D}}, \\ 0, & \text{otherwise.} \end{cases}$$

The Debye frequency enters here as a consequence of BCS theory incorporating electron-phonon interactions.

This Hamiltonian can be mapped to a spin Hamiltonian by introducing operators

$$S^z_{\mathbf{k}} = \frac{1}{2}(n_{\mathbf{k},\uparrow} + n_{\mathbf{k},\downarrow} - 1),\ S^+_{\mathbf{k}} = c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow},\ S^-_{\mathbf{k}} = c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}.$$

The Hamiltonian can then be written as

$$\begin{aligned}\mathcal{H} =& \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(2S^z_{\mathbf{k}} + 1) + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}(S^+_{\mathbf{k}} S^-_{\mathbf{k}'} + S^+_{\mathbf{k}'} S^-_{\mathbf{k}}) \\ =& H_0 + \sum_{\mathbf{k}} h_{\mathbf{k}} S^z_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}(S^x_{\mathbf{k}} S^x_{\mathbf{k}'} + S^y_{\mathbf{k}'} S^y_{\mathbf{k}}),\end{aligned}$$

with $h_{\mathbf{k}} = 2\epsilon_{\mathbf{k}}$. We also define states

$$|\downarrow\rangle_{\mathbf{k}} = |0\rangle\,,\ |\uparrow\rangle_{\mathbf{k}} = S^{+}_{\mathbf{k}}\,|0\rangle\,.$$

We will study this problem in the mean-field limit, with $\mathbf{S}_{\mathbf{k}} = \langle \mathbf{S}_{\mathbf{k}}\rangle + \delta\mathbf{S}_{\mathbf{k}}$. In the mean-field limit we find

$$\mathcal{H} = H_0 + \sum_{\mathbf{k}} h_{\mathbf{k}}(\langle S^z_{\mathbf{k}}\rangle + \delta S^z_{\mathbf{k}}) + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}((\langle S^x_{\mathbf{k}}\rangle + \delta S^x_{\mathbf{k}})(\langle S^x_{\mathbf{k}'}\rangle + \delta S^x_{\mathbf{k}'}) + (\langle S^y_{\mathbf{k}'}\rangle + \delta S^y_{\mathbf{k}'})(\langle S^y_{\mathbf{k}}\rangle + \delta S^y_{\mathbf{k}})).$$

Ignoring higher-order fluctuation terms and shifting the zero-level of the Hamiltonian we find

$$\begin{aligned}\mathcal{H} &= \sum_{\mathbf{k}} h_{\mathbf{k}}\delta S^z_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}(\langle S^x_{\mathbf{k}'}\rangle\,\delta S^x_{\mathbf{k}} + \langle S^x_{\mathbf{k}}\rangle\,\delta S^x_{\mathbf{k}'} + \langle S^y_{\mathbf{k}'}\rangle\,\delta S^y_{\mathbf{k}} + \langle S^y_{\mathbf{k}}\rangle\,\delta S^y_{\mathbf{k}'}) \\ &= \sum_{\mathbf{k}} h_{\mathbf{k}}\delta S^z_{\mathbf{k}} + 2\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}(\langle S^x_{\mathbf{k}'}\rangle\,\delta S^x_{\mathbf{k}} + \langle S^y_{\mathbf{k}'}\rangle\,\delta S^y_{\mathbf{k}}).\end{aligned}$$

We can now rotate the spin operators to write the Hamiltonian as

$$\mathcal{H} = -\sum_{\mathbf{k}} \mathbf{B}_{\mathbf{k}}\cdot\mathbf{S}_{\mathbf{k}},\ \mathbf{B}_{\mathbf{k}} = -2\epsilon_{\mathbf{k}}\mathbf{e}_z - 2\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\,\langle S^x_{\mathbf{k}'}\rangle\,\mathbf{e}_x.$$

The Superconducting Ground State Introducing

$$E_{\mathbf{k}} = \frac{1}{2}B_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta_0},\ \Delta_0 = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\,\langle S^x_{\mathbf{k}}\rangle\,,$$

we make the anzats that the ground state is

$$|\psi\rangle = \bigotimes_{\mathbf{k}} (u_{\mathbf{k}}\,|\downarrow\rangle_{\mathbf{k}} + v_{\mathbf{k}}\,|\uparrow\rangle_{\mathbf{k}}) = \left(\prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{-\mathbf{k},\downarrow}\right)\right)|0\rangle\,.$$

In the spin basis for a particular $\mathbf{k}$ we have

$$\mathcal{H} = -2\begin{bmatrix}\epsilon_{\mathbf{k}} & -\Delta_0 \\ -\Delta_0 & -\epsilon_{\mathbf{k}}\end{bmatrix}.$$

Its eigenvalues solve

$$\lambda^2 - 4\epsilon^2_{\mathbf{k}} - 4\Delta^2_0 = 0,$$

and are therefore equal to $\pm 2E_{\mathbf{k}} = \pm 2\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_0}$. The eigenvectors corresponding to the ground state solve

$$-2\begin{bmatrix}\epsilon_{\mathbf{k}} + E_{\mathbf{k}} & -\Delta_0 \\ -\Delta_0 & -\epsilon_{\mathbf{k}} + E_{\mathbf{k}}\end{bmatrix}\begin{bmatrix}v_{\mathbf{k}} \\ u_{\mathbf{k}}\end{bmatrix} = 0.$$

We therefore require

$$(\epsilon_{\mathbf{k}} + E_{\mathbf{k}})v_{\mathbf{k}} - \Delta_0 u_{\mathbf{k}} = 0,\ v^2_{\mathbf{k}} + u^2_{\mathbf{k}} = 1.$$

Combining them we find

$$\frac{(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})^2 + \Delta^2_0}{(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})^2}u^2_{\mathbf{k}} = \frac{2E_{\mathbf{k}}}{E_{\mathbf{k}} + \epsilon_{\mathbf{k}}}u^2_{\mathbf{k}} = 1,$$

hence

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)}.$$

We then have

$$v_{\mathbf{k}} = \frac{\Delta_0}{E_{\mathbf{k}} + \epsilon_{\mathbf{k}}}\sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)} = \sqrt{\frac{1}{2}\frac{\Delta^2_0}{E_{\mathbf{k}}(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})}} = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)}.$$

Now, the pseudomagnetic field can be parametrized in terms of an angle measured from the negative z-axis, given by

$$\sin(\theta_{\mathbf{k}}) = \frac{\Delta_0}{E_{\mathbf{k}}}.$$

At the same time we have

$$u_{\mathbf{k}} v_{\mathbf{k}} = \frac{1}{2}\sqrt{1 - \frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}} = \frac{1}{2}\sqrt{\frac{\Delta_0^2}{E_{\mathbf{k}}^2}},$$

hence we have

$$u_{\mathbf{k}} = \sin\left(\frac{\theta_{\mathbf{k}}}{2}\right),\ v_{\mathbf{k}} = \cos\left(\frac{\theta_{\mathbf{k}}}{2}\right).$$

The Gap in Superconductors We now find

$$\langle S_{\mathbf{k}}^x \rangle = 2u_{\mathbf{k}} v_{\mathbf{k}} = \sin(\theta_{\mathbf{k}}),$$

hence

$$\Delta_0 = V_0 \sum_{\mathbf{k}} \sin(\theta_{\mathbf{k}}) = V_0 \sum_{\mathbf{k}} \frac{\Delta_0}{E_{\mathbf{k}}},$$

where we here sum over $\mathbf{k}$ at energies $\hbar\omega_{\mathrm{D}}$ from the Fermi energy. Turning the summation into an integral and approximating the density of states to be constant, we find

$$D(0)V_0 \int_{-\hbar\omega_{\mathrm{D}}}^{\hbar\omega_{\mathrm{D}}} \mathrm{d}\epsilon\, \frac{1}{\sqrt{\epsilon^2 + \Delta_0^2}} = D(0)V_0 \sinh^{-1}\left(\frac{\hbar\omega_{\mathrm{D}}}{\Delta_0}\right) = 1,$$

implying

$$\Delta_0 = \frac{\hbar\omega_{\mathrm{D}}}{\sinh\left(\frac{1}{D(0)V_0}\right)} \approx 2D(0)\hbar\omega_{\mathrm{D}} e^{-\frac{1}{D(0)V_0}}.$$

At finite temperature the superconductor will be found in its energy eigenstates beyond the ground state, which are not created by the electronic creation and annihilation operators. The set of operators that do create the excited energy eigenstates are found by introducing a Bogolioubov transformation

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k},\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^\dagger,\ \beta_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k},\downarrow} + v_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^\dagger,$$

which satisfy fermionic commutation relations if

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1,\ u_{\mathbf{k}}^\star = u_{-\mathbf{k}},\ v_{\mathbf{k}}^\star = v_{-\mathbf{k}}.$$

The mean-field Hamiltonian then becomes

$$\mathcal{H} = \sum_{\mathbf{k}} E_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}).$$

At finite temperatures the energy gap is given by

$$\Delta(T) = V_0 \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle = V_0 \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \left\langle 1 - \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}^\dagger - \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}^\dagger \right\rangle.$$

Inserting thermal dependence we somehow find

$$\Delta(T) = V_0 \Delta(T) \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right).$$

Close to the critical temperature we expect the energy gap to vanish, yielding the self-consistency equation

$$1 = V_0 \sum_{\mathbf{k}} \frac{\tanh\left(\frac{\beta\epsilon_{\mathbf{k}}}{2}\right)}{2\epsilon_{\mathbf{k}}} \approx D(0)V_0 \int_{\hbar\omega_{\mathrm{D}}}^{\hbar\omega_{\mathrm{D}}} \mathrm{d}\epsilon \, \frac{\tanh\left(\frac{\beta\epsilon}{2}\right)}{2\epsilon} = D(0)V_0 \ln(A\hbar\omega_{\mathrm{D}}\beta_{\mathrm{c}}),$$

or

$$k_{\mathrm{B}}T_{\mathrm{c}} = A\hbar\omega_{\mathrm{D}} e^{-\frac{1}{D(0)V_0}}.$$

The new constant A is a purely numerical one, approximately equal to 1.13. Comparing this to the previous result for the energy gap we then find

$$\frac{2\Delta_0}{kT_{\mathrm{c}}} \approx 3.5.$$

Superconductor Condensation Energy Next we try to compute the condensation energy. We have for the normal state

$$\langle T \rangle_{\mathrm{n}} = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}}, \ \langle V \rangle_{\mathrm{n}} = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} (S^x_{\mathbf{k}} S^x_{\mathbf{k}'} + S^y_{\mathbf{k}'} S^y_{\mathbf{k}}) = \frac{1}{2} \sum_{\mathbf{k}} V_{\mathbf{k},\mathbf{k}},$$

as the latter sum is only non-zero if the $\mathbf{k}$ are identical. For the superconducting state we have

$$\begin{aligned}
\langle T \rangle_{\mathrm{n}} &= \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2 = \sum_{\mathbf{k}} \left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \\
\langle V \rangle_{\mathrm{n}} &= \langle V \rangle_{\mathrm{n}} - \sum_{\mathbf{k} \neq \mathbf{k}'} \langle S^x_{\mathbf{k}} \rangle \langle S^x_{\mathbf{k}'} \rangle = \langle V \rangle_{\mathrm{n}} - \sum_{\mathbf{k}} \frac{|\Delta_0|^2}{2E_{\mathbf{k}}}.
\end{aligned}$$

The condensation energy is then

$$\begin{aligned}
\Delta E =& \sum_{\mathbf{k}} \frac{|\Delta_0|^2}{2E_{\mathbf{k}}} - |\epsilon_{\mathbf{k}}| \left(1 - \frac{|\epsilon_{\mathbf{k}}|}{E_{\mathbf{k}}}\right) \\
=& |\Delta_0|^2 \sum_{\mathbf{k}} \frac{1}{\varepsilon_{\mathbf{k}} + E_{\mathbf{k}}} - \frac{1}{2E_{\mathbf{k}}} \\
\approx& 2D(0)|\Delta_0|^2 \int_0^{\infty} \mathrm{d}x \, \frac{1}{x + \sqrt{1+x^2}} - \frac{1}{2\sqrt{1+x^2}} = \frac{1}{2} D(0)|\Delta_0|^2.
\end{aligned}$$

The Bogolioubov-de Gennes Model The Bogolioubov-de Gennes model is a real-space model of superconductivity. Such a model is useful in cases where there is no translational symmetry (for instance in the presence of a magnetic field), which cannot be easily handled by the BCS Hamiltonian.

The model is based on the Fermi-Hubbard model defined by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c^\dagger_{j,\sigma} + c^\dagger_{j,\sigma} c^\dagger_{i,\sigma} - U \sum_i n_{j,\uparrow} n_{j,\downarrow} - \mu \sum_i n_{i,\uparrow} + n_{i,\downarrow}.$$

The presence of a magnetic field can be accounted for by adding a direction-dependent phase to the hopping term and changing the chemical potential depending on spin. By adding an on-site potential, disorder can also be introduced. Note that this Hamiltonian does not restrict the interactions to electrons at the Fermi surface, losing the physics of electron-phonon interactions. On the other hand, the interaction is no longer restricted to pairs with zero total momentum, allowing it to carry a net current. Thus some aspects are more realistic and some less.

The sum in the middle is quartic in the creation and annihilation operators, which is unfortunate. We remedy this by using a mean-field approximation, in which we obtain a new interaction term

$$\Delta = -\sum_i \Delta_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} + \Delta^\star_i c_{i,\downarrow} c_{i,\uparrow}.$$

For self-consistency we much have

$$\Delta_i = U \langle c_{j,\downarrow} c_{j,\uparrow} \rangle .$$

Now consider a gauge transformation of the operators according to

$$c(\mathbf{R}) \to e^{-i\frac{e}{\hbar c}\chi(\mathbf{R})} c(\mathbf{R}).$$

We then have

$$\Delta(\mathbf{R}) \to e^{-i\frac{2e}{\hbar c}\chi(\mathbf{R})} \Delta(\mathbf{R}),$$

and Δ transforms as if it had double charge.

The Chern-Simons Hamiltonian slightly generalizes the above to

$$\Delta = -\sum_{i,i} \Delta_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + \Delta^\star_{i,j} c_{j,\downarrow} c_{i,\uparrow}.$$

In this case, the symmetry of the spin part of the state is opposite of the symmetry of the $\Delta_{i,j}$. Assuming translational invariance we can Fourier transform to find

$$\Delta(\mathbf{k}) = \frac{1}{N} \sum_i \Delta(\mathbf{R}_i) e^{-i\mathbf{k}\cdot\mathbf{R}_i}.$$

In the presence of on-site pairing $\Delta_{i,j} = \Delta\delta_{ij}$ we find $\Delta(\mathbf{k}) = \Delta$.

We are now ready to define the Bogolioubov-de Gennes Hamiltonian. It has a kinetic term

$$H_0 = \sum_{i,j,\sigma} H_{0,i,j} c^\dagger_{i,\sigma} c_{i,\sigma},$$

as well as a term Δ. This can be neatly written in a matrix notation and the resulting matrix can be diagonalized, the corresponding eigenvectors being Bogolioubov transformed operators. Notable is the existence of an eigenvalue $-E$ for every eigenvalue E. If the latter has eigenvector (u, v), then the former has an eigenvector $(\mp v^\star, u)$, where the sign is determined by the symmetry of $\Delta_{i,j}$.

Josephson Junctions A Josephson junction is the junction between two electrically isolated superconductors. The electrons will tunnel across this junction due to the change in the phase θ, creating a current. Such junctions are very useful in measurements that require high precision.

We can describe Josephson junctions by defining a state $|m\rangle$ which describes m Cooper pairs tunnelling from one side to the other. We then introduce the tunnelling Hamiltonian

$$\mathcal{H} = \frac{1}{2} E_J \sum_m |m\rangle\langle m+1| + |m+1\rangle\langle m| .$$

The prefactor is called the Josephson coupling. The eigenstates are

$$|\phi\rangle = \sum_m e^{im\phi} |m\rangle ,$$

with eigenvalue $-E_J \cos(\phi)$. The corresponding current is

$$I(\phi) = \frac{2e}{\hbar} E_J \sin(\phi).$$

Defining the operator

$$n = \sum_m m |m\rangle\langle m| ,$$

the equations of motion are

$$I = 2e\frac{\mathrm{d}n}{\mathrm{d}t} = \frac{2ie}{\hbar}[\mathcal{H}, n] = -i\frac{e}{\hbar} E_J \sum_m |m\rangle\langle m+1| - |m+1\rangle\langle m| .$$

The energy eigenstates are thus also eigenstates of the current, with eigenvalue $I_C \sin(\phi)$. If there is a voltage drop we should add a term $U = -2eVn$. We also find

$$\partial_t \phi = \frac{2eV}{\hbar}.$$

This is similar to the semi-classical relations for a wavepacket in a potential.

The Kitaev Chain The Kitaev chain is a one-dimensional model in a similar vein to the Bogoulioubov-de Gennes model, used to describe Josephson junctions. The particles composing it are spinless fermions. Its Hamiltonian is

$$\mathcal{H} = -\sum_i t(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \mu c_j^\dagger c_j + \Delta(c_j^\dagger c_{j+1}^\dagger + c_{j+1} c_j).$$

In Fourier space it is

$$\mathcal{H} = \sum_k \epsilon_k c_k^\dagger c_k - \Delta(k) c_k^\dagger c_{-k} - \Delta^\star(k) c_{-k}^\dagger c_k,$$

where $\epsilon_k = -2t\cos(k) - \mu$ in units where $a = 1$, and $\Delta(k) = i\sin(k)$. The energies are

$$E_k = \sqrt{\epsilon_k^2 + 4|\Delta(k)|^2}.$$

We can introduce the Majorana representation

$$c_j^\dagger = \gamma_{2j} + \gamma_{2j+1},$$

for some new set of self-adjoint operators γ. Their commutation relations are $\{\gamma_i, \gamma_j\} = \frac{1}{2}\delta_{ij}$. In the particular case of $\mu = 0$ and $\Delta = t$ we find

$$\mathcal{H} = -4it \sum_i \gamma_{2j-1}\gamma_{2j},$$

which is notably independent of γ_0 and γ_{2N+1}.

SQUID Superconducting quantum interference devices (SQUID) use Josephson junctions to perform very accurate measurements of magnetic flux. The setup consists of two junctions wired in parallel, with some flux passing in the middle of the settup. The relative phase between the junctions will be the Aharanov-Bohm phase

$$\theta = 2\pi \frac{\Phi}{\Phi_0}.$$