Application of Quantum Mechanics

Michael Li

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Variational Principle
Variational principle, examples. [2]

Bound states and scattering states in one dimension
Bound states, reflection and transmission amplitudes. Examples. Relation between bound states and transmission amplitude by analytic continuation. [3]

Scattering theory in three dimensions
Classical scattering, definition of differential cross section. Asymptotic wavefunction for quantum scattering, scattering amplitude, cross section. Greenfis function, Born approximation to scattering on a potential. Spherically symmetric potential, partial waves and phase shifts, optical theorem. Low energy scattering, scattering length. Bound states and resonances as zeros and poles of S-matrix. [5]

Electrons in a magnetic field
Vector potential and Hamiltonian. Quantum Hamiltonian, inclusion of electron spin, gauge invariance, Zeeman splitting. Landau levels, effect of spin, degeneracy and filling effects, use of complex variable for lowest Landau level. Aharonov-Bohm effect. [4]

Particle in a one-dimensional periodic potential
Discrete translation group, lattice and reciprocal lattice, periodic functions. Blochfis theorem, Brillouin zone, energy bands and gaps. Floquet matrix, eigenvalues. Band gap in nearly-free electron model, tight-binding approximation. [3]

Crystalline solids
Introduction to crystal symmetry groups in three dimensions, Voronoi/Wigner-Seitz cell. Primitive, body-centred and face-centred cubic lattices. Reciprocal lattice, periodic functions, lattice planes, Brillouin zone. Bloch states, electron bands, Fermi surface. Basics of electrical conductivity: insulators, semiconductors, conductors. Extended zone scheme. Bragg scattering. Vibrations of crystal lattice, quantization, phonons. [7]

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1 Approximation Theory

1.1 Variational Method

The method is as followed:

- we cook up a class of states (aka wavefunctions) parametrized by some parameter α.
- We find $E(\alpha)$, the energy of that state.
- Since we know any state can be decomposed into eigenstates, we must have $E(\alpha) > E_0$ for all α. So we find the minimum $E(\alpha)$ and call it a day! Furthermore, if we know the ground state has parity, and our cooked-up wavefunction set has a different parity, then we are estimating the energy of the first excited state!

Example (Virial Theorem)**.** Suppose we have a particle in d dimensions, moving in the potential $V(x) = Ar^n$. This means the potential scales as $V(\lambda x) = \lambda^n V(x)$. Then assume there is a normalized ground state $\psi_0(x)$ with energy $E_0 = T_0 + V_0$. Then consider the trial class $\psi(x;\alpha) = \alpha^{d/2}\psi_0(\alpha x)$, so that $\psi(x;\alpha)$ is normalized for all α. Then from the scaling property we can see that $E(\alpha) = \alpha^2 T_0 + \alpha^{-n} V_0$. And the minimum gives:

$$\frac{\mathrm{d}E}{\mathrm{d}\alpha} = 2\alpha T_0 = n\alpha^{-n+1} V_0 = 0$$

But the minimum must be at $\alpha = 1$ as this is the true ground state, so we must hav $2T_0 = nV_0$, which is the *generalized Virial Theorem.*

1.2 Perturbation Theory

We recall from PQM, for a state $|\psi\rangle$ satisfying $H+\mu V|\psi\rangle = E|\psi\rangle$ and that approaches $|r\rangle$ with $H|r\rangle = E_r|r\rangle$ as $\mu \to 0$ for some small parameter in V, we have:

$$E = E_r + \mu\langle r|V|r\rangle + \mu^2 \sum_{j\neq r} \frac{|\langle j|V|r\rangle|^2}{E_r - E_j} + \cdots$$

Where E is the energy of the state $|\psi\rangle$.

2 Band Structure

2.1 Electrons in One Dimension

2.1.1 Tight-Binding Model

Consider a 1D lattice of N electrons evenly separated in space and denote $|n\rangle$ as the state when the electron sits on the nth atom. We have the Hamiltonian:

$$H = E_0 \sum |n\rangle\langle n| - t \sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right)$$

The first term describs electrons remaining at an atom, and the second term describes hopping to a neighbouring atom. t is the *hopping parameter*.

Oh yeah, what about the edges? Here our solution is to declare that the lattice is periodic and identify $|N+1\rangle = |1\rangle$.

For a general state $|\psi\rangle = \sum_m \psi_m |m\rangle$, we substitute into our equation $h|\psi\rangle = E|\psi\rangle$ to get the following linear equation set:

$$E_0\psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

For each n. These are solved by the ansatz $\psi_n = e^{ikna}$ where k is called the *wavenumber*, and the quantity $p = \hbar k$ plays a similar role as momentum. Note that k is not unique so we limit $k \in [-\frac{\pi}{a}, \frac{\pi}{a})$ and call this the *Brillouin zone*. The periodicity requirement gives $e^{ikNa} = 1$, or k is a multiple of $\frac{2\pi}{aN}$.

We also see that this gives $E = E_0 - 2t\cos(ka)$, where states with $k > 0$ describe right-moving electrons and vice versa.

2.1.2 Nearly Free Electrons

This model is the exact opposite of the model above. We assume that the electron is free to move anywhere and we mimic the lattice by a periodic potential $V(x)$ such that $V(x+a) = V(x)$. Without the potential we have eigenfunctions $\psi_k(x) = \frac{1}{\sqrt{L}}e^{ikx}$ where k is quantized by $\frac{2\pi}{L}$, and the energy is $E_0(k) = \frac{\hbar^2 k^2}{2m}$. So now we want to consider the potential. Perturbation theory it is.

2.1.2.1 Not-so-Simple^{TM} Perturbation Theory

From PQM, we know the first thing to do is to check if the states are degenerate. Here k and $-k$ are degenerate, but we need to check if the states actually interact! Expand $V(x)$ in fourier series:

$$V(x) = \sum_{n\in Z} V_n e^{2\pi i n x/a} \quad V_n = V_{-n}^* \quad V_n = \frac{1}{a}\int_0^a \mathrm{d}x V(x) e^{-2\pi i n x/a}$$

So we now calculate $\langle k|V|k'\rangle = \sum_{n\in Z} V_n \delta_{k-k',2\pi n/a}$, so we have mixing only when $k = k' + \frac{2\pi n}{a}$ or when $k = \frac{\pi n}{a}$ as $k' = -k$. But this is the edge of Brillouin Zone (BZ)! Hmmm....Let's investigate the energy spectrum.

Low Momentum Using the perturbation formula listed in section one, the first order correction is just V_0 from the fourier sum above and we ignore the second order terms. So the particle just moves as if there is no potential.

At the edge of BZ Here we know that we need degenerate perturbation theory. Write the energy eigenstates as $\alpha|k\rangle + \beta|k'\rangle$ to leading order. Then the Schrodinger waveequation becomes:

$$\begin{pmatrix} \langle k|H|k\rangle & \langle k|h|k'\rangle \\ \langle k'|h|k\rangle & \langle k'|H|k'\rangle \end{pmatrix} \begin{pmatrix}\alpha\\ \beta\end{pmatrix} = E\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

But we know what are the individual elements, and take $k = -k'$:

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} + V_0 & V_n \\ V_n^* & \frac{\hbar^2 k^2}{2m} + V_0 \end{pmatrix} \begin{pmatrix}\alpha\\ \beta\end{pmatrix} = E\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

Which gives the eigenvalues $E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_m|$. Gaps appear!

Near edge of BZ Consider $k = \frac{n\pi}{a} + \delta$. We do the same perturbation theory as above to get that:

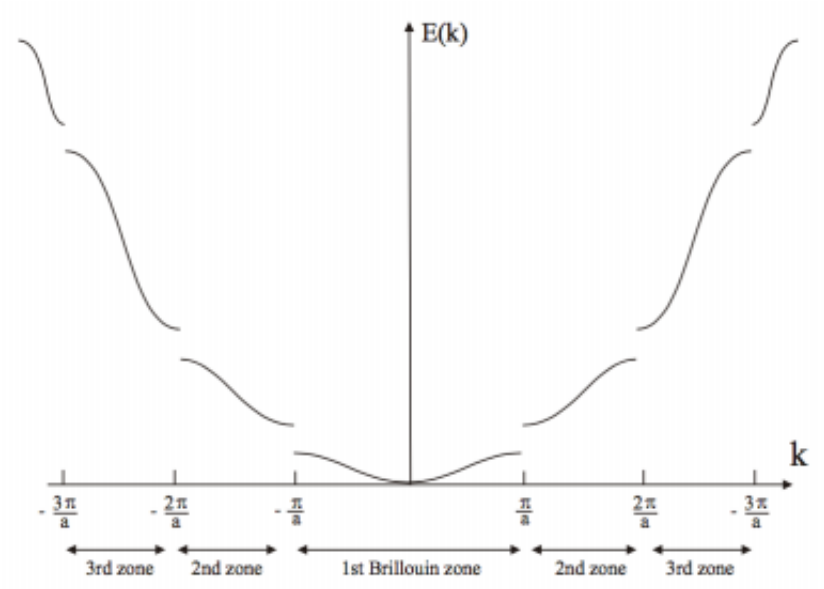
$$E_\pm = \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} + \delta^2\right) + V_0 \pm \sqrt{|V_n|^2 + \left(\frac{\hbar^2 2n\pi\delta}{2ma}\right)^2}$$

Expand this when $\delta \ll V_n$:

$$E_{pm} \approx \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} + \delta^2\right) + V_0 \pm |V_n|^2 + \frac{\hbar^2}{2m}\left(1 + \pm\frac{1}{|V_n|}\frac{n^2\hbar^2\pi^2}{ma^2}\right)^2 \delta^2$$

So we see that as we approach the gaps, the energy is quadratic in momentum δ.

Now this gives us all the information we need to draw the Energy diagram in terms of k!



The relationship $E(k)$ is called the *dispersion relation*.

2.2 Band Structure

The gaps in the spectrum are *very* important. Here is another way to see them. Consider

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) = E\phi$$

Here we have $V(x+a) = V(x)$ so for the two linearly independent solutions $\psi_1(x)$ and $\psi_2(x)$, $\psi_1(x+a)$ and $\psi_2(x+a)$ are also solutions. So we define:

$$\begin{pmatrix}\psi_1(x+a)\\ \psi_2(x+a)\end{pmatrix} = F(E)\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}$$

where $F(E)$ is the *Floquet Matrix*.

Theorem. $\det F = 1$

Proof. We introduce the Wronskian from 1A Differential Equations, and thus we have $W(x+a) = F(E)W(x)$. But it is simple to check that $(\det W)' = 0$, meaning $\det W(x+a) = \det W(x)$. Thus $\det F(E) = 1$. □

Now by standard linear algebra, the eigenvalues obey $\lambda^2 - \operatorname{tr} F\lambda + 1 = 0$. And thus we either have two complex eigenvalues $e^{\pm ika}$, which give :

$$\psi_\pm(x+a) = e^{\pm ika}\psi_\pm(x)$$

And there are plane-wave-like states.

Or we have two real ones so that $\psi_\pm(x+a) = e^{\pm\mu a}\psi_\pm(x)$. These states are unbounded as $x \to \pm\infty$, so this is where gaps appear.

2.3 Discrete Translational Invariance

In the absence of a lattice, we label states by momentum $p = \hbar k$ because we have translational symmetry and Noether's theorem, which tell us $[p, H] = 0$ so we can simutaneously diagonalize p and H. With a lattice we only have discrete translational invariance $x \to x + a$. Define a translation operator T_l such that $T_l\psi = \psi(x+l)$.

We claim that T_l is unitary.

Proof.

$$\begin{aligned} <\phi|T_l|\psi> &= \int \mathrm{d}x \phi^*(x) T_l \psi(x) \\ &= \int \mathrm{d}x \phi^*(x)\psi(x+l) \\ &= \int \mathrm{d}x \phi^*(x-l)\psi(x) \\ &= \int \mathrm{d}x [T_{-l}\phi]^*(x)\psi(x) \end{aligned}$$

Thus $T_l^* = T_{-l} = T_l^{-1}$. □

By Taylor expansion we can see that $T_l = e^{ilp/\hbar}$.

A system is said to be invariant under translations by l if $[H, T_l] = 0$. For discrete translational symmetry, we can simultaneously diagonalize H and T_l.

Theorem (Bloch's Theorem in 1D)**.** In a periodic potential $V(x) = V(x+a)$, all energy eigenstates can be writeen as $\psi_k(x) = e^{ikx}U_k(x)$ where $U_k(x) = U_k(x+a)$ and $k \in [\frac{-\pi}{a}, \frac{\pi}{a}]$.

Proof. Take $\psi_k(x)$ to be an eigenstate of T_a. Then

$$\psi_k(x+a) = e^{ika}\psi_k(x)$$

Thus $U_k(x+a) = U_k(x)$. □

The quantity $p = \hbar k$ is called the crystal momentum. It is *not* mass times velocity. It is conserved $\mod \frac{2\pi\hbar}{a}$. And thus we can draw $E(k)$ vs k in either the extended zone scheme (the figure two pages above) or the reduced zone scheme, shown onthe right.

Note that the ends are identified. In the reduced zone scheme, states are labelled by $\psi_{n,h}(x)$.

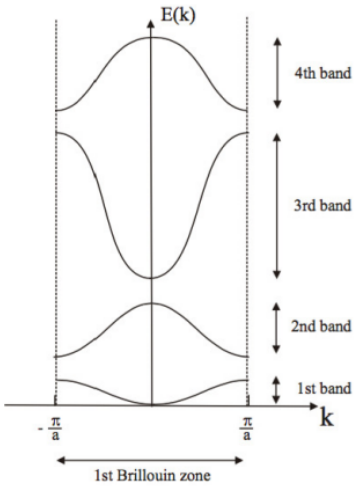


Figure 1: Reduced Zone Scheme

2.4 Lattices

We want to describe an election moving in a $2D$ or $3D$ signal. A *Bravais Lattice* is a periodic array of points defined by integer sums of linearly independent basis vectors $\mathbf{a}_i$. These *primitive lattice vectors* $\mathbf{a}_i$ are not unique, as for the square lattice below we can take e_i as the vectors, or e_1 along with the rightward or the leftward diagonal as the primitive vectors.

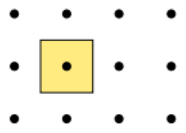


Figure 2: Bravais Lattice

A *primitive unit cell* is a region of space which, when translated by $\mathbf{a}_i$, tessellates the space. They are not unique.

The *Wigner-Seitz cell* Γ, also known as the *Voronoi cell*, is a canonical primitive unit cell that is defined by the region of space closest to a certain lattice point.

In $2D$, there are 5 different Bravais lattice, and in $3D$, there are 14 of those. However, we are only really interested in 3 of these in the $3D$ case and we would ignore the $2D$ case:

Cubic This has $\mathbf{a}_i = a\mathbf{e}_i$.

Body-centered Cubic (BCC) $\mathbf{a}_1 = a\mathbf{e}_1$, $\mathbf{a}_2 = a\mathbf{e}_2$, and $\mathbf{a}_3 = \frac{a}{2}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)$.

Face-centered Cubic (FCC) $\mathbf{a}_1 = a(\mathbf{e}_2 + \mathbf{e}_3)$, $\mathbf{a}_2 = a(\mathbf{e}_1 + \mathbf{e}_3)$, and $\mathbf{a}_3 = a(\mathbf{e}_1 + \mathbf{e}_2)$.

Given a Bravais lattice Λ, the reciprocal lattice is defined by:

$$\Lambda^* = \{\mathbf{k} = \sum n_i \mathbf{b}_i, n \in \mathbb{Z}$$

where $a_i \cdot b_j = 2\pi\delta_{ij}$.

In 3D, we can construct $\mathbf{b}_i$ by:

$$\mathbf{b}_i = \frac{\pi}{V}\epsilon_{ijk}\mathbf{a}_j \times \mathbf{a}_k$$

Note.
- $(\Lambda^*)^* = \Lambda$.
- The reciprocal lattice lies in Fourier or momentum space.

The Wigner-Seitz cell of the reciprocal lattice is called the *Brillouin zone*. In 1d, a lattice with spacing a has a reciprocal lattice with spacing $b = \frac{2\pi}{a}$. The Wigner-Seitz cell is those points in $[-\frac{b}{2}, \frac{b}{2}]$, which is what we saw previously.

The BZ is also called the 1st BZ. The nth BZ is those points in recriprocal space that are nth closest to the origin. All those higher BZ have the same volume as the first one.

To construct BZ boundaries, draw perpendicular bisectors between the origin and all other points. Cross $n-1$ bisectors from the origin and you are in the nth BZ.

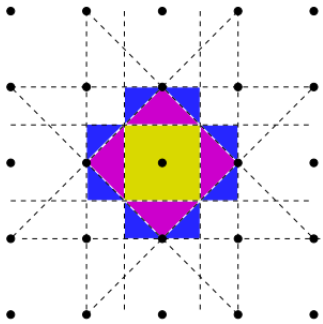


Figure 3: First Three BZs of Square Lattice

We can map higher BZ into the first BZ by translation by $q \in \Lambda^*$. The edges of the BZ are identified, so that for a d-dimensional lattice, the BZ is a torus T^d.

2.5 Band Structure in 3D

We still have Bloch's theorem, and the proof is entirely the same. The label $\mathbf{k}$ is called the crystal momentum (actually strictly $\hbar\mathbf{k}$).$\mathbf{k}$ is ambiguous as if we add an vector in the recirpocal lattice to it, it has the same eigenvalues by definition.

As in ID, we can choose to restrict $\mathbf{k}$ to lie in the 1st BZ. In this case, we label states by $\mathbf{k} \in BZ$ and by a band index $n \in \mathbb{Z}$. This is the *reduced zone scheme.* Alternatively, it may be useful to label states by $\mathbf{k} \in \mathbb{R}^d$. This is the *extended zone scheme.*

2.5.1 Tight-binding in 3D

We can redo our tight-binding model or a general bravais lattice Λ. The electron can sit in states $|\mathbf{r}>, r \in \Lambda$. We can write a tight-binding Hamiltonian as:

$$\begin{aligned} H &= E_0 \sum |r\rangle\langle r| - \sum_{\langle r,r'\rangle} t_{r-r'}(|r\rangle\langle r'| + |r'\rangle\langle r|) \\ &= \sum (E_0|r\rangle\langle r| - \sum_a t_a(|r\rangle\langle r'| + |r'\rangle\langle r|) \end{aligned}$$

Where the second sum is summing over all r' that is adjacent to r.

Again, this is easily solved with:

$$|\psi(k)\rangle = \frac{1}{\sqrt{N}} \sum_{r\in\lambda} e^{ik\cdot r}|r\rangle$$

Where N is the number of total lattice sites. Similar to 1D, this has energy:

$$E(k) = E_0 - \sum_a 2t_a \cos(k \cdot a)$$

2.5.2 Nearly Free Electrons in 3D

Consider an electron in $\mathbb{R}^3$ in a potential $V(x) = V(x+r)$ for all $r \in \Lambda$. We will work perturbatively, starting from plane wave states $|k\rangle$ with $\langle x|k\rangle = e^{ikx}$ and $E_0(k) = \frac{h^2k^2}{2m}$. We will need the Fourier transform:

$$V(k) = \int e^{-ikx} V(x) \mathrm{d}^3x$$

Claim. $V(k) = 0$ unless $k \in \Lambda^*$.

Proof.

$$\begin{aligned} V(k) &= \sum \int \mathrm{d}^3x e^{-k(x+r)} V(x+r) \\ &= \sum e^{-ikr} \int \mathrm{d}^3x e^{-ikx} V(x) \end{aligned}$$

Define $\Delta(k) = \sum e^{-ikr}$. Then:

$$\Delta(k) = \sigma(k_1)\sigma(k_2)\sigma(k_3)$$

where $\sigma(k) = \sum_{-\infty}^{\infty} e^{-2\pi ikn}$. Consider:

$$\sigma_N(k) = \sum_{-N/2}^{N/2} e^{-2\pi ikn} = \frac{e^{-2\pi ik(N/2+1)} - e^{2\pi ikN/2}}{e^{-2\pi ik} - 1}$$

So $\Sigma_N(k) = \frac{\sin(N+1)\pi k}{\sin \pi k}$. Now we can prove that (through drawing and kind of hand-waving) :

$$\lim_{N\to\infty} \sigma_N(k) = \sum_{-\infty}^{\infty} \delta(k-n)$$

Thus $\Delta(k) = V^* \sum \delta(k-q)$. This thus means that we can write:

$$V(x) = \sum_{q\in\Lambda^*} e^{iqx} V_q$$

From perturbation theory we have:

$$\langle k|V(x)|k'\rangle \sim \int \mathrm{d}^3x e^{i(k'-k)x} V(x) = 0$$

unless $k' - k = q$ with $q \in \Lambda^*$.

This means that a state k can only scatter off to be k' if the difference $q = k' - k$ can be absorbed by the lattice. □

how does the energy change?

- For low momentum, $|k\rangle$ can only scatter into $|k+q\rangle$ which has very different energy $\Rightarrow$ non-degenerate perturbation so the spectrum is unchanged.
- iF $|k\rangle$ has the same energy as $|k+q\rangle$, $q \in \Lambda^*$, then we need degenerate perturbation theory. This gives that:

$$k^2 = (k+q)^2 \Rightarrow 2kq + q^2 = 0$$

Thus $k = -\frac{1}{2}q + k_\perp$ where $k_\perp \dot{q} = 0$. Thus, k lives on the bisector between 0 and $-q$, so k is the boundary of BZ.

For degenerate perturbation, a gap opens up a boundary of BZ and note that the gap would vary as we move around the boundary.

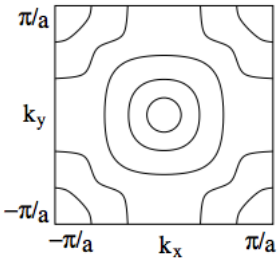


Figure 4: Energy contours for 2D square lattice

After knowing what the energy looks like, we want to know how many states are in the BZ:

Claim. The number of states in the BZ is equal to N, the number of sites on the spatial lattice Λ.

Proof. Consider a lattice $r = \sum n_i a_i$ of finite size where $0 \leq n_i \leq N_i$. The total number of sites is $N = N_1 N_2 N_3$.

We impose periodic boundary conditions $\psi(x + N_i a_i) = \psi(x)$. Then Bloch's theorem tell us that $e^{-n_i a_i k} = 1$. This gives:

$$k = \sum_i \frac{m_i}{N_i} b_i$$

where b_i are the primitice vectors of the reciprocal lattice. Now we can think of each state occupying a unit volume in the reciprocal lattice of volume $\frac{V^*}{N}$, so the number of states is precisely N. □

3 Electron Dynamics in Solids

We would start by doing something wrong: Ignore interactions between electrons. This is *completely* unjustified, but it turns out the results we are going to get are the same.

3.0.1 Fermi Surfaces

Electrons are fermions that obey the *Pauli exlcusion principle*: no two electrons can sit in the same state. To start, suppose there is no lattice, and the electrons sit in a cubic box, with sides of length L:

$$E = \frac{h^2 k^2}{2m} \quad k_1 = \frac{2\pi n_i}{L}$$

Thus we fill out a ball of electrons in momentum space as energy levels get filled. This is called the *Fermi sea*, and the boundary of the ball is called the *Fermi surface*. The states on the fermi surface have *Fermi momentum* $\hbar k_F$ and *Fermi energy* $E_F = \frac{\hbar^2 k_F^2}{2m}$.

Then in a lattice, the following happens:

- The energy spectrum splits into bands. (Remember Brillouin Zones)
- Each band can accommodate $2N$ electrons, where N is the number of lattice sites, as electrons have two spin states.

But there is one further important fact. In a solid, each atom typically donates some number Z of electrons which are free to roam around. Z is an integer and is called the *valency*. Now let's look at the case $Z = 1$:

Thus we have N electrons, which can comfortably fit within the first BZ. Consider the BZ for a 2d square lattice. If there is no lattice, the fermi surface fills a circle with area half of the square.

The effect of the lattice is to lower energy close to the BZ boundary and distort the Fermi surface so that is increasingly looks like a wide cross, shown below.

Figure 5: Fermi surface for increasing lattice strengths

Therefore, in this case, we can start to classify *metals* and *insulators*. If we perturb the system then the electrons near the Fermi surface can respond by moving into unoccupied states. For example, if we apply a small electric field, the electrics respond and a current flows. A material with a Fermi surface is called a *metal*.

For $Z = 2$, the same thing happens, but for a lattice suitably strong, we have E_{min} in second BZ is larger than E_{max} in the first BZ, so the fermi sea fills the whole square (as we have $2N$ electrons) and there is no fermi surface as there is an energy gap to excite any electron. For small perturbations, the electrons don't move.

Materials with no Fermi surface are called *insulators*.

3.1 Graphene

Finally, some actual example. Graphene is a two-dimensional lattice of carbon atoms arranged on a honeycomb lattive. It was discovered in 2004. It is best thought of

as a triangular Bravais lattice but each site has two connected carbon atoms. $\mathbf{a}_1 = \frac{\sqrt{3}a}{2}(\sqrt{3}, 1)$, $\mathbf{a}_2 = \frac{\sqrt{3}a}{2}(\sqrt{3}, -1)$. The sublattice A is $\mathbf{r} = n_a\mathbf{a}_1, n_2\mathbf{a}_2$, sublattice B is $\mathbf{r} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \mathbf{d}$, with $\mathbf{d} = -a(1, 0)$.

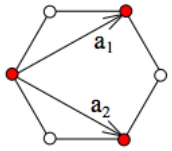


Figure 6: A: Red dots; B: White dots

Now the reciprocal lattice span a triangular lattice, and we look at two adjacent corners of the hexagonal BZ, denoted $\mathbf{K}$ and $\mathbf{K}'$. Now we work with the tight-binding model:

$$H = -t\sum_{r\in A}[|r;A\rangle\langle r;B| + |r;A\rangle\langle r+a_1;B| + |r;A\rangle\langle r+a_2;B| + \cdots]$$

where $|r;A\rangle$ is on the A-sublattice. We solve using the ansatz:

$$|\psi(k)\rangle = \frac{1}{\sqrt{2N}}\sum e^{ikr}(c_A|r;A\rangle + c_B|r;B\rangle)$$

Solving the Schrodinger equation with this gives $E(k) = \pm|\gamma(k)|$, where:

$$\gamma(k) = -t(1 + e^{ika_1} + e^{ika_2})$$

Now if we expand it out:

$$E(k) = \pm t\sqrt{1 + 4\cos(\frac{3k_xa}{2})\cos(\frac{\sqrt{3}k_ya}{2}) + 4\cos^2(\frac{\sqrt{3}k_ya}{2})}$$

There are two bands as we have two sublattices. The two bands meet at $\mathbf{k} = \mathbf{K}$, and $\mathbf{k} = \mathbf{K}'$. Now graphene has valency $z = 1$, so the lower states are filled and the higher states are not. The fermi surface is just two points, $k = K$, and $k = K'$. These are *Dirac points*.

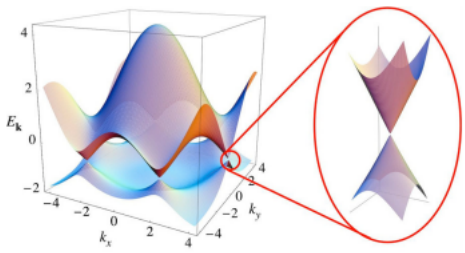


Figure 7: Band Structure of Graphene

In the vicinity of Dirac points, $\mathbf{k} = \mathbf{K} + \mathbf{q}$, where $\mathbf{q}$ is some small momentum. A taylor expansion gives $E(\mathbf{k}) \approx \pm\frac{3ta}{2}|\mathbf{q}|$. This is the dispersion relation for a massless relativistic particle: $E = |p|c$. We have $E(\mathbf{k}) \approx \hbar v_F|q|$, where $v_F = \frac{3ta}{2\hbar}$ is the speed of the electron. In graphene, this is about $\frac{1}{300}$ of the speed of liight. But the low energy physics of graphene is described by relativistic equations.

Close to $\mathbf{k} = \mathbf{k}$, we can expand γ and get that :

$$\gamma(\mathbf{k}) \approx v_F\hbar(iq_x - q_y)$$

Near the Dirac point, we have:

$$H = v_F\hbar \begin{pmatrix} 0 & iq_x - q_y \\ -iq_x - q_y & 0 \end{pmatrix} = -v_F\hbar\mathbf{q}\cdot\sigma$$

where $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}]$, $\sigma^y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $\sigma = (\sigma^y, \sigma^x)$. This si the *Dirac equation* for a massless relativistic fermion in two spatial dimensions. For Dirac, the two components of H were the spin, in graphene they denote A, B sublattice. Of course, real electrons also have spin $|\uparrow\rangle$ and $|\downarrow\rangle$. Therefore, the excitations of graphene consist of 4 species of massless relativistic particles, two from K and two from K'.

3.2 Dynamics of Bloch Electrons

Consider a single elecrton in a band with energy $E(k)$, $k \in BZ$.

Claim. The velocity is $v = \frac{1}{\hbar}\frac{\partial E}{\partial k}$.

Proof. The velocity is defined as $v = \frac{1}{m}\langle\psi| - ih\nabla|\psi\rangle$. From Bloch's theorem we have $\psi_k(x) = e^{ikx}U_k(x)$. Then the schrodinger equation becomes:

$$H_k u_k(x) = E(k)u_k(x)$$

where $H_k = \frac{\hbar^2}{2m}(-i\nabla + k)^2 + V(x)$. Consider $H_{k+q} = H_k + \frac{\partial H_k}{\partial k}q + \frac{1}{2}\frac{\partial^2 H_k}{\partial k^i \partial k^j}q^i q^j$. The 1st order perturbation theory gives:

$$\Delta E = \langle u_k|\frac{\partial H_k}{\partial k}q|u_k\rangle$$

But the exact result is $E(k+q) = E(k) + \frac{\partial E}{\partial k}q + \cdots$. Then equating the two:

$$\frac{\partial E}{\partial k} = \langle u_k|\frac{\partial H_k}{\partial k}|u_k\rangle = \frac{\hbar^2}{m}\langle u_k|(-i\nabla + k)|u_k\rangle = \frac{\hbar}{m}\langle\psi_k| - i\hbar\nabla|\psi_k\rangle = \hbar v$$

□

From this, we have two more claims:

Claim.
- A filled band has no electric current $j = -ev$.
- A filled band has no heat current:

$$j_H = 2\int \frac{\mathrm{d}^3k}{(2\pi)^3}(Ev)$$

Proof. -

$$j = -\frac{2e}{\hbar}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\partial E}{\partial k} = 0$$

-

$$j_H = 2\int \frac{\mathrm{d}^3k}{(2\pi)^3}(Ev) = \frac{1}{\hbar}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\partial(E^2)}{\partial k} = 0$$

As both here are total derivatives of periodic functions in k. □

Definition. The effective mass tensor is defined to be:

$$m^*_{ij} = \hbar^2\left(\frac{\partial^2 E}{\partial k^i \partial k^j}\right)^{-1}$$

For isotropic system, we have $m^*_{ij} = m^*\delta_{ij}$.

3.3 Semi-classical Equations of Motion

Suppose we add an external force to the electron $F = -\nabla U(x)$. The *semi-classical approximation* views the quantum particle as a wavepacket with some average k and x. Consider the total energy of the particle to be:

$$E = E(k) + U(x) \quad \Rightarrow \quad \frac{\partial E}{\partial k}\frac{\partial k}{\partial t} + \nabla U\frac{\partial x}{\partial t} = v\left(\hbar\frac{\partial k}{\partial t} + \nabla U\right) = 0$$

So we have:

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = -\nabla U = F$$

This is Newton's 2nd law for a Bloch electron. In general, we have to solve:

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = F \quad v = \frac{1}{\hbar}\frac{\partial E}{\partial k}$$

We can also retrieve Newton's second law of motion $m^*\frac{\mathrm{d}v}{\mathrm{d}t} = F$.

Example. An electron in a constant electric field E experiences a force $F = -eE$. Then we have $k(t) = k(0) - \frac{eE}{\hbar}t$. Consider $E = -C\cos(ka)$,a one-dimensional system with a tight-binding form of band-structure, then:

$$v(k) = -\frac{Ca}{\hbar}\sin(ka)$$

Which oscillates in time. Therefore, a DC current produces AC oscillations! but sadly, in real life, it gets destroyed by impurities.

3.3.1 Holes

Consider a completely filled band and remove one electron. The vacancy acts as if its a particle in its own right. It's called a *hole*. Expanding about the top of the band, the electron dispersion relation is :

$$E_k = E_{max} + \frac{\hbar^2}{2m}|k - k_{max}|^2$$

where $m_* < 0$ here (look at the dispersion relation graph and think what happens at the top). As the hole moves away from the top of the band, it costs more energy (as we are subtracting less). we write:

$$E_{hole}(k) = -E(k) = -E_{max} + \frac{\hbar^2}{2m^*_{hole}}|k - k_{max}|^2$$

Since we are taking away an electron with momentum k, the resulting hole has momentum $-k$. However, we have that:

$$v_{hole} = \frac{1}{\hbar}\frac{\partial E_{hole}}{\partial k_{hole}} = \frac{1}{\hbar}\frac{\partial E}{\partial E} = v$$

So the velocity is the same as the removed electron. These definitions give rise to the equation:

$$m^*_{hole}\frac{\mathrm{d}v_{hole}}{\mathrm{d}t} = -F$$

So in an electric field, we can see holes as carrying a positive $+e$ charge.

3.4 An Example - Electrons in a Magnetic Field

3.4.1 Semi-Classical Motion

Our semi=classical equation of motion gives:

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = -ev \times B \qquad v = \frac{1}{\hbar}\frac{\partial E}{\partial k}$$

Then using these equations we can see that:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\partial E}{\partial k}\cdot\frac{\partial k}{\partial t} = -3v\cdot(v \times B) = 0$$

So the energy is constant and the component of k parallel to b is constant. Then we know the electrons orbit the fermi surface (constant energy) perpendicular to B. Then we consider the path in the plane perpendicular to B:

$$\hat{\mathbf{B}} \times \hbar\dot{\mathbf{k}} = -eB\dot{\mathbf{r}}_\perp$$

Then we can solve this by integrating time and getting:

$$\mathbf{r}_\perp(t) = \mathbf{r}_\perp(0) - \frac{\hbar}{eB}\hat{\mathbf{B}} \times (\mathbf{k}(t) - \mathbf{k}(0))$$

For free electrons, since in k space electrons move in circles, this moves in circles too and we reproduce the classical result.

3.4.2 Cyclotron Frequency

Now the time taken to travel between two points is:

$$t_2 - t_1 = \int_{k_1}^{k_2}\frac{\mathrm{d}k}{|\dot{k}|} = \frac{\hbar^2}{eB}\int_{k_1}^{k_2}\frac{\mathrm{d}k}{|\frac{\partial E}{\partial k}_\perp|}$$

Then if we consider another orbit with $E+\Delta E$ with momentum $k' = k + \frac{\partial E}{\partial k}_{\perp}\Delta(k)$, then the energy difference is:

$$\Delta E = |\frac{\partial E}{\partial k}_{\perp}|\Delta(k)$$

So the total time is:

$$t_2 - t_1 = \frac{\hbar^2}{eb}\frac{1}{\Delta E}\int_{k_1}^{k_2}\Delta(k)\mathrm{d}k$$

But the integral is just the area difference between the two orbits in k-space! So:

$$T = \frac{\hbar^2}{eb}\frac{\partial A(E)}{\partial E}$$

And for free electrons we can check this confirms our high-school intuition.

4 Phonons

4.1 Lattices in 1 Dimension

Consider N identical, equally spaced atoms. The nth atom has position x_n, $N = 1, \cdots, N$. In equilibrium, we have $x_n = na$. The potential that holds them in place takes the form $\sum_n V(x_n - x_{n-1})$. If we taylor expand about $x_n = na$, we will generally find a harmonic oscillator. For small deviations, we write:

$$u_n(t) = x_n(t) - na$$

The hamiltonian is then:

$$H = \sum_n \frac{p_n^2}{2m} + \frac{\lambda}{2}\sum_n (u_n - u_{n-1})^2$$

The equation of motion is:

$$m\ddot{u}_n = -\lambda(2u_n - u_{n-1} - u_{n+1})$$

The solution takes the form $u_n = Ae^{-i(\omega t + kna)}$, where we really take real and imaginary parts for the solution. Once again, $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$, the BZ. Periodicity requires $u_{N+1} = u_1$, so we have:

$$k = \frac{2\pi}{Na}l$$

with $l = -\frac{N}{2}, \cdots, \frac{N}{2}$. Now substituting the solution into the equation of motion gives that $\omega = 2\sqrt{\frac{\lambda}{m}}|\sin(\frac{ka}{2})|$. For small $k > 0$, we can expand this in k, and $\omega \approx \sqrt{\frac{\lambda}{m}}ak$. The phonon dispersion relation is thus reminiscent of light, and we call $\sqrt{\frac{\lambda}{m}}a$ the speed of sound.

4.1.1 Diatomic Chain

Now similarly as above, but consider a chain of atoms of alternating type. The equations of motions are:

$$m\ddot{u_2}n = -\lambda(2u_{2n} - u_{2n-1} - u_{2n+1}$$

$$M\ddot{u_{2n+1}} = -\lambda(2u_{2n+1} - u_{2n} - u_{2n+2}$$

We use the ansatz:

$$u_{2n} = Ae^{-w\omega t - 2ikna} \qquad u_{2n+1} = Be^{-i\omega t - 2ikna}$$

Then we can determine ω to be:

$$\omega_{\pm}^2 = -\frac{\lambda}{mM}[m + M \pm \sqrt{(M-m)^2 + 4Mm\cos^2(ka)}]$$

The $+$ branch is called the optical branch, and the $-$ branh is the acoustic branch. If we look at the eigenvalues of the schrodinger equation as $k \to 0$, we have $A = 1, B = 1$ for the lower branch so they move in phase and create sound waves, and $A = M, B = -m$ for the upper branch, so the atoms move out of phase. Since often the different sites of the lattrice contains ions of opposite charge, and this creates a dipole with some frequency that can emit/absorb light, and thus the name *optical branch*.

4.1.2 Peierls Transition

Consider electrons moving in a 1d monatomic lattice that can also vibrate. Valency $z = 1$ gives a half-filled band and thus it is a conductor. Now consider a distortion of the lattice in which successive pairs of atoms move closer together. This costs a lot of energy as the lattice is out of equilibrium:

$$U_{lattice} \sim N\lambda(\delta x)^2$$

where δx is the shift away from normal. This also has an effect on the electrons. Since the lattice periodicity is now $2a$, the BZ is $k \in [-\frac{\pi}{2a}, \frac{\pi}{2a}]$. We expect a gap to open up at $k = \pm\frac{\pi}{2a}$. Filled states will have lower energy, unfilled states will have higher energy. Does this lowered energy beat the cost of distorting the lattice? The energy gain is:

$$U_{electron} = -\frac{2Na}{2\pi}\int_{-\pi/2a}^{\pi/2a} \mathrm{d}k(E_0(k) - E_-(k))$$

where the 2 on the top is to account for the spin-degree of freedom, and $\frac{Na}{2\pi}$ is the density of states of the electrons.

Now we look at the region near $k = \frac{\pi}{2a}$. Taylor expanding, we have:

$$E_0(k) \approx \mu + v(k - \frac{\pi}{2a})$$

Now using a result from the energy dispersion close to BZ edge (from long long ago):

$$E_{\pm}(q) = \mu \pm \sqrt{v^2q^2 + \frac{\Delta^2}{4}}$$

So:

$$U_{electron} \approx -\frac{Na}{\pi}\int_{-\Lambda}^{0} \mathrm{d}q(vq+\sqrt{v^2q^2+\Delta^2/4}) = -\frac{Na}{\pi}\left[\frac{\Delta^2}{16v^2\Lambda} - \frac{\Delta^2}{8\mu}\log(\frac{\Delta}{2v\Lambda})\right]$$

Now the first term competes with $U_{lattice}$ but the second term always beats $U_{lattice}$ when Δ is small! This shows that a half-filled conductor in 1d cannot exist! It is unstable to a lattice distortion that turns it into an insulator.

5 Particles in Magnetic Fields

5.1 Gauge Fields

Recall from Electromagnetism, the electric field E and magnetic field B can be written as:

$$E = -\nabla\phi - \frac{\partial A}{\partial t} \qquad B = \nabla \times A$$

A and ϕ are called *gauge fields*. A particle of mass m and charge q has Lagrangian:

$$L = \frac{m}{2}\dot{x}^2 + q\dot{x}A - q\phi$$

The classical equation of motion from this Lagrangian is:

$$m\ddot{x} = q(E + \dot{x} \times B)$$

5.1.1 The Hamiltonian

Definition. The *canonical momentum* is defined as $\mathbf{p} = m\dot{x} + qA$.

And the Hamiltonian is given by the Legendre transformation of L, which is:

$$H = \dot{x} \cdot p - L = \frac{1}{2m}(p - qA)^2 + q\phi$$

5.1.2 Gauge Transformation

Well from Electromagnetism we know we can change ϕ and A around as:

$$\phi \to \phi - \frac{\partial \alpha}{\partial t} \qquad A \to A + \nabla\alpha$$

In this transformation, we have $p \to p + q\nabla\alpha$ so the numerical value of p have zero meaning but the Hamiltonian and the velocity are both gauge invariant. The schrodinger equation changes as:

$$\psi \to e^{iq\alpha/\hbar}\psi$$

And this is seen most easily if we define:

$$D_t = \frac{\partial}{\partial t} + \frac{iq}{\hbar}\phi \qquad D_i = \frac{\partial}{\partial x^i} - \frac{iq}{\hbar}A_i$$

Because then the schrodinger equation becomes:

$$i\hbar D_t\psi = -\frac{\hbar}{2m}D^2\psi$$

And these transform nicely.

5.2 Landau Levels

Let's consider cool cases! No. We will have a vanishing electric field and a constant magnetic field. That's it.

The Hamiltonian is $h = \frac{1}{2m}(p - qA)^2$. Take $\mathbf{B} = (0, 0, B)$ and we take the *Landau gauge*, which defines

$$\mathbf{A} = (0, xB, 0)$$

Then the Hamiltonian becomes:

$$H = \frac{1}{2m}(p_x^2 + (p_y - qBx)^2 + p_x^2)$$

Here it is actually better to work with ladder operators:

$$a = \frac{1}{\sqrt{2q\hbar B}}(\pi_x + i\pi_y) \qquad a^\dagger = \frac{1}{\sqrt{2q\hbar B}}(\pi_x - i\pi_y)$$

Which satisfy the same commutation relation as the *ladder operators* in PQM for harmonic oscillators and we can work from there. [Check Example Sheet 3]

But we can also use the ansatz:

$$\psi(x) = e^{ik_y y + ik_z z}\chi(x)$$

And we get that:

$$E = \hbar\omega_B\left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m} \quad \omega_B = \frac{qB}{m}$$

And with wavefunctions:

$$\psi(x, y) \sim e^{ik_y y + ik_z z} H_n(x - k_y l_B^2) e^{-(x - k_y l_B^2)^2/2l_B^2} \quad l_B = \sqrt{\frac{\hbar}{qB}}$$

And where H_n are the hermite polynomial wavefunctions of the harmonic oscillator.

This looks like a harmonic oscillator, and it will be obvious if one uses the ladder operators.

5.2.1 Degeneracy

We will now say bye to the z dimension by taking $k_z = 0$. Then these levels are called *Landau levels.*

We see the energy does not depend on k_y, so we expect a lot of degeneracy. Let's draw a rectangular $L_x \times L_y$ box. Then in the y-direction we must have the periodic condition (like any good old harmonic oscillator in a box), so k_y is quantized in units of $\frac{2\pi}{L_y}$.

Now the x direction is harder. Why? Because we do *not* have translational invariance in this gauge for A. Since the wavefunctions are exponentially localized around $x = k_y l_B^2$, then we would expect $0 \leq k_y \leq L_x/l_B^2$ since $0 \leq x \leq L_x$. Then the number of states in each Landau level is:

$$n = \frac{L_y L_x}{2\pi l_B^2} = \frac{qBA}{2\pi\hbar}$$

where A is the area of the sample. This is huge!

5.2.2 Symmetric Gauge

We can also work in the symmetric gauge:

$$A = \frac{B}{2}(-y, x, 0)$$

Where there is no translational symmetry but there is rotational symmetry. So let's introduce the angular momentum:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{qB}{2m}L_z + \frac{q^2B^2}{8m}(x^2+y^2) \qquad L_z = xp_y - yp_x$$

Then take it into the complex plane of $w = x+iy$, $\bar{w} = x-iy$, and $\partial = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)$, we have:

$$H = -\frac{2\hbar^2}{m}\partial\bar{\partial} - \frac{\omega_b}{2}L_z + \frac{m\omega_B^2}{8}w\bar{w}$$

Then it is simple to check the lowest Landau level states obey:

$$psi_0(w, \bar{w}) = f(w)e^{-|w|^2/4l_B^2}$$

for *any* holomorphic $f(w)$. But the requirement that they are also eigenvalues of L_z brings $f(w) = w^M$ where $M \in \mathbb{Z}^+$.

5.3 Aharonov-Bohm Effect

You see, A and ϕ are actually physical; they are just a bit *discreet*.

5.3.1 Particles around a Flux Tube

Let's take a good old cylindrical solenoid of area A carrying a megnatic field B inside and thus having a A with $A_\phi = \frac{\Phi}{2\pi r}$ where $\Phi = BA$ is the magnetic flux. Consider a charged quantum particle restricted on a ring of radius r outside the solenoid. Using our hamiltonian and $\psi = \frac{1}{\sqrt{2\pi r}}e^{in\phi}$ as the eigenstates we see the spectrum is:

$$E = \frac{\hbar^2}{2mr^2}(n - \frac{\Phi}{\Phi_0})^2$$

where $\Phi_0 = \frac{2\pi\hbar}{q}$ is the *quantum of flux*. Thus we see that if Φ is an integer multiple of Φ_0 then nothing happens. But if it is not, the particle knows about the flux! Even though it can be arbitrarily far away.

Now the gauage field is a total divergence $A = \nabla\alpha$ with $\alpha = \frac{\Phi\phi}{2\pi}$. So we can try to remove this problem discussed above by redefining $\psi \to e^{-iq\alpha/\hbar}\psi$. But this only works (single-valuedly) when Φ is a multiple of $\Phi_0 = \frac{2\pi\hbar}{q}$. Aw Snap.

5.4 Magnetic Monopoles

A magnetic monopole is an object that satisfies:

$$B = \frac{g\hat{r}}{4\pi r^2}$$

Where g is the magnetic charge.

WAIT, WAIT, WAIT, $\nabla \cdot B = 0$ man. Can't happen.

Well, it turns out there is a physicist called Dirac that is smarter than most of the people and found a loophole...

Note. It is also rumored that Dirac found a loophole in the Constitution of USA.

5.4.1 Dirac Quantization

We know from above that when a charge particle q moves in a closed path in the background of some $A(x)$ the particle wavefunction picks up a phase $e^{iq\alpha/\hbar}$ with $\alpha = \oint_C A \cdot \mathrm{d}x$.

now we place our magnetic charge (don't object yet) at the center, and place our electric particle in the background of it. Then we have:

$$\alpha = \oint A \cdot \mathrm{d}x = \int_S B \cdot \mathrm{d}S$$

If the surface makes a solid angle Ω, then using the fact that $\int_{S^2} B \cdot \mathrm{d}S = g$, we have $\alpha = \frac{\Omega g}{4\pi}$. But we can equally integrate over its complement, which gives:

$$\alpha' = -\frac{(4\pi - \Omega)g}{4\pi}$$

This gives the quantization condition that:

$$qg = 2\pi\hbar n$$

with $n \in Z$ as $e^{iq\alpha/\hbar} = e^{iq\alpha'/\hbar}$.

5.4.2 Patching Gauge Fields

This derivation still leaves open the question of how we can have $B = \nabla \times A$ and $\nabla \cdot B \neq 0$. To see this consider the following:

$$A^N_\phi = \frac{g}{4\pi r}\frac{1 - \cos\theta}{\sin\theta}$$

Now we can do a quick calculation to verify that $B = \nabla \times A = \frac{g\hat{r}}{4\pi r^2}$.

*Wait, wait, wait....*I see what you are doing here. A is singular at $\theta = \pi$! That isn't right. But don't worry, just tag along for now. We can similarly define:

$$A^s_\phi = -\frac{g}{4\pi r}\frac{1 + \cos\theta}{\sin\theta}$$

And it would have the same B. This is not defined on the half-line $\theta = 0$. Now the important part comes: we would use A^N in the Northern hemisphere and A^S in the southern hemisphere. These two *are* related by a gauge transformation so it doesn't matter that they don't match at the equator! The gauge transformation is:

$$A^n_\phi = A^S_\phi + \frac{1}{r\sin\theta}\partial_\phi \alpha$$

Where $\alpha = \frac{g\phi}{2\pi}$. But we run into a new problem. α is not single valued, and we do want our wavefunction ψ to be single-valued. Under this gauge transformation, we have:

$$\psi \to e^{iq\alpha/\hbar}\psi$$

And ψ is single valued only if $qg = 2\pi\hbar n$, $n \in Z$. This is Dirac quantization again.

5.5 Spin in a Magnetic Field

Particles carry an intrinsic sngular momentum called *spin*, S. Angular momentum of charged particle give rises to magnetic moment m which couples to the magnetic field by:

$$H = -m \cdot B$$

The question is: what's the relationship between spin S and m? Consider a particle of charge q and mass m moving in a circle. From electromagnetism, $m = -\frac{q}{2}r \times v = -\frac{q}{2m}L$. By analogy, we would expect $m = g\frac{q}{2m}S$. An important result is that $g_e = 2$, while $g_p \approx 5.588$, $g_n \approx -3.823$, as the latter two are composite particles.

5.5.1 Spin Precession

The spin of an electron with $q = -e$ couples to a magnetic field $H = \frac{e\hbar}{2m}\sigma \cdot B$. If $B = (0, 0, B)$ the two eigenstates are $|\uparrow\rangle$ and $|\downarrow\rangle$ with $H|\uparrow\rangle = \frac{\hbar\omega B}{2}|\uparrow\rangle$, $H|\downarrow\rangle = \frac{-\hbar\omega B}{2}|\downarrow\rangle$, where $\omega = \frac{eB}{m}$. In general we can write:

$$|\psi(\theta, \psi)\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + e^{i\phi}\sin\frac{\theta}{2}|\downarrow\rangle$$

And using time-dependent Schrodinger's equation we have that:

$$|\psi(\theta, \psi, t)\rangle = e^{i\omega_B t/2}\left[\cos\frac{\theta}{2}|\uparrow\rangle + e^{i(\phi-\omega_b t)}\sin\frac{\theta}{2}|\downarrow\rangle\right]$$

Thus the effect of the magnetic field is to cause the spin to precess about the $\mathbf{B}$ axis.

5.5.2 Zeeman Effect

6 Scattering Theory

6.1 Scattering in 1 Dimension

We work in 1D to see most of the intuition as in 3D all is lost except calculations. We know the solutions to the time-independent Schrodinger equation can be separated into two types:

Bound States These have normalizable wavefunctions, $E < 0$, and the particle is trapped within the potential.

Scattering States These have non-normalizable wavefucntions, $E > 0$, and the particle can be "anywhere". Asymptotically they must look like plane waves e^{ikx} (right moving) and e^{-ikx} (left moving).

6.1.1 Some Review

We know from 1B quantum mechanics that scattering can be seen as:

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to \infty \end{cases}$$

For particles coming in from the left (and change sign for the right), with reflection probability $|r|^2$ and transmission probability $|t|^2$. From IB we also know there is a conserved probability current:

$$J(x) = -i\frac{\hbar}{2m}\left(\psi^* \frac{\mathrm{d}\psi}{\mathrm{d}x} - \psi \frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right)$$

6.1.2 The New Stuff and The Parity Basis

Now since $V(x)$ is real so $\psi_R^*(x)$ is also a solution. Then:

$$\psi_R^*(x) - r^*\psi_R(x) \sim \begin{cases} (1-|r|^2)e^{-ikx} & x \to -\infty \\ t^*e^{-ikx} - r^*te^{ikx} & x \to \infty \end{cases}$$

This has the same form as $\psi_L(x)$ except a factor so they must agree after dividing through t^*, thus, for the scattering from the right with t' and r', we know:

$$t' = t \qquad r' = -\frac{r^*t}{t^*}$$

6.1.2.1 S-Matrix

Note. This is one of the most important concepts in this chapter. Seriously.

Now we write the incoming basis as $I_R = e^{ikx}$ $x \to -\infty$ and $I_L = e^{-ikx}$ $x \to \infty$, and the outgoing basis as $O_R = e^{ikx}$ $x \to \infty$ and $O_L = e^{-ikx} x \to -\infty$. Then:

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} I_R \\ I_L \end{pmatrix} + S\begin{pmatrix} O_R \\ O_L \end{pmatrix}$$

where:

$$S = \begin{pmatrix} t' & r \\ r' & t \end{pmatrix}$$

Some initial properties of S matrix:

- S is unitary.
- $S^*(k) = S(-k)$ as flipping k and $-k$ along with complex conjugation doesn't change the basis.

6.1.2.2 Parity Basis

It is useful to work with eigenfunctions of the parity operator $P : \psi(x) \to \psi(-x)$. For symmetric potentials with $V(x) = V(-x)$ we have $\psi_k(x) = \psi_k(-x)$. It is better to wotk with asymptotic states which are eigenstates of P.

$$\psi_+(x) = \psi_R(x) + \psi_L(x) = \psi_R(x) + \psi_R(-x)$$

And similarly $\psi_-(x) = \psi_R(x) - \psi_L(x)$.

Example. We look at a potential well with width a and height V_0, centered at 0. The parity even state is:

$$\psi_+(x) = A(e^{iqx} + e^{-iqx})$$

The match at $x = \frac{a}{2}$ gives:

$$r + t = -e^{-ika}\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik}$$

And similarly for the parity odd one we can find that:

$$r - t = -e^{ika}\frac{ik\tan(qa/2) + q}{ik\tan(qa/2) + q}$$

There is no need to check the $-\frac{a}{2}$ one as by parity we are done!

In general we define incoming and outgoing asymptotic states as:

Incoming The parity $+$ state is $\mathcal{L}_+ = e^{-ik|x|}$, and the $-$ state is $\mathcal{L}_- = sgn(x)e^{-ik|x|}$.

Outgoing The parity $+$ state is $e^{ik|x|}$, and the parity $-$ state is $-sgn(x)e^{ik|x|}$. Now we have:

$$\begin{pmatrix}\mathcal{L}_+\\ \mathcal{L}_-\end{pmatrix} = M\begin{pmatrix}\mathcal{L}_R\\ \mathcal{L}_L\end{pmatrix}$$

Where $M = \begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}$, and similarly for the outgoing state.

Now the S-matrix with respect to parity basis is:

$$\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix} = \begin{pmatrix}\mathcal{L}_+\\ \mathcal{L}_-\end{pmatrix} + \mathcal{S}^p\begin{pmatrix}\theta_+\\ \theta_-\end{pmatrix}$$

Where $\mathcal{S}^P = MSM^{-1} = \begin{pmatrix}t + \frac{1}{2}(r + r') & \frac{1}{2}(r - r')\\ \frac{1}{2}(r - r') & t - \frac{1}{2}(r + r')\end{pmatrix}$. Note that S and $\mathcal{S}$ are unitary, and if $V(x) = V(-x)$, then $r = r'$, and thus S_{++} and S_{--} are both phases, as their magnitude has to be 1. [Remember that $r' = \frac{-r^*t}{t^*}$] Thus we write:

$$S_{++} = e^{2i\delta_+(k)} \qquad S_{--} = e^{-2i\delta_-(k)}$$

The S-matrix encodes many properties of the potential $V(x)$.

6.1.3 Bound States

If we know the S-matrix, we can resoncstruct the band state spectrum. The trick is to analytically continue $S(k)$ to $K \in \mathbb{C}$. Consider $V(x) = V(-x)$ and parity even states. Asymptotically,

$$\psi_+(x) = L_+(x) + S_{++}\theta_+(x) \sim \begin{cases} e^{ikx} + S_{++}e^{-ikx} & x \to -\infty \\ e^{-ikx} + S_{++}e^{ikx} & x \to \infty \end{cases}$$

Now we set $k = i\lambda$ and divide through S_{++} so we have:

$$\psi_+(x) \sim \begin{cases} S_{++}^{-1}e^{-\lambda x} + e^{\lambda x} & x \to -\infty \\ S_{++}^{-1}e^{\lambda x} + e^{-\lambda x} & a \to \infty \end{cases}$$

The wavefunction is normalizable whenever $S_{++}(k) \to \infty$ as $k \to i\lambda$ for $\lambda > 0$. The upshot is that poles in the S-matrix on the positive imaginary k-axis correspond to bound states with energy $-\frac{\hbar^2\lambda^2}{2m}$. The same story holds for S_{--}.

Example. Now we look at our potential well again. Here $S_{++}(k) = -e^{-ika}\frac{q\tan(qa/2)-ik}{q\tan(qa/2)+ik}$. If we set $k = i\lambda$, then this has a pole when:

$$\lambda = q\tan\frac{qa}{2} \qquad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

Which is what we had during IB QM! SImilarly we can do this for the parity odd ones.

6.1.4 Resonances

Let's look at parity-even functions and assume S_{++} has a pole at $k = k_0 - i\gamma$ and of course $-k^*$ (generally). The energy is $E = E_0 - i\frac{\Gamma}{2}$ where $E_0 = \hbar^2\frac{k_0^2-\gamma^2}{2m}$ and $\Gamma = \frac{2\hbar^2 k_0}{m}$.

The imaginary energy is to remind us that this state (which evolves as $e^{-iET/\hbar}$) decays over time and $\tau = 1/\Gamma$ is its half-life. These kind of states appear when we have a high but *positive* potential well in which the particle eventually escapes but not for a long while. An example can be seen on the third example sheet with a pair of delta functions.

6.2 Scattering in Three Dimensions

Finally, we get to the topic of interest. Our hamiltonian is

$$H = \frac{p^2}{2m} + V(r)$$

This could be thought as the motion fo a single particle or the *relative motion* of 2 particles separated by distance r and interacting through $F = -\nabla V(r)$. To make our lives easier and pay no attention to 3D whatsoever, we will only consider rotaionally invariant potentials.

6.2.1 Cross-Section and A Lot Of Definitions

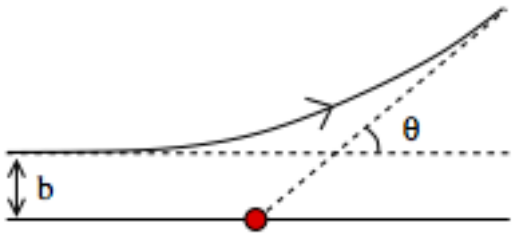


Figure 8: Classical Scattering

Here b is the closest approach point without scattering, or *impact parameter* and θ is the *scattering angle*. Consider a uniform circular beam of particles at b impact paramter. Let σ be the incoming cross-sectional area of the beam, and let Σ be the outgoing beam cross-sectional area, then we have $\mathrm{d}\sigma = b\mathrm{d}\phi\mathrm{d}b$ and $\mathrm{d}\Sigma = \sin\theta\mathrm{d}\phi\mathrm{d}\theta$, so we define the following:

Definition. - The *differential cross-section* is defined as:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Sigma} = \frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|$$

This is the ratio of the incoming and outgoing cross-sectional areas.

- The *total cross-section* is defined as:

$$\sigma_T = \int \mathrm{d}\Sigma \frac{\mathrm{d}\sigma}{\mathrm{d}\Sigma}$$

This, intuitively, tells us how "strong" the scattering is.

- The scattering amplitude $f(\theta)$ is defined as the θ coefficient of the scattering of a plane wave:

$$\psi_{scattered}(\mathbf{r}) = f(\theta)\frac{e^{ikr}}{r}$$

And we also have that $\frac{\mathrm{d}\sigma}{\mathrm{d}\Sigma} = |f(\theta)|^2$.

6.2.2 Partial Waves

We know that for spherical waves we have an expansion in terms of partial waves:

$$\psi(r,\theta) = \sum R_l(r)P_l(\cos\theta)$$

Where $P_l(\cos\theta)$ are *Legendre polynomials*. Remember they are eigenfunctions of the angular momentum operator of eigenvalue $\hbar^2 l(l+1)$. Then the Schrodinger equation becomes:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} - U(r) + k^2\right)R_l(r) = 0$$

Where we have rescaled the potential $U(r) = \frac{2m}{\hbar^2}V(r)$.

6.2.2.1 Asymptotic Waves

Now assume asymptotically the potential drops off quickly enough so that waves obey $U(r) = 0$. Then we have $R_0(r) = \frac{e^{\pm ikr}}{r}$. And for $l \neq 0$ the solutions are called *spherical Bessel functions*. Another solution is of course the plane wave e^{ikz} and with sufficient determination, we can write this as:

$$e^{ikr} = \sum_{l=0}^{\infty} \frac{2l+1}{2ik} \left[\frac{e^{ikr}}{r} - (-1)^l \frac{e^{-ikr}}{r} \right] P_l(\cos\theta)$$

So the plane wave decomposes into an outgoing spherial wave and an ingoing one (second term).

6.2.3 Scattering Amplitude, and Unitarity Bounds

We consider a plane wave coming in the z direction with e^{ikz} and we want to calculate solutions with the asymptotic form $\psi(r) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$. Expanding $f(\theta)$ into legendre polynomials with $f(\theta) = \sum \frac{2l+1}{k} f_l P_l(\cos\theta)$,we have:

$$\psi(r) \sim \sum \frac{2l+1}{2ik} \left[(-1)^{l+1} \frac{e^{-ikr}}{r} + (1 + 2if_l) \frac{e^{ikr}}{r} \right] P_l \cos\theta$$

Note for each l we have an ingoing and outgoing wave. This is 1D! For rotationally invaraint potentials, the 3D S-matrix S is diagonal in the angular momentum basis with $S_l = 1 + 2if_l = e^{2i\delta_i}$ where the second equality follows as S_l must be a phase. Then we have:

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta)$$

The differential cross section is then:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Sigma} = \frac{1}{k^2} \sum_{l,l'} (2l+1)(2l'+1) f_l f_{l'}^* P_l(\cos\theta) P_{l'}(\cos\theta)$$

The total cross section then can be evaluated using the orthogonality of Legendre polynomials to give:

$$\sigma_T = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$$

Then comparing to our $f(\theta)$ expansion we see:

$$\sigma_T = \frac{4\pi}{k} \operatorname{Im} f(0)$$

This is called the *optical theorem*. If we think of the total cross-section instead as built from the cross-sections for each partial wave, then we have:

$$\sigma_T = \sum \sigma_l \quad \sigma_l = \frac{4\pi}{k^2}(2l+1) \sin^2 \delta_l$$

Now each contribution is maximized when $\delta_l = \pm\frac{\pi}{2}$, called the unitarity bound.

6.2.4 An Example - The Hard Sphere

Ok, ok, let's do an actual example. Our scattering region is a hard sphere with infinite potential inside $r = a$ and 0 outside. We similarly decompose it in partial waves, and the radial part obeys:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{l(l+1)}{\rho^2} + 1\right)(\rho R_l(\rho)) = 0$$

where $\rho = kr$. The solutions to these are the spherical bessel functions $j_l(\rho)$ and $n_l(\rho)$ where:

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\sin\rho}{\rho} \qquad n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\cos\rho}{\rho}$$

The asymptotic forms are:

$$j_l(\rho) \to \frac{\sin(\rho - \frac{1}{2}l\pi)}{\rho} \quad n_l(\rho) \to \frac{\cos(\rho - \frac{1}{2}l\pi)}{\rho} \quad \rho \to \infty$$

And:

$$j_l(\rho) \to \frac{\rho^l}{(2l+1)!!} \quad n_l(\rho) \to -(2l-1)!!\rho^{-(l+1)}$$

Out of all of this, the only really useful thing is to see that n_l diverges at the origin and j_l does not.

The general solution for the radial equation is then:

$$R_l(r) = A_l\left[\cos\alpha_l j_l(\rho) - \sin\alpha_l n_l(\rho)\right]$$

The asymptotic form is $\sim \frac{1}{\rho}\sin(\rho - \frac{1}{2}l\pi + \alpha_l)$. While the expected form (remember the plane wave expansion) is:

$$R_l(r) \sim \frac{e^{i\delta_l}e^{i\pi l/2}}{\rho}\left[-e^{-i(\rho+\delta_l-\pi l/2)} + e^{i(\rho+\delta_l-\pi l/2)}\right]$$

And we see that they agree if $\alpha_l = \delta_l$, so we found our phase shift!

The boundary condition imposed by the sphere gives $R_l(a) = 0$, or in terms of phase shift:

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)}$$

For very low momentum, we can then expand this in powers of ka and get that:

$$\sigma_T = 4\pi a^2(1 + O((ka)^4))$$

which is a factor of 4 bigger than the corresponding classical πa^2 result. We also have $\delta_l \sim (ka)^{2l+1}$ at low momentum, so the scattering is dominated by the $l = 0$ wave which we can write as:

$$\delta_0 \sim -ka_s + O(k^3)$$

We call a_s the *scattering length.*

6.2.5 Bound States

We then consider a sphere of radius a again, but with potential $-V_0$ inside. Define $U(r) = \frac{2mV(r)}{\hbar^2}$ and $\gamma^2 = \frac{2mV_0}{\hbar^2}$. Then outside we have the free Schrodinger equation:

$$\psi(r) = \frac{A\sin(kr + \delta_0)}{r}$$

Where a similar argument as in the example above would show that δ_0 is the phase shift for the 0th partial wave. Inside the sphere we have:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 + \gamma^2\right)(r\psi) = 0$$

which gives the solution:

$$\psi(r) = \frac{B\sin(\sqrt{k^2+\gamma^2}r)}{r}$$

As the wavefunction needs to be regulat at $r = 0$. We patch the two solutions together and get the condition:

$$\frac{\tan(ka + \delta_0)}{ka} = \frac{\tan(\sqrt{k^2+\gamma^2}a)}{\sqrt{k^2+\gamma^2}a}$$

At low energies $k^2 \ll \gamma^2$ with $\frac{\tan(ka+\delta_0)}{ka} \approx \frac{\tan(\gamma a)}{\gamma a}$, we can rearrange the equation to get:

$$\tan\delta_0 = ka\left(\frac{\tan(\gamma a)}{\gamma a} - 1\right) + O(k^3)$$

So $a_s = a - \frac{\tan(\gamma a)}{\gamma}$. We see that the scattering length is negative for small γ (pulls into the scattering region) and it also has poles. We can do a similar derivation (but too boring to show here) that bound states exist exactly at the points which γ diverges and these are also exactly the points where the spherical wave component of the S matrix, $S_0(k)$ has poles.

6.2.6 Resonance

Again, if poles occur at energy $E = E_0 - \frac{i\Gamma}{2}$, then the S-matrix, which is a phase, must take the form:

$$S(E) = e^{2i\theta(E)}\frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}$$

By taylor expanding the solution (uninteresting). Set $\theta = 0$ to see the physics. Then we have:

$$\sin^2\delta = \frac{\Gamma^2}{4(E-E_0)+\Gamma^2}$$

Then using the expansion of σ_T in $\sin^2\delta_l$, we know that:

$$\sigma_T \approx \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2}{4(E-E_0)+\Gamma^2}$$

This is called the *Breit-Wigner distribution*, which looks like the following:

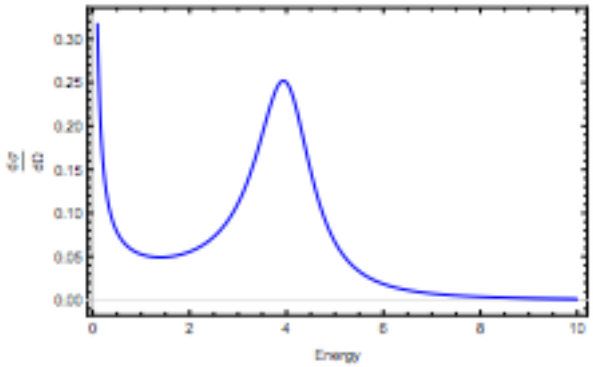


Figure 9: Breit-Wigner distribution

This is what the LHC is always looking for! This peak indicates scattered off particles and we try to measure its property.

6.3 Lippmann-Schwinger Equation

For the general time-independent Schrodinger equation, write $H_0 = -\frac{\hbar^2\nabla^2}{2m}$ and ϕ a state that satisfies $h_0|\phi\rangle = E|\phi\rangle$. Then we can rearrange the Schrodinger equation to:

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0}V|\psi\rangle$$

This is called the *Lippmann-Schwinger equation.*

6.3.1 The Green's Function

Note that the inverse operator $E - h_0$ is exactly the Green's function that obeys:

$$\left(E + \frac{\hbar^2\nabla^2}{2m}\right)G_0(E; r, r') = \delta(r - r')$$

Write $E = \frac{\hbar^2k^2}{2m}$ and rewrite the equation as:

$$(\nabla^2 + k^2)G_0(k; r - r') = \frac{2m}{\hbar^2}\delta(r - r')$$

Where the sneaky change in G_0 to $r - r' = q$ is by translational invaraince. We solve by Fourier transform:

$$\tilde{G}_0(k; q) = \int e^{-iqx}G_0(k; x)$$

This gives:

$$(-q^2 + k^2)\tilde{G}(k; q) = \frac{2m}{\hbar^2}$$

This is something we can solve! The answer is:

$$\tilde{G}_0(k;q) = -\frac{2m}{\hbar^2}\frac{1}{q^2-k^2}$$

Before one gets too excited, let's move back to position space:

$$G_0(k;x) = -\frac{2m}{\hbar^2}\int \frac{\mathrm{d}^3q}{(2\pi)^3}\frac{e^{iqx}}{q^2-k^2}$$

This integral, sadly, is not well-defined due to the singularity at $q = \pm k$. To resolve this, we use:

$$G_0^+(k;x) = -\frac{2m}{\hbar^2}\int \frac{\mathrm{d}^3q}{(2\pi)^3}\frac{e^{iqx}}{q^2-k^2-i\epsilon} \qquad \epsilon \to 0^+$$

We could have also used $+i\epsilon$, and it would have given us a different answer. We would see what they mean later. Now we polar transform:

$$\begin{aligned} G_0^+(k;x) &= -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^{2\pi}\mathrm{d}\phi\int_{-1}^{+1}\mathrm{d}(\cos\theta)\int_0^{\infty}\mathrm{d}q\frac{q^2e^{iqx\cos\theta}}{q^2-k^2-i\epsilon} \\ &= \frac{-2m}{\hbar^2}\frac{1}{(2\pi)^2ix}\int_{-\infty}^{\infty}\mathrm{d}q\frac{qe^{iqx}}{(q-k-i\epsilon)(q+k+i\epsilon)} \end{aligned}$$

The expansion here is valid as $\epsilon \to 0^+$ so we are safe. Then we complete a half circle in the upper half-plane using complex methods, which includes the pole at $k + i\epsilon$

$$= \frac{-2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ik|r-r'|}}{|r-r'|}$$

If we had picked $+\epsilon$ to start with, we would have ended up with a minus sign in the exponent. We now rewrite the Schrodinger equation as:

$$\psi(k;r) = e^{ikr} - \frac{2m}{\hbar^2}\int \mathrm{d}^3r'\frac{e^{ik|r-r'|}}{4\pi|r-r'|}V(r')\psi(k;r')$$

The interpretation is that e^{ikr} is the incident wave while the second term is a scattered wave. Therefore, it would be quite unphysical if we took reverse signs: A spherical wave would come in and turn into a plane wave!

Asymptotically, when rr', we have:

$$|r-r'| = \sqrt{r^2-2rr'+r'^2} \approx r - \frac{r\cdot r'}{r} + \cdot$$

Then we have:

$$G_0^+(k, r-r') \approx \frac{-2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}e^{-ikrr'}$$

So substituting in, we have:

$$\psi(r) \sim e^{ikr} + f(\theta,\phi)\frac{e^{ikr}}{r}$$

where $f(\theta,\phi) = \frac{-2m}{\hbar^2}\frac{1}{4\pi}\int \mathrm{d}^3r'e^{-ik\hat{r}r'}V(r')\psi(k;r')$. Wait, but we haven't actually solved it! That is true: we just got the form of it. To get more information, we need another tool:

6.4 The Born Approximation

We want to solve:

$$\psi(k,r) = e^{ikr} + \int \mathrm{d}^3 r G_0^+(k; r-r')V(r')\psi(k,r')$$

So we series expand! With $\psi(r) = \sum_0^\infty \phi_N(r)$, with $\phi_0(r) = e^{ikr}$. This gives that:

$$\phi_{n+1}(r) = \int \mathrm{d}^3 r' G_0^+(k; r-r')V(r')\phi_n(r')$$

Roughly speaking, this converges if V is like small.We truncate this by the leading term and say:

$$\psi(r) = e^{ikr} - \frac{2m}{4\pi\hbar^2}[\int \mathrm{d}^3 r' e^{iqr'} V(r')]\frac{e^i kr}{r}$$

Where $q = k - k\hat{r}$. But this is just the fourier transform. So the scattering amplitude is:

$$f(\theta,\phi) = \frac{-m}{2\pi\hbar^2}\tilde{V}(q)$$

Where $\tilde{V}$ is the fourier transform of V.

Example. We introduce the Yukawa potential $V(r) = \frac{Ae^{-\mu r}}{r}$. The fourier transform is:

$$\tilde{V}(q) = \frac{4\pi A}{q^2+\mu^2}$$

So the differential cross section is just $|f(\theta,\phi)|^2$, which is:

$$\left(\frac{2Am}{\hbar^2\mu^2 + 8mE\sin^2(\frac{\theta}{2})}\right)^2$$

6.5 Scattering off a Lattice

Note. This is the *final* topic of the entire course. I know, it is long indeed.

Denoting $k' = k\hat{r}$ as the scattered momentum (effectively replacing θ, ϕ), we know that if a wave localized at 0 is scattered off a potential which is localized around $\mathbf{R}$ then:

$$\psi(r) \sim e^{ik(r-R)} + f(k,k')\frac{e^{ik|r-R|}}{|r-R|}$$

Now let us have $r \to \infty$ and expand $|r-R| \approx r - \hat{r}\cdot R$. Then:

$$\psi(r) \sim e^{-ik\cdot R}\left[e^{ikr} + f(k,k')e^{-i(k'-k)\cdot R}\frac{e^{ikr}}{r}\right]$$

So we see that our effective scattering amplitude is $f(k)e^{iqR}$ where $q = k - k'$. Then if we have a lattice of points Λ , then :

$$f_\Lambda(k,k') = f(k,k')\sum_{R\in\Lambda} e^{iqR}$$

But we know what the sum is. From a long time ago when we were still talking about lattices, this vanishes unless $q \in \Lambda^*$. Then there is scattering from a lattice iff

$$k - k' \in \Lambda^*$$

This is known as the *Laue condition.*

6.5.1 The Bragg Condition, or Explaining to a Physicist^{TM}

There is an equivalent phrasing in real space. If we define $k \cdot k' = k^2 \cos\theta$, then taking the square of this gives:

$$|q| = 2k \sin(\theta/2)$$

Now each $q \in \Lambda^*$ defines a set of parallel planes in Λ known as Bragg planes and have $a \cdot q = 2\pi n$. The distance between successive planes is then $d = \frac{2\pi}{|q|}$. Furthermore, k corresponds to a wavelength $\lambda = \frac{2\pi}{k}$. Thus we have:

$$n\lambda = 2d \sin(\theta/2)$$

BUT WAIT! This is high school physics! If we treat the waves as scattering off successive planes, then they achieve constructive interference iff this condition is satisfied! (See Young's double slit experiment in high school)

This is the physicist's interpretation of *Laue's condition* and it is actually hard to justify that the particles scattering off planes, but *oh well.* They need some kind of heuristic explanation.

Note. I have nothing against physicists. I am just a faithful note copier. :).

6.5.2 The Structure Factor

If the lattice is not Bravais and instead described by a Bravais lattice and some atoms displaced by vectors d_i, then the scattering amplitude is replaced by $f(k.k') = \Delta(q)S(q)$ where $S(q) = \sum_i f_i(k.k')e^{iq \cdot d_i}$. The function $S(q)$ is called the geometric structure factor.

We are done!