

# **Advanced Quantum Engineering**

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# Chapter 1

## Perturbing Potentials in Engineered Systems

### I Perturbation Methods of Quantum Mechanics

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In quantum engineering, we encounter many scenarios where the Hamiltonian describing our potential is not analytically solvable. In order to investigate of such Hamiltonians, we have to succumb to a practical technique known as **perturbation theory**. In this context, we will be considering a class of Hamiltonian that is consisted of two distinct parts:

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{known}} + \underbrace{\hat{H}_1}_{\text{perturbed}} .$$

We do not know the eigen-spectrum of  $\hat{H}_1$ , but we now want to find the new eigenstates and eigenfunctions of the total Hamiltonian  $\hat{H}$ . There are two important assumptions that we have to make here:

1. The dominating Hamiltonian,  $\hat{H}_0$ , is known; as in, we know all the eigenenergies and eigenstates of  $\hat{H}_0$ .
2. The perturbing Hamiltonian,  $\hat{H}_1$ , is “small”.

The general strategy that we will apply here is to expand in terms of solutions to  $\hat{H}_0$ . Given that the Hamiltonian eigenvalue equation looks like,

$$\underbrace{\hat{H}_0 + \hat{H}_1}_{\hat{H}|\psi_\alpha\rangle + E_\alpha|\alpha\rangle},$$

where  $E_\alpha$  is the eigenenergy and  $|\psi_\alpha\rangle$  is the eigenstate of the full Hamiltonian, we can write the full eigen-spectrum as follows.

**Theorem 1.1: Ansatz for the Total Eigenspectrum**

$$\begin{aligned} |\psi_\alpha\rangle &= |\psi_\alpha^{(0)}\rangle + |\psi_\alpha^{(1)}\rangle + |\psi_\alpha^{(2)}\rangle + \cdots + |\psi_\alpha^{(n)}\rangle \\ E_\alpha &= E_\alpha^{(0)} + E_\alpha^{(1)} + E_\alpha^{(2)} + \cdots + E_\alpha^{(m)} \end{aligned}$$

There are two sub-classes of the Hamiltonian we are considering - if  $\hat{H}_1$  is time-independent, or if  $\hat{H}_1(t)$  is time-dependent.

## I.1 Time-Independent Perturbation Theory

We will first be considering the case if  $\hat{H}_1$  is independent of time. Plugging in the boxed substitution above into the original eigenvalue problem, we find,

$$\begin{aligned} & \left( \hat{H}_0 + \hat{H}_1 \right) \underbrace{\left( |\psi_\alpha^{(0)}\rangle + |\psi_\alpha^{(1)}\rangle + |\psi_\alpha^{(2)}\rangle + \cdots + |\psi_\alpha^{(n)}\rangle \right)}_{|\psi_\alpha\rangle} \\ &= \underbrace{\left( E_\alpha^{(0)} + E_\alpha^{(1)} + E_\alpha^{(2)} + \cdots + E_\alpha^{(m)} \right)}_{E_\alpha} \underbrace{\left( |\psi_\alpha^{(0)}\rangle + |\psi_\alpha^{(1)}\rangle + |\psi_\alpha^{(2)}\rangle + \cdots + |\psi_\alpha^{(n)}\rangle \right)}_{|\psi_\alpha\rangle} \end{aligned}$$

Define the **order** of our perturbation to be the sum  $n + m$ . For instance, a term with  $|\psi_\alpha^{(2)}\rangle$  and  $E_\alpha^3$  has order 5. Every order of the LHS should be equal to the order of the RHS. Thus, we can break the expression above into all the different orders. The zeroth-order equation looks like,

$$\hat{H}_0 |\psi_\alpha^{(0)}\rangle = E_\alpha^{(0)} |\psi_\alpha^{(0)}\rangle.$$

The first order equation would be a combination terms that yield  $n + m = 1$ , which are,

$$\hat{H}_0 |\psi_\alpha^{(1)}\rangle + \hat{H}_1 |\psi_\alpha^{(0)}\rangle = E_\alpha^{(0)} |\psi_\alpha^{(1)}\rangle + E_\alpha^{(1)} |\psi_\alpha^{(0)}\rangle.$$

If we dot both sides of the expression above with  $\langle \psi_\alpha^{(0)} |$ , the above equation becomes,

$$\begin{aligned} \langle \psi_\alpha^{(0)} | \hat{H}_0 | \psi_\alpha^{(1)} \rangle + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle &= \langle \psi_\alpha^{(0)} | E_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle + \langle \psi_\alpha^{(0)} | E_\alpha^{(1)} | \psi_\alpha^{(0)} \rangle \\ \langle \psi_\alpha^{(0)} | \hat{H}_0 | \psi_\alpha^{(1)} \rangle + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle &= E_\alpha^{(0)} \langle \psi_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle + E_\alpha^{(1)} \langle \psi_\alpha^{(0)} | \psi_\alpha^{(0)} \rangle \end{aligned}$$

Notice that, by definition, each order of the perturbation are linearly independent, as in the follows.

### Theorem 1.2: Linear Independence of $n$ -th Order Perturbations

$$\langle \psi_\alpha^{(m)} | \psi_\alpha^{(n)} \rangle = \delta_{mn}.$$

This is because if they are not orthogonal, there exists a component of  $|\psi_\alpha^{(m)}\rangle$  in  $|\psi_\alpha^{(n)}\rangle$ . If  $m > n$ , the extra component can simply be absorbed into  $|\psi_\alpha^{(m)}\rangle$  such that the two components are now orthogonal to each other. With that in mind, the above expression becomes,

$$\langle \psi_\alpha^{(0)} | \hat{H}_0 | \psi_\alpha^{(1)} \rangle + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle = E_\alpha^{(0)} \delta_{01} + E_\alpha^{(1)} \delta_{00}$$

Since the Hamiltonian operator is Hermitian, the Hermitian transpose of the Schrödinger equation becomes,

$$\hat{H}_0 |\psi_\alpha^{(0)}\rangle = E_\alpha^{(0)} |\psi_\alpha^{(0)}\rangle \leftrightarrow \langle \psi_\alpha^{(0)} | \hat{H}_0 = \langle \psi_\alpha^{(0)} | E_\alpha^{(0)}.$$

Using the Schrödinger equation, the above expression becomes,

$$\underbrace{E_\alpha^{(0)} \langle \psi_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle}_0 + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle = E_\alpha^{(1)}$$

Therefore, the first order perturbation of the energy would be as follows.

**Theorem 1.3: First Order Energy Correction**

$$E_\alpha^{(1)} = \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle$$

Going back to the first order eigenvalue equation, dotting both sides with  $\langle \psi_m^{(0)} |$ , where  $m \neq \alpha$ , would be,

$$\begin{aligned} \langle \psi_m^{(0)} | (\hat{H}_0 | \psi_\alpha^{(1)} \rangle + \hat{H}_1 | \psi_\alpha^{(0)} \rangle) &= \langle \psi_m^{(0)} | (E_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle + E_\alpha^{(1)} | \psi_\alpha^{(0)} \rangle) \\ \langle \psi_m^{(0)} | \hat{H}_0 | \psi_\alpha^{(1)} \rangle + \langle \psi_m^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle &= \langle \psi_m^{(0)} | E_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle + \underbrace{\langle \psi_m^{(0)} | E_\alpha^{(1)} | \psi_\alpha^{(0)} \rangle}_{m \neq \alpha} \\ E_m^{(0)} \langle \psi_\alpha^{(0)} | \psi_\alpha^{(1)} \rangle + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle &= E_\alpha^{(0)} \langle \psi_m^{(0)} | \psi_\alpha^{(1)} \rangle. \end{aligned}$$

Thus, the we see that the projection (coefficient) of  $|\psi_\alpha^{(1)}\rangle$  with  $|\psi_m^{(0)}\rangle$  would be,

$$\langle \psi_m^{(0)} | \psi_\alpha^{(1)} \rangle = \frac{\langle \psi_m^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle}{E_\alpha^{(0)} - E_m^{(0)}}$$

Thus, resolving the identity, we find that the first-order perturbed eigenstate can be written as,

**Theorem 1.4: First Order Eigenstate Correction**

$$|\psi_\alpha^{(1)}\rangle = \sum_{m \neq \alpha} \left( \langle \psi_m^{(0)} | \psi_\alpha^{(1)} \rangle \right) |\psi_m^{(0)}\rangle = \sum_{m \neq \alpha} \frac{\langle \psi_m^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle}{E_\alpha^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle$$

Now, we can solve perturbatively to the second order: the second-order terms of the eigenvalue equation would be,

$$\hat{H}_0 |\psi_\alpha^{(2)}\rangle + \hat{H}_1 |\psi_\alpha^{(1)}\rangle = E_\alpha^{(0)} |\psi_\alpha^{(2)}\rangle + E_\alpha^{(1)} |\psi_\alpha^{(1)}\rangle + E_\alpha^{(2)} |\psi_\alpha^{(0)}\rangle.$$

Dotting both sides by  $\langle \psi_\alpha^{(0)} |$ , the above equation becomes,

$$\underbrace{\langle \psi_\alpha^{(0)} | \hat{H}_0 | \psi_\alpha^{(2)} \rangle}_{\text{dies}} + \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(1)} \rangle = \underbrace{\langle \psi_\alpha^{(0)} | E_\alpha^{(0)} | \psi_\alpha^{(2)} \rangle + \langle \psi_\alpha^{(0)} | E_\alpha^{(1)} | \psi_\alpha^{(1)} \rangle}_{\text{dies}} + \langle \psi_\alpha^{(0)} | E_\alpha^{(2)} | \psi_\alpha^{(0)} \rangle$$

Simplifying the equation above yields,

$$\langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(1)} \rangle = E_\alpha^{(2)}.$$

However, the first order perturbation was already solved above. Substituting the known first-order perturbation from above, we see,

$$\begin{aligned} E_\alpha^{(2)} &= \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_\alpha^{(1)} \rangle \\ &= \sum_{m \neq \alpha} \underbrace{\frac{\langle \psi_m^{(0)} | \hat{H}_1 | \psi_\alpha^{(0)} \rangle}{E_\alpha^{(0)} - E_m^{(0)}}}_{\text{constant}} \left( \underbrace{\langle \psi_\alpha^{(0)} | \hat{H}_1}_{\text{not from } |\psi_\alpha^{(1)}\rangle} | \psi_m^{(0)} \rangle \right). \end{aligned}$$

Recognise the left term is the complex conjugate of the right term. Thus, the above summation, which is the second-order energy perturbation, can be written as,

**Theorem 1.5: Second Order Energy Correction**

$$E_\alpha^{(2)} = \sum_{m \neq \alpha} \frac{\left| \langle \psi_\alpha^{(0)} | \hat{H}_1 | \psi_m^{(0)} \rangle \right|^2}{E_\alpha^{(0)} - E_m^{(0)}}$$

Now, we will make a cute observation. Notice that if  $E_\alpha^{(0)}$  is the ground state, as in,

$$E_\alpha^{(0)} < E_m^{(0)} \quad \forall m,$$

then the denominator of the  $E_\alpha^{(2)}$  will be negative. Therefore, a very important sanity check we can make for the second-order perturbation would be as follows.

**Theorem 1.6: Second Order Energy Correction of the Ground State**

The energy of the ground state is always lowered by the second-order energy correction.

Now, we will try an interesting example.

**Problem 1.1: Perturbation of an Infinite Square Well**

Consider an unperturbed Hamiltonian corresponding to the square well of width  $a$  with infinitely high walls (hard walls). A particle of mass  $m$  is in this well. Now, as a perturbation, introduce a delta function potential in the middle of the well of strength  $\alpha$ . **a.** What is the first-order correction to the energy of the ground state? **b.** The second-order correction to the energy of the ground state can be expressed as an infinite series that can be summed exactly. Write down the expression for the second-order correction as a sum and then sum it exactly to provide a compact expression for the second-order correction. **c.** Which is larger: the first-order or second-order correction? Does the answer of which is larger depend on the parameters of the square well?

**Solution.** The  $n$ th eigenfunction  $\psi_n(x)$  for the infinite square well centred at the origin with length  $L$ , according to Shankar obeys the form and contains the eigenenergy

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & \text{odd } n \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & \text{even } n \end{cases}, \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2ML^2},$$



where  $L$  is the total width of the curve, and  $M$  is the mass of the particle.

**a.** Assume now we are engaging in a perturbation,

$$\hat{H} = \underbrace{\hat{H}_{\text{well}}}_{\hat{H}^0} + \underbrace{\hat{H}_{\text{delta function}}}_{\hat{H}^1} = \hat{H}^0 + \alpha\delta(x-0).$$

According to Shankar (17.1.7), the first-order energy correction due to the now additional  $\hat{H}^1$  Hamiltonian would be,

$$E_n^1 = \langle n^0 | \hat{H}^1 | n^0 \rangle.$$

Assuming  $n = 1$  to be in the ground state, we see that the above inner product can be written in integral form,

$$E_n^1 = \int_{-\infty}^{\infty} \psi_0^*(x) \hat{H}^1 \psi_0(x) dx = \int_{-\infty}^{\infty} \alpha \cos^2\left(\frac{\pi x}{a}\right) \delta(x) dx$$

Using the property of the Dirac delta function,

$$\int_{-\infty}^{\infty} f(x) \delta(x-x') dx = f(x'),$$

the above integral collapses into,

$$\boxed{E_1^1 = \alpha}$$

**b.** The second order energy correction can be written as the summation,

$$E_n^2 = \langle n^0 | \hat{H}^1 | n^1 \rangle = \sum_{m \neq n} \frac{|\langle n^0 | \hat{H}^1 | m^0 \rangle|^2}{E_n^0 - E_m^0}.$$

Again, expanding inner product above using integral form and substituting the eigenenergies according to the eigensystem of the infinite square well listed above, we see that the second-order correction becomes,

$$E_{\text{ground}}^2 = \sum_{m \neq \text{ground}} \frac{2M}{\hbar^2 \pi^2 (1 - m^2)} \left[ \int_{-\infty}^{\infty} \psi_{\text{ground}}^* \alpha \delta(x) \psi_m dx \right]^2$$

which, evaluating the Dirac delta function, becomes,

$$E_{\text{ground}}^2 = \sum_{m \neq \text{ground}} \frac{2\alpha M}{\hbar^2 \pi^2 (1 - m^2)} \left[ \underbrace{\sqrt{\frac{2}{a}}}_{\cos 0 = 1} \psi_m(0) \right]^2$$

However, we know that  $\sin 0$  will always equal to zero, therefore all the even  $m$  above will become zero. Thus, we only need to consider the odd terms in the summation above, which becomes,

$$\boxed{E_{\text{ground}}^2 = \frac{8\alpha M}{\hbar^2 \pi^2 a^2} \sum_{\text{odd } m > 1} \frac{1}{1 - m^2}}$$

Writing the above summation in terms of a telescoping series,

$$\frac{1}{1 - m^2} = \frac{1}{2(m+1)} - \frac{1}{2(m-1)},$$

we can express the above summation as,

$$\begin{aligned}
 \sum_{\text{odd } m > 1} \frac{1}{1 - m^2} &= \frac{1}{1 - 3^2} + \frac{1}{1 - 5^2} + \frac{1}{1 - 7^2} + \cdots \\
 &= \frac{1}{2(3+1)} - \frac{1}{2(3-1)} + \frac{1}{2(5+1)} - \frac{1}{2(5-1)} + \frac{1}{2(7+1)} - \frac{1}{2(7-1)} + \cdots \\
 &= \frac{1}{2(4)} - \frac{1}{2(2)} + \frac{1}{2(6)} - \frac{1}{2(4)} + \frac{1}{2(8)} - \frac{1}{2(6)} + \cdots = -\frac{1}{4}
 \end{aligned}$$

since every  $n$ th and  $n + 3$ rd term cancels each other out. Thus, substituting this into the above equation, we see,

$$E_{\text{ground}}^2 = -\frac{2\alpha M}{\hbar^2 \pi^2 a^2},$$

which validates the theorem that the second time-independent perturbation of every ground state will be negative.

**c.** *There are two interpretations of this problem: the magnitude of the energy shift, or the value of the energy shift.*

- Magnitude of the energy shift: The ratio between the first and second order energy correction would be,

$$\frac{E_{\text{ground}}^2}{E_{\text{ground}}^1} = \frac{2\alpha M}{\hbar^2 \pi^2 L^2} \frac{1}{\alpha} = \frac{2M}{\hbar^2 \pi^2 a^2}$$

The relative size of the first and second order corrections **depend on the parameters of the square well**: precisely, the **mass** and the **size** of the box. If  $2M/\hbar^2 \pi^2 L^2 > 1$ , then  $E^2$  is larger, if  $2M/\hbar^2 \pi^2 L^2 < 1$ , then  $E^1$  is larger.

- Value of energy shift: Assuming that  $\alpha$  is always positive, the first order perturbation is positive and the second order perturbation is negative. Thus, first order correction is greater than the second order perturbation, regardless of other parameters of the well.

## 1.2 Time-Dependent Perturbation Theory

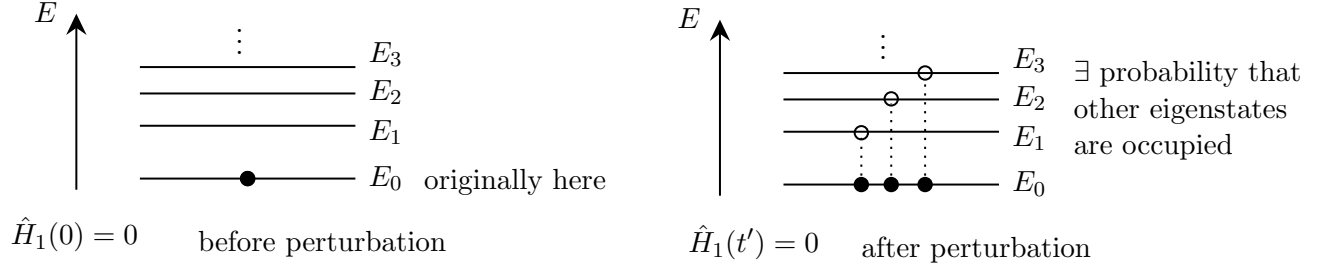
We will now be considering the case if the perturbing Hamiltonian is time-dependent, as in,

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t).$$

Again, we are expected to know the full solution to the unperturbed Hamiltonian. While  $H^0$  has a well-defined eigensystem,  $H(t)$ , and subsequently,  $\hat{H}(t)$  does not have a full eigensystem. Thus, instead of finding the  $n$ th order corrections to the eigensystem, we are trying to find the **transitions**, or the probability that another eigenstate other than the original eigenstate is occupied. We can visualise our objective as follows:

In typical situations the perturbation  $H^1(t)$  vanishes for  $t < t_0$ , exists for some finite time, and then vanishes for  $t > t_f$ . We ask ourselves the central question of time-dependent perturbation theory:

What is the probability for our particle to be in the new eigenstate  $|f^{(0)}\rangle$  at a later time  $t$ , if the particle was originally in the initial eigenstate  $|i^{(0)}\rangle$ ?



Originally, when there were not any time-dependent perturbation, the full time-dependent wavefunction of a quantum particle would be,

$$|\Psi(t)\rangle = \sum_{\alpha} c_{\alpha}(t) |\psi_{\alpha}(t=0)\rangle,$$

where, according to the Schrödinger equation, the time evolution of each coefficient would be,

$$c_{\alpha}(t) = c_{\alpha}(0) \exp\left(-\frac{iE_{\alpha}t}{\hbar}\right).$$

Now, it is different. Using the above form of the time-dependent wavefunction, we guess that our new wavefunction due to a time-dependent perturbation will look like,

**Theorem 1.7: Ansatz for a Time-Dependent Perturbation**

$$|\Psi(t)\rangle = \sum_{\alpha} d_{\alpha}(t) \exp\left(-\frac{iE_{\alpha}t}{\hbar}\right) |\psi_{\alpha}^{(0)}\rangle$$

Plugging this ansatz into the Schrödinger equation,

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = (\hat{H}_0 + \hat{H}_1(t)) |\Psi(t)\rangle,$$

we can get the time-dependence of the  $d_{\alpha}$  coefficient for the  $|f\rangle$  state,  $d_f$ , to be,

$$\dot{d}_f(t) = -\frac{i}{\hbar} \langle f^{(0)} | \hat{H}_1(t) | i^{(0)} \rangle \exp(i\omega_{f \leftarrow i} t), \text{ where } \omega_{f \leftarrow i} \equiv \frac{E_f^{(0)} - E_i^{(0)}}{\hbar}.$$

The  $d_n$  coefficients can be interpreted as the **transition probability amplitude** for the transition  $|i\rangle \rightarrow |f\rangle$ ; in other words, the probability amplitude for measuring a particle of with original eigenvalue  $E_i^{(0)}$  to be in the new eigenvalue  $E_f^{(0)}$ . Integrating the equation above with respect to time, we yield the transition probability amplitude to be,

**Theorem 1.8: Transition Probability Amplitude**

The transition probability amplitude (in the first order) due to a time-dependent perturbation can be expressed as,

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar} \int_0^t \langle f^{(0)} | \hat{H}_1(t') | i^{(0)} \rangle \exp(i\omega_{f \leftarrow i} t') dt' \text{ where } \omega_{f \leftarrow i} \equiv \frac{E_f^{(0)} - E_i^{(0)}}{\hbar}.$$

To find the actual probability (density) of finding the particle in state  $|f\rangle$  starting from  $|i\rangle$ , we simply square the modulus of the  $d_f$  coefficient.

**Theorem 1.9: The Transition Probability**

$$P(\text{finding state in } |\psi_f^0\rangle \text{ at time } t) = |d_f(t)|^2$$

We will now do another very instructive example.

**Problem 1.2: Time Dependent Perturbation of the Infinite Square Well**

Consider the hard wall square well of width  $a$ . A particle of mass  $m$  is in the ground state of this well. At time 0 a perturbation begins, in which a potential  $V_0$  becomes present in the left half of the well. **a.** At time  $T > 0$  the energy of the particle is measured. What is the probability that the energy of the particle is measured to be that of the first excited state in the quantum well? Treat the calculation perturbatively (e.g. do not consider excitations to other states that then lead to population of the first excited state). **b.** What is the first time after  $T = 0$  that the probability is zero?

**Solution.**

**a.** The perturbation Hamiltonian after  $t > 0$  would look like,

$$H_1(t > 0) = \begin{cases} V_0 & -\frac{L}{2} < x < 0 \\ 0 & \text{otherwise} \end{cases}.$$

Thus, we can compute the matrix element due to this perturbation between the ground ( $|1\rangle$ ) and the first excited state ( $|2\rangle$ ) in function space to be,

$$\langle 2 | \hat{H}_1(t) | 1 \rangle = \int_{-\infty}^{\infty} \psi_2^*(x) \hat{H}_1(x, t > 0) \psi_1(x) dx = \frac{2}{L} \int_{-a/2}^0 \cos\left(\frac{\pi x}{a}\right) V_0 \sin\left(\frac{2\pi x}{a}\right) dx = -\frac{4V}{3\pi}.$$

Moreover, the Bohr frequency between the ground and first excited state would be,

$$\omega_{2 \leftarrow 1} = \frac{1}{\hbar} \left[ \frac{\hbar^2 \pi^2 (2)^2}{2Ma^2} - \frac{\hbar^2 \pi^2 (1)^2}{2Ma^2} \right] = \frac{3\hbar \pi^2}{2Ma^2}$$

Thus, the probability amplitude equation becomes,

$$\dot{d}_2(t) = -\frac{i}{\hbar} \left( -\frac{4V}{3\pi} \right) \exp(i\omega_{2 \leftarrow 1} t).$$

Integrating the equation above yields,

$$\begin{aligned} d_2(t) &= -\frac{4V_0 i}{3\pi \hbar} \int_0^T \exp(i\omega_{2 \leftarrow 1} t) dt = -\frac{8a^2 m V_0}{9\pi^3 \hbar^2} i [\exp(i\omega_{2 \leftarrow 1} T) - 1] \\ &= \frac{16a^2 m V_0}{9\pi^3 \hbar^2} \left[ \frac{\exp(i\omega_{2 \leftarrow 1} T/2) - \exp(-i\omega_{2 \leftarrow 1} T/2)}{2i} \right] \exp(i\omega_{2 \leftarrow 1} T/2) \\ &= \frac{16a^2 m V_0}{9\pi^3 \hbar^2} \sin(\omega_{2 \leftarrow 1} T/2) \exp(i\omega_{2 \leftarrow 1} T/2). \end{aligned}$$

Finding the magnitude squared of the probability amplitude coefficient yield the total probability of finding the state (and eigenenergy)  $|f\rangle, E_f$  at time  $t$ , which would be,

$$P\left(\text{finding state in } |\psi_f^{(0)}\rangle \text{ at time } t\right) = |d_{2\leftarrow 1}(t)|^2 = \left(\frac{16a^2mV_0}{9\pi^3\hbar^2}\right) \sin^2\left(\frac{3\hbar\pi^2}{4Ma^2}t\right).$$

b. The zeroes of the  $\sin^2(x)$  function occurs when  $x = n\pi$ , where  $n$  is an integer. Simply setting  $n = 1$ , we see the next time the  $\sin^2$  function reaches zero would be,

$$\frac{3\hbar\pi^2}{4Ma^2}T = \pi, \quad \rightarrow \quad T = \frac{4Ma^2\pi}{3\hbar\pi^2}.$$

### I.3 Different Pictures of Quantum Mechanics

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In the above derivation, both the wavefunction  $|\Psi(t)\rangle$  and the operator  $\hat{H}_1(t)$  are evolving in time. However, can we find a new description of quantum mechanics - i.e. **picture** - such that the state is independent of time?

In theory, not really. However, in practice, we often really only care about the expected value of an operator,  $\langle\hat{O}\rangle$ , and we can manipulate the expected value however mathematically we want. First, we discuss the time evolution and the expected value in the typical course of quantum mechanics: in this case, the wavefunction is time-dependent. This picture of quantum mechanics is called the **Schrödinger picture**, thus the subscript  $S$ .

$$i\hbar\frac{\partial|\Psi_S(t)\rangle}{\partial t} = \hat{H}_S|\Psi_S(t)\rangle, \quad \leftrightarrow \quad \Psi_S(t) = \exp\left(-i\frac{\hat{H}_S t}{\hbar}\right)|\Psi_S(t=0)\rangle.$$

Thus, an operator  $\hat{O}$  will obey the form,

$$\hat{O}_S = \hat{O} \exp\left(-i\frac{\hat{H}_S t}{\hbar}\right)|\Psi_S(t=0)\rangle,$$

and its expected value becomes,

$$\begin{aligned} \langle\hat{O}\rangle &= \langle\Psi(t)|\hat{O}_S|\Psi(t)\rangle = \exp\left(i\frac{\hat{H}_S t}{\hbar}\right)\langle\Psi_S(t=0)|\hat{O}|\Psi_S(t=0)\rangle\exp\left(-i\frac{\hat{H}_S t}{\hbar}\right) \\ &= \langle\Psi_S(t=0)|\hat{O}|\Psi_S(t=0)\rangle. \end{aligned}$$

The exponent factor in the above computation of the expected value cancels each other out due to complex conjugation; thus, the expected value is time independent. However, we can regroup the computation of the expected value by defining a new operator  $\hat{O}_H$  to be,

$$\langle O \rangle = \langle \Psi(t=0) | \underbrace{e^{i\hat{H}t/\hbar} \hat{O} e^{-i\hat{H}T/\hbar}}_{\hat{O}_H} | \Psi(t=0) \rangle \equiv \langle \Psi(t=0) | \hat{O}_H | \Psi(t=0) \rangle$$

In this case, the wavefunction becomes independent of time, while the operator now varies with time - this formalism of quantum mechanics is called the **Heisenberg picture**. The wavefunction and the operators in the Heisenberg picture is defined as follows.

**Theorem 1.10: Wavefunction and Operators in the Heisenberg Picture**

$$|\Psi_H\rangle \equiv |\Psi_S(t=0)\rangle$$

$$\hat{O}_H(t) \equiv e^{i\hat{H}t/\hbar} \hat{O}_S e^{-i\hat{H}t/\hbar}$$

## II Photon Absorption

In this section, we will develop intuition on Fermi's Golden rule and how to use it properly.

### II.1 Fermi's Golden Rule

The Fermi's Golden Rule is essentially an application of time-dependent perturbation theory to periodic potentials, as in,

$$\hat{H}_1(t) = \hat{V} \cos(\omega t).$$

Fermi's Golden Rule gives us the **transition rate**, the probability of a transition per unit time, from one eigenstate  $|i\rangle$  to another  $|f\rangle$ . The transition rate is defined as follows.

**Theorem 1.11: the Transition Rate**

he transition rate from one eigenstate  $|i\rangle$  to another  $|f\rangle$  would be,

$$R_{i \rightarrow f} \equiv \frac{P_{i \rightarrow f}}{T} = \frac{|d_f(t)|^2}{T}$$

where  $T$  is the time duration for the given transition to happen.

Fermi's Golden Rule states the following.

**Theorem 1.12: Fermi's Golden Rule**

If there exists a constant<sup>a</sup>, sinusoidal perturbing Hamiltonian in the form  $\hat{H}_1 = \hat{V} \cos(\omega t)$ , then the transition rate between the eigenstates  $|i\rangle$  and  $|f\rangle$  would be,

$$R_{i \rightarrow f} = \frac{2\pi}{\hbar^2} |\langle f | \hat{V} | i \rangle|^2 \delta(\omega_{f \leftarrow i} - \omega), \text{ where } \omega_{f \leftarrow i} = \frac{E_f - E_i}{\hbar}.$$

<sup>a</sup>As in, it does not stop for a *very* long time.

**Proof.** From previous discussions, we have seen that the probability amplitude of transitions between an initial state  $|i\rangle$  to  $|f\rangle$  due to a time-dependent perturbation  $\hat{H}^{(1)} = \hat{V}_0 \cos \omega t$  for time  $T$  would be,

$$P_{i \rightarrow f} = P_{f \rightarrow i} = \frac{|E_0 P_{if}|^2}{\hbar^2 (\omega_{if} - \omega)^2} \sin^2 \left( \frac{(\omega_{if} - \omega)T}{2} \right) = \frac{|E_0 P_{if}|^2 T^2}{\hbar^2 4} \left( \frac{\sin x(T)}{x(T)} \right)^2,$$

where the function  $x(T)$  is defined as,

$$x(t) = \frac{\omega_{if} - \omega}{2} T.$$

Now, we define the function  $\delta_t(\alpha)$  to be,

$$\delta_t(\alpha) \equiv \frac{\sin^2 \alpha t}{\pi \alpha^2 t},$$

which we know that the function has the properties,

$$\delta_t(\alpha) \begin{cases} = t/\pi & \text{for } \alpha = 0 \\ \leq 1/\pi \alpha^2 t & \text{otherwise} \end{cases}, \quad \int_{-\infty}^{\infty} dy \frac{\sin^2 y}{y^2} = \pi.$$

Therefore, for a test function  $F(\alpha)$ , one has,

$$\lim_{t \rightarrow \infty} \int_{-\infty}^{\infty} d\alpha \delta_t(\alpha) F(\alpha) = \lim_{t \rightarrow \infty} \int_{-\infty}^{\infty} dy \frac{\sin^2 y}{\pi y^2} F\left(\frac{y}{t}\right) = F(0),$$

and thus the sequence of functions  $\delta_t(\alpha)$  is a representation of the Dirac delta function,

$$\lim_{t \rightarrow \infty} \delta_t(\alpha) = \delta(\alpha).$$

Thus, for long times, we obtain from the previous equation,

$$P_{i \rightarrow f} = T \frac{2\pi |V_{nm}|^2}{\hbar^2} \delta(E_n - E_m)$$

From this, we can obtain the transition rate, that is, the transition probability per unit time,

$$R_{i \rightarrow f} \equiv \frac{P_{i \rightarrow f}}{T} = \frac{2\pi}{\hbar^2} |\langle f | \hat{V} | i \rangle|^2 \delta(\omega_{f \leftarrow i} - \omega), \text{ where } \omega_{f \leftarrow i} = \frac{E_f - E_i}{\hbar} \quad \square$$

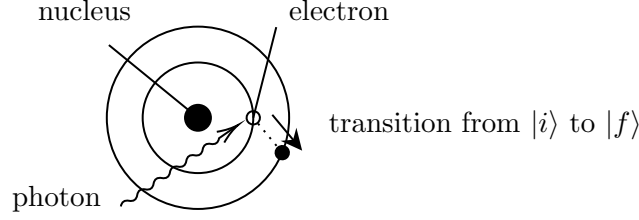
However, if we are treating transitions into states of (almost of) continuous spectrum, we are more interested in the transition rate to *a group of states*. We suppose that the matrix elements of all these final states are equal, and introduce the density of states  $\rho(E_n)$ , where  $\rho(E_n)dE_n$  gives the number of states with energy between  $E_n$  and  $E_n + dE_n$ . The transition rate into this set of states would therefore be,

$$R_{i \rightarrow \text{group}} = \sum_f R_{i \rightarrow f} = \int dE_f \rho(E_f) R_{if} = \frac{2\pi}{\hbar^2} |\langle f | \hat{V} | i \rangle|^2 \rho(E_f).$$

## II.2 Photon Absorption in Atomic Systems

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We will now perform two examples of Fermi's golden rule to various systems. First, let's look at bound electrons in an atom.



### Bound Electrons in an Atom

If we shine an electromagnetic wave on an atom, we know that the electron in the atom will transition from one state to another, as in,  $|i\rangle$  to  $|f\rangle$ , due to the **absorption** of a photon. A diagram of the situation is as follows.

Here, the interaction between the atom and the electron is best described by a **dipole interaction Hamiltonian**,

$$\hat{H}_1 = -e \underbrace{\vec{E}(r)}_{\text{electric field}} \cos(\omega(t)) \cdot \underbrace{\vec{r}}_{\text{pos. of electron}} \equiv \boxed{\vec{d} \cdot \vec{E}_0 \cos(\omega t)}$$

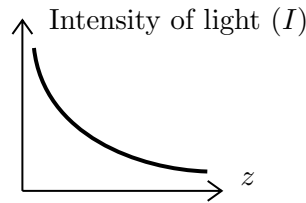
Here, the operator  $\hat{d}$  is called the **dipole operator**, and is defined as follows,

$$\boxed{\hat{d} \equiv q\vec{r}}.$$

For an electron,  $q = -e$ . In essence, we are suggesting that the nucleus-electron pair *approximately* acts as a dipole from the centre. We will now try to derive the **dielectric function**, or the function describing the interaction of light with the atom. Precisely, the dielectric function describes how much of the light is absorbed and reflected in the process.

### Step 1: Absorption rate of a photon by an atom.

We will first consider the macroscopic decay of optical waves along the  $+z$  direction. We expect our light wave to obey the following position-intensity graph. The most simple function of intensity



that models this process would be an exponential decay, as in,

$$I(z) = I_0 \exp(-\alpha z).$$

The  $\alpha$  coefficient here is called the **absorption coefficient**, and is proportional to the  $1/L$ . The time derivative of intensity would be, q

$$\frac{dI}{dt} = \frac{dI}{dz} \frac{dz}{dt} = \underbrace{-\alpha I}_{dI/dz} \underbrace{\left(\frac{c}{n}\right)}_{dz/dt, \text{ wavespeed.}}$$

where  $n$  is the index of refraction.



Due to the conservation of energy, whatever energy that is decayed must go *somewhere*: we know that the light got absorbed by the atom, and we can use Fermi's golden rule to find out how much light was absorbed. The absorption intensity would be the absorption rate  $R_{if}(\omega)$  multiplied by the amount of energy *per absorption* as follows.

$$\underbrace{-\alpha I \left( \frac{c}{n} \right)}_{\text{decay of intensity}} = \underbrace{-R_{if}(\omega)\omega}_{\text{absorption by atom}}.$$

Therefore, can solve for  $\alpha$  to be, while substituting the intensity of light with the electric field,

$$\alpha = \frac{R(\omega)\hbar\omega}{I(c/n)} \xrightarrow{I=n^2 E^2/8\pi} \boxed{\alpha = \frac{8\pi\hbar\omega}{nc} \frac{R(\omega)}{E^2(\omega)}}.$$

### Step 2: Imaginary part of $\epsilon$ .

The electric field of the propagating electric field would look like,

$$E(z, t) = E_0 \exp -i(kz - \omega t),$$

assuming that it only travels in one direction. Here, the wavenumber of the EM wave as it interacts with the atom would be,

$$k \equiv \sqrt{\epsilon} \frac{\omega}{c},$$

where  $\epsilon$  behaves like a permittivity factor. However, since there is dissipation, there will be both a real and an imaginary part to the permittivity and, as expected, the dielectric constant,

$$\epsilon = \epsilon_R + i\epsilon_I, \quad \kappa = \kappa_R + i\kappa_I.$$

Expanding the square root of the permittivity, we yield<sup>1</sup>,

$$\epsilon^{1/2} = (\epsilon_R + i\epsilon_I)^{1/2} \approx \sqrt{\epsilon_R} \left( 1 + \frac{i\epsilon_I}{2\epsilon_R} \right),$$

therefore, we can get the imaginary part of the dielectric constant to be,

$$\kappa_I = \frac{\epsilon_I}{2n} \frac{\omega}{c}.$$

Here,  $\kappa_I$  can be directly related to  $\alpha$  via the expression,

$$I \propto E^2 \xrightarrow[k=\sqrt{\epsilon}\omega/c]{\kappa_I \propto \omega/c} \exp(-2\kappa_I z) \xrightarrow[\text{from intensity decay}]{\propto} \exp(-\alpha z).$$

Thus, we can solve  $\alpha$  to be,

$$\boxed{\alpha = \frac{\epsilon_I}{n} \frac{\omega}{c}} \xrightarrow[\text{from previous}]{=} \frac{8\pi\hbar\omega}{nc} \frac{R(\omega)}{E^2(\omega)}.$$

Therefore, solving for  $\epsilon_I$  yields,

$$\epsilon_I = \frac{nc}{\omega} \frac{8\pi\hbar\omega}{nc} \frac{R(\omega)}{E^2(\omega)} = 8\pi\hbar \frac{R(\omega)}{E(\omega)^2}.$$

<sup>1</sup>As a reminder, the index of refraction and the permittivity are related via  $n = \sqrt{\epsilon_R}$ .

According to Fermi's golden rule, we know that,

$$R_{if}(\omega) = \frac{2\pi}{\hbar^2} |\langle f | \hat{V} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega).$$

However, we also know that the perturbing Hamiltonian takes the form,

$$\hat{V} = \hat{d} \cdot \hat{E}_0 = (q\hat{r}) \cdot \hat{E}_0.$$

Thus, we see, substituting  $q = -e$  for an electron,

$$R_{if}(\omega) = \frac{e^2}{E^2(\omega)} \frac{2\pi}{\hbar^2} |\langle f | \hat{r} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega).$$

Substituting  $R_{if}(\omega) = R(\omega)$  into our expression of  $\epsilon_I$ , we yield,

$$\epsilon_I = 16\pi^2 e^2 |\langle f | \hat{r} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega).$$

### Step 3: Some Complex Analysis\*

We will be using some relations from complex analysis that we don't need to go into great details of. Once we know the imaginary part of the permittivity, we can actually solve for the real part using the **Kramers–Kronig relations**, which follows the following form.

$$\begin{aligned} \epsilon(\omega) &= \epsilon_R(\omega) + i\epsilon_I(\omega) \\ \epsilon_R(\omega) &= \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\epsilon_I(\omega')}{\omega' - \omega} d\omega' \\ \chi_I(\omega) &= -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\chi_R(\omega')}{\omega' - \omega} d\omega', \end{aligned}$$

where  $\mathcal{P}$  is the **Cauchy principal value** operator. We will also use a mathematical trick,

$$2\pi\delta(\omega - \omega_0) = \lim_{\delta \rightarrow 0} \text{Im} \left[ \frac{1}{\omega_0 - \omega + i\delta} \right],$$

which then yield the full permittivity function to be as follows<sup>2</sup>,

#### Theorem 1.13: The Dielectric Function

The **dielectric function** describes the response of a given material to an external electric field; the dielectric function due to an absorption of a photon by an electron from  $|i\rangle$  to  $|f\rangle$  would be,

$$\epsilon(\omega) = \lim_{\delta \rightarrow 0} \frac{8\pi e^2 |\langle f | \hat{r} | i \rangle|^2}{E_f - E_i - \hbar\omega + i\delta} = \epsilon(\omega) = \lim_{\delta \rightarrow 0} \frac{8\pi |\langle f | \hat{d} | i \rangle|^2}{E_f - E_i - \hbar\omega + i\delta}$$

Physically, the matrix element  $\langle \psi_f | \hat{r} | \psi_i \rangle$  is the magnitude of transition, called the **transition dipole moment**. Once the full dielectric function is known, a number of other optical properties can also be calculated - for instance, the complex refractive index,  $N(\omega)$ , which is related directly to the complex dielectric function via the relationship,

$$N(\omega) = \sqrt{\epsilon(\omega)}$$

<sup>2</sup>Here is a useful reference on the same topic: <https://spiral.imperial.ac.uk/bitstream/10044/1/9174/1/Ratcliff-LE-2012-PhD-Thesis.pdf>

### How to calculate the matrix element?

The matrix element  $\langle \psi_f | \hat{d} | \psi_i \rangle$  is a scalar value that can be calculated through an integral. For instance, if we have an electron in a hydrogen atom with an electron starting in the  $2p$  orbital and moving into the  $2s$  orbital, the transition dipole moment for this process can be written as  $\langle \psi_{2p} | \hat{d} | \psi_{2s} \rangle$ . Recall that the dipole operator  $\hat{d}$  can be rewritten as  $\hat{d} = q\hat{r}$ . To calculate the matrix element, we simply sandwich the dipole operator with the wavefunctions,

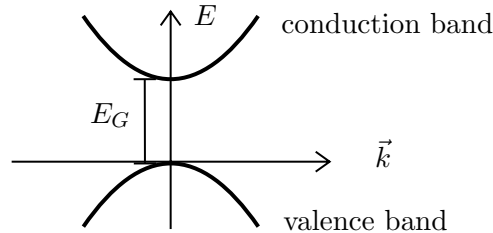
$$\langle \psi_{2p} | \hat{p} | \psi_{2s} \rangle = e \langle \psi_{2p} | \hat{r} | \psi_{2s} \rangle = -e \int \psi_{2p}^* \vec{r} \psi_{2s} d^3r = \boxed{-e \iiint \psi_{2p}^*(r) \psi_{2s} d^3r}$$

Again, we can write the wavefunctions of the  $2p$  and  $2s$  wavefunctions in position basis and evaluate the numerical result of the integral above.

## II.3 Dielectric Function of a Direct Band Gap Semiconductor

In the previous section, we found the dielectric function for a particle where  $\langle \hat{r} \rangle$  is pretty well-defined in the atom. However, in many situations,  $\langle \hat{r} \rangle$  might not be well-defined. Can we still find a dipole operator and thus find the dielectric function of these objects?

The answer is, of course, yes. We will now consider the dielectric function of a **direct band gap semiconductor**, for instance, Gallium arsenide (GaAs). Attached in the figure below is the dispersion curve for the energy band of the Dirac band gap semiconductor -electrons only have eigenstates within a certain **energy band**. In the case of a Dirac band gap semiconductor, there are two modes of energy per wavelength  $|k\rangle$ , as seen below.



The above energy band can actually be very well approximated using the expressions,

$$\boxed{E_c(k) \approx E_G + \frac{\hbar^2 k^2}{2m_C}, \quad E_V(k) \approx -\frac{\hbar^2 k^2}{2m_V}},$$

where  $m_C$  and  $m_V$  are the *effective* electron masses in the respective bands.

### Step 1: Find interaction Hamiltonian.

To solve for the dielectric function of a direct band gap semiconductor, we first need to write the Hamiltonian this system obeys. Classical electrodynamics dictate that the Hamiltonian field of an EM field would be,

$$\hat{H} = \frac{(\hat{p} - e\hat{A}/c)^2}{2m} + q\phi$$

where  $\hat{p}$  is the momentum operator (for the electron),  $\hat{A}$  is the vector potential (due to the EM wave), and  $\phi$  is the scalar potential. Expanding  $\hat{H}$ , we see that the Hamiltonian can be partitioned into three parts.

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + q\phi}_{\text{Hamiltonian of free electron}} + \underbrace{\frac{e^2}{2mc^2}\hat{A}^2}_{\text{property of EM wave}} + \underbrace{-\frac{e}{2mc}(\hat{p} \cdot \hat{A} + \hat{A} \cdot \hat{p})}_{\text{coupling strength}}.$$

Since the Hamiltonian of the free electron and the third term will *always* be there whenever we have an atom and EM wave, the strength of the coupling will be contingent to the last two terms of the above expression. Thus, we can consider the coupling strength Hamiltonian to be the perturbing Hamiltonian,

$$\hat{H}_1 = -\frac{e}{2mc} (\hat{p} \cdot \hat{A} + \hat{A} \cdot \hat{p})$$

Choosing the **Coulomb gauge** such that  $[\hat{p}, \hat{A}] = \nabla \cdot \hat{A} = 0$ , the perturbing Hamiltonian can be written as,

$$\boxed{\hat{H}_1 = -\frac{e}{2mc} \hat{A} \cdot \hat{p}}$$

From classical electrodynamics, we know that the relationship between the vector potential and the electric field would be,

$$\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t}.$$

Assuming that the scalar potential is negligible, we can relate the vector potential and a sinusoidally oscillating electric field via the relationship,

$$\vec{E} = \vec{E}_0 \exp(i\omega t), \rightarrow \boxed{-i\omega\vec{A} = \vec{E}}.$$

Therefore, we can write the perturbing Hamiltonian as,

$$\hat{H}_1 = -\frac{e}{2mc} \left( -\frac{1}{i\omega} \vec{E} \right) \cdot \hat{p} = \frac{\vec{E} \cdot \vec{p}}{i\omega} \frac{e}{mc} = \boxed{\frac{\vec{E}_0 \cdot \hat{p}}{i\omega} \frac{e}{mc} \exp(i\omega t)}.$$

Since our perturbing potential is time-dependent and periodic, it would naturally be wise to use Fermi's golden rule.

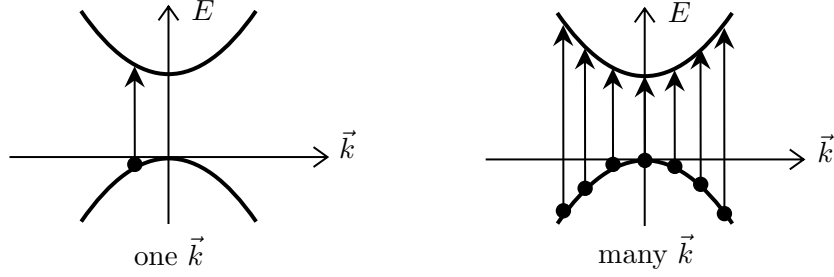
## Step 2: Compare with known results.

In the previous section, the Hamiltonian that we dealt with yields the dielectric function,

$$\hat{H}_1 = \hat{d} \cdot \vec{E}, \rightarrow \epsilon(\omega) = \lim_{\delta \rightarrow 0} \frac{8\pi \left| \langle f | \hat{d} | i \rangle \right|^2}{E_f - E_i - \hbar\omega + i\delta}.$$

Since our Hamiltonian here is in the exact same form<sup>3</sup> as the previous section, we can get the dielectric function for our current extended function to be,

$$\hat{H}_{1,\text{extended system}} = \frac{1}{i\omega} \frac{e}{mc} [\hat{p} \cdot \vec{E}], \quad \boxed{\epsilon_{\text{extended}}(\omega) = \frac{8\pi e^2}{\omega^2 (mc)^2} \lim_{\delta \rightarrow 0} \frac{8\pi \left| \langle f | \hat{p} | i \rangle \right|^2}{E_f - E_i - \hbar\omega + i\delta}}.$$



However, in reality, there could be more than one contribution of  $\vec{k}$  to the conduction band: the total transition (absorption) from the valence gap to the conduction gap does not occur for only one value of  $k$ , seen as follows.

Therefore, to find the full dielectric constant, we actually need to sum up the transitions over all of the valence band, as follows,

$$\epsilon_{\text{total}}(\omega) = \sum_{\text{all } k} \frac{8\pi e^2}{\omega^2 (mc)^2} \lim_{\delta \rightarrow 0} \frac{8\pi |\langle f | \hat{p} | i \rangle|^2}{E_f - E_i - \hbar\omega + i\delta}.$$

Again, we can interpret the matrix elements  $\langle f, k | \hat{p} | i, k \rangle$  to be the **transition dipole moment** of our extended system. Since  $\hat{p}$  is the momentum operator for the electron we are considering, we can calculate the above matrix element again by writing out the integral in position basis,

$$\langle \psi_{f,k} | \hat{p} | \psi_{i,k} \rangle = \iiint \psi_{f,k}^* \left[ \underbrace{-i\hbar \nabla}_{\hat{p}} \psi_{i,k} \right] d^3$$

Usually, this matrix element is a constant with respect to  $k$ . Therefore, we can calculate the absorption of this extended system by considering the imaginary part of the dielectric function. The initial state we are considering here is the valence band, while the final state here is the conduction band. The dielectric function therefore becomes,

$$\epsilon_I(\omega) = \frac{16\pi^2 e^2}{\omega^2 (mc)^2} \underbrace{P_{CV}^2}_{\text{transition dipole moment}} \sum_k \delta(E_C(k) - E_V(k) - \hbar\omega)$$

Substituting in the energy of the conduction and valence band, respectively, with respect to  $k$ , the above equation becomes,

$$\begin{aligned} \epsilon_I(\omega) &= \frac{16\pi^2 e^2}{\omega^2 (mc)^2} P_{CV}^2 \sum_k \delta \left( \underbrace{E_G + \frac{\hbar^2 k^2}{2m_C}}_{E_C(k)} - \underbrace{\frac{\hbar^2 k^2}{2m_V}}_{E_V(k)} - \hbar\omega \right) \\ &= \frac{16\pi^2 e^2}{\omega^2 (mc)^2} P_{CV}^2 \sum_k \delta \left( E_G - \hbar\omega + \frac{\hbar^2 k^2}{2\mu} \right). \end{aligned}$$

Here,  $\mu$  is the **reduced mass** of the electron, defined conveniently as,

$$\frac{1}{\mu} = \frac{1}{m_C} + \frac{1}{m_V}.$$

<sup>3</sup>Notice that  $[\hat{p}, \vec{E}] = 0$ , so that we can switch their positions.

### III Superconducting Quantum Circuits

#### III.1 The Current Operator

Recall that the current of a circuit is how much charged particles are moving forward in time. Naturally, we can link the current operator with the momentum operator,

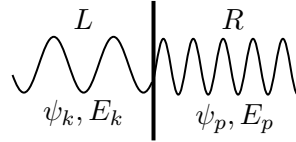
$$\hat{h} = -i\hbar\nabla, \quad \boxed{\hat{\rho} = \frac{q}{m}\hat{p}}.$$

The expected value of the current operator can therefore be written as,

$$\langle \hat{\rho} \rangle = \frac{ce\hbar}{m} \langle \psi | \nabla | \psi \rangle,$$

where  $|\psi\rangle$  is the wavefunction of the electrons in the circuit.

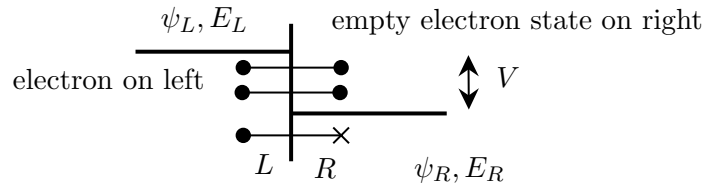
Now we will consider a special case<sup>4</sup>. Consider two distinct materials in contact, and we want to look at the tunneling rate between the two materials. We can express the current that goes from



the left side  $L$  to the right side  $R$  via the Hamiltonian,

$$\langle \psi_k | \hat{H}_i | \phi_p \rangle = T_0,$$

where  $\hat{H}_0$  is called the **tunnelling coefficient** and  $T_0$  is the **tunnelling probability**. Now, let's introduce voltage bias to the system as follows. Again, we will need to add up all the *available*



electron states from the left to the right. However, for an electron in the left to the right, according to Fermi's golden rule, the transition rate would be,

$$R_{L \rightarrow R} = \frac{2\pi}{\hbar} \left| \langle \psi_k | \hat{H}_T | \psi_p \rangle \right|^2 \delta(E_K - E_P).$$

To get the total current, we have to integrate over all possible transitions,

$$\int_E R_{L \rightarrow R} = \int_E \frac{2\pi}{\hbar} \left| \langle \psi_k | \hat{H}_T | \psi_p \rangle \right|^2 \delta(E_K - E_P)$$

<sup>4</sup>This apparatus is actually the Bardeen's approach solution for finding the tunneling current of a scanning tunneling microscope.

The term  $\delta(E_K - E_P)$  can be thought of as the density of states of the tip at energy  $E_K$ . Thus, integrating all the possible initial energies  $E_K$ , the above transition rate becomes,

$$R^{\text{total}} = \int_E R_{L \rightarrow R} = \int_E \frac{2\pi}{\hbar} \left| \langle \psi_k | \hat{H}_T | \psi_p \rangle \right|^2 \delta(E_K - E_P) = \frac{2\pi}{\hbar} \left| \langle \psi_k | \hat{H}_T | \psi_p \rangle \right|^2 \rho(E_K - E_P)$$

where  $\rho_R(E)$  is the number of energy levels between the energies  $E$  and  $E + \delta E$ .

The total current is therefore the sum of little contributions over all these energies, which will be the charge multiplied by the transition rate. The current is thus be proportional to the density of states on the left AND the **empty levels** on the right. Once we integrate over all of that, we find that we end up formulating<sup>5</sup> energy difference between the two sides, where  $E_{F,k}$  is the Fermi energy on the left hand side,

$$I = (e) \frac{2\pi}{\hbar} |T_0|^2 \rho_L(E) \rho_R(E) (E_{F,k} - E_{R,k}),$$

which simplifies into,

$$I = \frac{2\pi e^2}{\hbar} \rho_L \rho_R |T_0|^2 V.$$

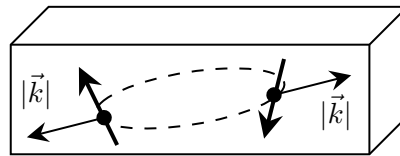
Note that the expression above essentially simplifies into Ohm's law, as in,  $I \propto V$ .

## III.2 Cooper Pairs

We will now be discussing superconductors; specifically, the BCS (Bardeen-Cooper-Schrieffer) model of superconductors. A **superconductor** is an object with no electrical resistance below a certain critical temperature, such that once set in motion, a persistent electric current will flow in the superconducting loop forever without any power loss. The **BCS model** is a model that describes effective interactions of electrons in the superconductor with crystal lattices.

Electrons are, of course, negatively charged. The negative electron will attract nearby positive ions in the lattice, and subsequently cause a vibration (i.e. creating a **phonon**) throughout the lattice. Since phonons propagate in a metal by acoustic vibrations, there will be certain regions in the solid are more positive than others. Thus, effectively, the phonon can cause pairs of electrons to be attracted to each other, forming objects called **Cooper pairs**.

From the lens of statistical mechanics, small attraction between electrons in a metal can cause a paired state of electrons to have a lower energy than the Fermi energy, which implies that the pair is in a bound state.



The two electrons forming a Cooper pair has opposite properties. For instance, if one electron has spin up, another must be spin down. Therefore, a Cooper pair, when acting as an individual particle, behaves like a boson, even when its contingent compartments act as fermions.

<sup>5</sup>This is because for an energy  $E$ , the particle obeys the Fermi-Dirac distribution, and when we integrate the current with respect to all possible energies, the the “extrema” energy pops out due to the chain rule.

## Phase of a Superconductor

At low temperatures, macroscopic numbers of Cooper pairs can occupy the same ground states<sup>6</sup>, forming a **Cooper pair condensate**. The wavefunction of this condensate would be that of a multiparticle system,

$$|\Psi_{\text{BCS}}\rangle = \prod_k \left( u_k \underbrace{|0\rangle}_{\text{no pair}} + v_k \underbrace{|1\rangle}_{\text{one pair}} \right),$$

combine all  $\vec{k}$

where the basis ket states  $|N\rangle$  implies the follows<sup>7</sup>,

$$|N\rangle \equiv N \text{ pairs of electrons with opposite momentum vectors } \vec{k}$$

The amplitudes  $u_k$  and  $v_k$  are complex numbers that satisfies the normalisation condition,

$$|u_k|^2 + |v_k|^2 = 1,$$

while also having a phase when multiplied, we can get the **superconducting order parameter**  $u_k v_k$ ,

$$u_k v_k = |u_k v_k| \exp i\phi.$$

It turns out that  $|\Psi_{\text{BCS}}\rangle$  is called a **coherent superposition** of Cooper pairs, for the phase  $\phi$  is constant for all Cooper pairs. In other words, it is only possible for a superconductor to have zero or one Cooper pair in the system. As this sounds quite non-intuitive, we will need to qualitatively answer two questions that might arise.

### Does the size of the superconductor matter?

**No.** It doesn't matter if our superconductor is of dimension 1 mm or 1 metre. As long as the superconductor act as one system<sup>8</sup>, the distortion of an electron can cause lattice vibrations in the metal, which will propagate throughout the entire metal. In other words, a Cooper pair can be formed by a coupling from one end of the superconductor, regardless of how far apart they are from another.

### Is the number state $|2\rangle$ possible?

**No.** Although a Cooper pair acts as a boson, it is a bound state of two fermions. Number states of two fermions with a given wavenumber  $\vec{k}$  can only be  $|0\rangle$  or  $|1\rangle$ . There are two possible ways we can explain this phenomenon.

1. An electron in a metal is described by its eigenenergy  $\vec{k}$  and its spin. According to the Pauli exclusion principle, two identical fermions must not occupy the same state. Therefore, the only possible combination of two electrons in a metal with wavevector magnitude  $|\vec{k}|$  would be between electrons positive or negative spin. If there are two electrons with the same  $\vec{k}$  and same spin, there would be no wavefunction due to the antisymmetry of fermionic systems. Thus, only  $|0\rangle$  and  $|1\rangle$  exists.

<sup>6</sup>lowest energy states of the superconductor.

<sup>7</sup>These are actually called Fock states.

<sup>8</sup>where it is possible to get from one side of the superconductor to another without going through other materials.



2. Let's say, hypothetically, that two Cooper pairs with  $\vec{k}$  exists (as in, the state  $|2\rangle$  exists). There will be cross interactions between the Cooper pairs (6 possible ways the 4 electrons can "pair up"), and the physics of the Cooper pairs break down.

### III.3 the Superconducting Order Parameter

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We can now consider the energy it takes to create or break a Cooper pair back in the  $|N\rangle$  basis. Defining the **superconducting Hamiltonian** as,

$$\hat{H}_{SC} \equiv |0\rangle_k \langle 1|_k,$$

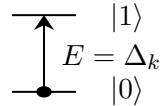
we can get the matrix element as follows,

$$\underbrace{\langle N|}_{N \text{ pairs}} \underbrace{|0\rangle_k \langle 1|_k}_{\hat{H}_{SC}} \underbrace{|N+1\rangle}_{N \text{ pairs}} = u_k v_k = u_k v_k = |u_k v_k| \exp i\phi.$$

Notice that the diagonal terms of the matrix elements become zero, and that the off diagonal matrix elements are actually negative of each other. Thus, the magnitude of the energy required to create or break a Cooper pair to free electrons would simply be,

$$E = \Delta_k = u_k v_k,$$

where  $\Delta_k$  is defined as the **superconducting order parameter** for the momentum  $\vec{k}$ . The order parameter  $\Delta(\vec{r})$ , can be considered as a macroscopic wave function of a Cooper pair, normalised to the density of Cooper pairs. The energy state diagram is as follows.



The order of magnitude of this energy is approximately a few Kelvins. That's why most superconductors only exist at very low temperatures: at high temperatures, a lot of the thermal energy can be absorbed by the quantum states, thus actually destroying the Cooper pairs in process.

### III.4 Transmon Qubits

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The *macroscopic* wavefunction for a Cooper pair, normalised to the density of Cooper pairs<sup>9</sup> would be,

$$\Psi_S(\vec{r}) = \sqrt{n_S(\vec{r})/2} \exp(i\phi(\vec{r})),$$

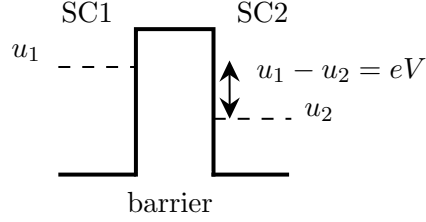
where  $\vec{r}$  are *parameters* of the wavefunction, and  $\Psi_S(\vec{r})$  is the probability density of finding a Cooper pair in  $\vec{r}$ . Note that the phase  $\phi$  here is exactly the same as in the BCS wavefunction. Now, consider what happens if we want a Cooper pair to tunnel through a potential barrier as follows.

Here, SC1 and SC2 are wells that the Cooper pair tunnels from and to, respectively. Assume that the Cooper pairs on both side of the well follows the wavefunction,

$$\psi_1(\vec{r}) = \sqrt{n_{s1}/2} \exp i\phi_1, \quad \psi_2(\vec{r}) = \sqrt{n_{s2}/2} \exp i\phi_2.$$

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<sup>9</sup>i.e., half the density of electrons in the condensate,  $n_S(\vec{r})$



The two basis states that we will use would be,  $|\text{SC1}\rangle$  and  $|\text{SC2}\rangle$ , as in, if the particle is left or right of the potential barrier. Thus, the above wavefunction can be written in matrix form as,

$$|\psi\rangle_{\text{Josephson}} = \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_2(\vec{r}) \end{pmatrix} = \begin{pmatrix} \sqrt{n_{s1}/2} \exp i\phi_1 \\ \sqrt{n_{s2}/2} \exp i\phi_2 \end{pmatrix}.$$

The Hamiltonian that the two systems, if there is a potential bias of  $V$ , would be,

$$\hat{H} = \begin{pmatrix} eV & K \\ K & -eV \end{pmatrix},$$

where  $K$  is the coupling/tunneling strength due to the potential barrier. Thus, substituting the wavefunction and the Hamiltonian into the Schrödinger equation, we yield,

$$i\hbar \frac{d}{dt} \begin{pmatrix} \sqrt{n_{s1}/2} \exp i\phi_1 \\ \sqrt{n_{s2}/2} \exp i\phi_2 \end{pmatrix} = \begin{pmatrix} eV & K \\ K & -eV \end{pmatrix} \begin{pmatrix} \sqrt{n_{s1}/2} \exp i\phi_1 \\ \sqrt{n_{s2}/2} \exp i\phi_2 \end{pmatrix}.$$

Solving the system, we yield two equations. The first equation we yield would be,

$$\frac{dn_{s1}}{dt} = -\frac{dn_{s2}}{dt} = \frac{2Kn_S}{\hbar} \sin(\phi_2 - \phi_1).$$

Since  $n_{s_i}$  is simply the electron density left/right of the barrier, the above equation is suggesting that no Cooper pairs are created or destroyed during this process. Since the current is defined as  $dq/dt$ , we can actually write down the equation current going through the potential. This is called the **DC Josephson Effect**.

#### Theorem 1.14: DC Josephson Effect

A non dissipative electric current called the **Josephson current** flows through the barrier with the equation,

$$I_J = I_C \sin(\phi_1 - \phi_2).$$

The amplitude of this current which is determined only by the phase difference between the superconductors and the properties of the junction, swept into a coefficient known as the **critical current**  $I_C$ . If we supply a current with  $I < I_C$ , then the Josephson junction is superconducting. However, as soon as  $I > I_C$ , the Josephson junction will become a resistor.

The second equation to be solved is as follows,

$$\frac{d(\phi_1 - \phi_2)}{dt} = \frac{2eV}{\hbar}$$

This relation describes the **AC Josephson Effect** as described in the following theorem. If we integrate both sides of the equation with time, we yield,

$$\phi_2 - \phi_1 = \frac{2eVt}{\hbar}.$$

**Theorem 1.15: AC Josephson Effect**

If somehow voltage is applied between the two superconducting banks, then the superconducting phase difference between them will grow with the relationship,

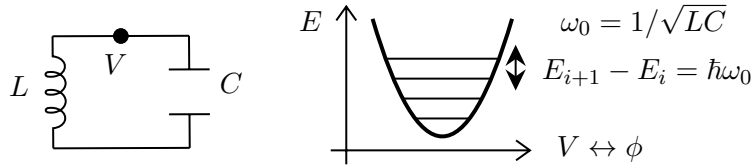
$$\phi_2 - \phi_1 = \frac{2eVt}{\hbar}$$

The Josephson junction in essence behaves as an inductor with the inductance,

$$L = \frac{c^2 V}{dI/dt} = \frac{vc^2}{-eV/\hbar I_C \cos(2eVt/\hbar)} = -\frac{\hbar c^2}{2eI_C \cos \phi}$$

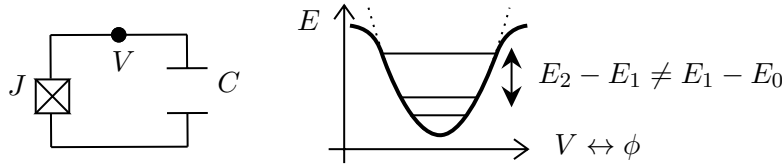
which is a function of the voltage applied. We can thus say that the Josephson junction is a nonlinear inductor - this is a crucial advancement for quantum information science.

Let's us first consider the energy levels of a regular **quantum LC circuit** as follows. Here, we



see that the energy difference of every energy level is the same, which is  $E_{i+1} - E_i = \hbar\omega_0$ , where  $\omega_0$  is the natural frequency of the quantum LC circuit. Since all the energy levels have the same difference, we can't really use the quantum LC circuit to encode anything.

Now, let's replace the original inductor with our new inductor, the Josephson junction. The circuit and energy diagram now looks as follows, Using the dotted line as a reference to the LC



circuit, we now yield an energy curve that is anharmonic (not quadratic), and therefore the energy levels are not equidistant anymore. Thus, we can actually know whether we are on the ground state or the first excited state, since the energy it takes to excite them will be different.

The ground states and the first energy states considered here are *different* than the states of the Cooper pairs before - the states presented here correspond to the amount of energy each level of the current in the Josephson junction have. The ground state has a less energetic current, while the first excited state has a more energetic current. Thus, we can actually use the zeroth and first states as **qubits** because all the excitations are different from each other. The qubits formed using the currents of the Josephson junction are called the **transmon qubits**.

Now, we should try an advanced example<sup>10</sup>.

<sup>10</sup>This problem was inspired by the paper, Clemens Müller et al 2019 *Rep. Prog. Phys.* **82** 124501, *Towards understanding two-level-systems in amorphous solids - Insights from quantum circuits*.

**Problem 1.3: TLS and Transmon Qubits**

Two-level-systems (TLS) are common quantum mechanical objects in amorphous solids that arises from random disorders of the atomic lattices. It can be modeled as two minima in a double well potential which are separated by a barrier. At low temperatures, the dynamics of the TLS are governed by quantum tunneling through the barrier.

- a. Suppose a typical potential wells configuration of a TLS as shown in the figure below. The difference between the two ground-state eigenenergies of the two wells is  $\epsilon$ . The matrix element for the tunnelling through the barrier is  $\langle L | \hat{H}_T | R \rangle = \Delta/2$ . Find the two lowest energy eigenstates and eigenenergies. Treating the TLS as a qubit, what is its transition frequency?
- b. The tunneling energy  $\Delta$  is a function of the barrier height  $V$ , barrier width  $d$  and the effective mass of the particle  $m$ ,

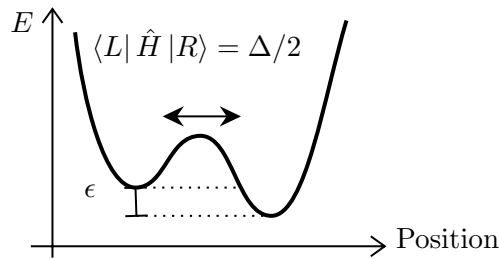
$$\Delta = \hbar\omega_0 \exp(-\lambda),$$

Where  $\lambda = \sqrt{2mV/\hbar^2}d$ . Due to its random nature, ensembles of TLS exhibit a range of parameters in  $\lambda$  and  $\epsilon$  with uniform probability. That is,

$$P(\epsilon, \Delta) d\epsilon d\lambda = P_0 d\epsilon d\lambda.$$

Assuming there is a minimum tunneling energy  $\Delta_0$ , find the density of states of TLS,  $D(E)$  by integrating over all possible  $\Delta$  values. Here,  $E$  is the transition energy of the TLS.

- c. In superconducting circuits, TLS are commonly present in the material interfaces within the Josephson junction. This causes a coupling of superconducting transmon qubit to a bath of TLSs. Given a SC qubit (of frequency  $\omega_0$ ) to TLS coupling matrix element of JTLS, use Fermis golden rule to calculate the decay rate of a SC qubit initially in the excited state due to resonant interaction with the TLSs.


**Solution.**

- a. From the energy diagram supplied by the problem, we know that the particle localised at  $|R\rangle$  would have an energy of  $E_R$ , as in,

$$\langle R | \hat{H} | R \rangle = E_R.$$

Similarly, the particle localised at  $L$  would thus have an energy of,

$$\langle L | \hat{H} | L \rangle = E_R + \epsilon.$$

It would therefore be convenient to introduce the quantity  $E_0$  where,

$$E_0 = \frac{E_R + (E_R + \epsilon)}{2}.$$

Therefore, since  $\langle L | \hat{H}_T | R \rangle = \Delta/2$ , the Hamiltonian for the total TLS would be,

$$\hat{H} = \begin{pmatrix} E_0 - \epsilon/2 & \Delta/2 \\ \Delta/2 & E_0 + \epsilon/2 \end{pmatrix}$$

where  $\hat{H}_{11}$  is defined as  $\langle R | \hat{H} | R \rangle$ . Using Wolfram Mathematica, we know that the eigenvalues and the eigenvectors of the Hamiltonian would be,

$$E_1 = E_0 - \frac{\sqrt{\Delta^2 + \epsilon^2}}{2}, \quad |\psi_1\rangle = \frac{1}{\sqrt{\left(\frac{\epsilon + \sqrt{\Delta^2 + \epsilon^2}}{\Delta}\right)^2 + 1}} \left( -\frac{\epsilon + \sqrt{\Delta^2 + \epsilon^2}}{\Delta} |R\rangle + |L\rangle \right)$$

Similarly, the second eigensystem would be,

$$E_2 = E_0 + \frac{\sqrt{\Delta^2 + \epsilon^2}}{2}, \quad |\psi_2\rangle = \frac{1}{\sqrt{\left(\frac{\epsilon + \sqrt{\Delta^2 + \epsilon^2}}{\Delta}\right)^2 + 1}} \left( -\frac{\epsilon - \sqrt{\Delta^2 + \epsilon^2}}{\Delta} |R\rangle + |L\rangle \right)$$

The transition frequency can be calculated via Schrödinger's equation,

$$\begin{aligned} i\hbar \frac{\partial |\psi\rangle}{\partial t} &= \hat{H} |\psi\rangle \\ i\hbar \begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} &= \begin{pmatrix} E_0 - \epsilon/2 & \Delta/2 \\ \Delta/2 & E_0 + \epsilon/2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} aE_0 - a\epsilon/2 + b\Delta/2 \\ a\Delta/2 + bE_0 + b\epsilon/2 \end{pmatrix} \end{aligned}$$

Assuming that  $a$  and  $b$  takes the form,

$$a = A \exp(-i\omega_0 t), \quad b = B \exp(-i\omega_0 t),$$

where  $A$  and  $B$  are complex numbers (to include phase), we yield the system,

$$\begin{cases} \dot{a} = \frac{1}{i\hbar} \left[ a \left( E_0 - \frac{\epsilon}{2} \right) + b \frac{\Delta}{2} \right] \\ \dot{b} = \frac{1}{i\hbar} \left[ a \frac{\Delta}{2} + b \left( E_0 + \frac{\epsilon}{2} \right) \right] \end{cases}$$

which then yields,

$$\begin{cases} A\hbar\omega_0 \exp(i\omega_0 t) = A \exp(-i\omega_0 t) \left( E_0 - \frac{\epsilon}{2} \right) + B \exp(-i\omega_0 t) \frac{\Delta}{2} \\ B\hbar\omega_0 \exp(i\omega_0 t) = A \exp(-i\omega_0 t) \frac{\Delta}{2} + B \exp(-i\omega_0 t) \left( E_0 + \frac{\epsilon}{2} \right). \end{cases}$$

Removing the  $\exp(-i\omega_0 t)$  dependence, we yield,

$$\begin{cases} A\hbar\omega_0 = A \left( E_0 - \frac{\epsilon}{2} \right) + B \frac{\Delta}{2} \\ B\hbar\omega_0 = A \frac{\Delta}{2} + B \left( E_0 + \frac{\epsilon}{2} \right) \end{cases}, \quad \xrightarrow{X \equiv A/B} \begin{cases} X\hbar\omega_0 = X \left( E_0 - \frac{\epsilon}{2} \right) + \frac{\Delta}{2} \\ \hbar\omega_0 = X \frac{\Delta}{2} + \left( E_0 + \frac{\epsilon}{2} \right) \end{cases}$$

Solving for  $X$  and  $\omega_0$  of the above system, we yield,

$$\omega_0 = \frac{1}{\hbar} \left[ E_0 \pm \frac{\sqrt{\Delta^2 + \epsilon^2}}{2} \right]$$

b. The transition energy<sup>11</sup> is defined as,

$$E \equiv E_2 - E_1 = \sqrt{\Delta^2 + \epsilon^2}.$$

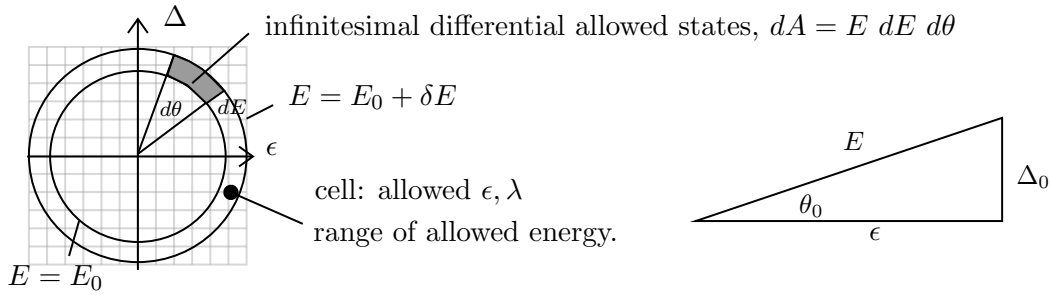
First, taking the derivative of  $\Delta$  with respect to  $\lambda$ , we yield,

$$d\Delta = -\hbar\omega_0 \exp(-\lambda) d\lambda = -\Delta d\lambda.$$

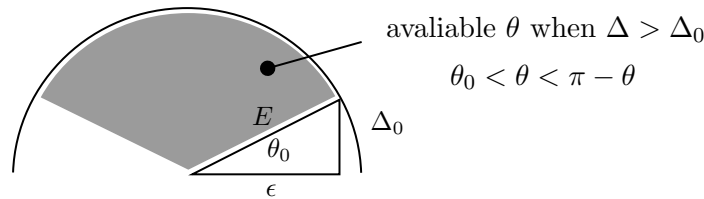
Since the probability distribution function appears as,

$$P(\epsilon, \Delta) d\epsilon d\lambda = P_0 d\epsilon d\lambda = -P_0 d\epsilon \left( \frac{d\Delta}{\Delta} \right) = -\frac{P_0}{\Delta} d\epsilon d\Delta.$$

In phase space, the relationship between  $d\epsilon d\Delta$  can be plotted in the graph below.



We can interpret the density of states as the volume between the energy levels  $E$  and  $E + \delta E$  in phase space. Thus, the allowed ranges of  $\theta$  such that  $\Delta > \Delta_0$  can therefore be visualised as the “strip” in the figure below.



Thus, we can convert the probability density function into the density of states function using the relationship,

$$\iint P(\epsilon, \Delta) d\epsilon d\lambda = \iint \frac{-P_0}{\Delta} \underbrace{d\epsilon d\Delta}_{\text{density of available states}} = \iint \frac{-P_0}{\Delta} E dE d\theta \equiv \int D(E) dE$$

However, given that there exists a minimum  $\Delta_0$ , the possible  $\theta$ s would be, Using the triangle relating  $\theta$ ,  $E$ ,  $\Delta$ , and  $\epsilon$  above, we see,

$$\sin \theta = \frac{\Delta}{E}, \quad \rightarrow \quad \Delta = E \sin \theta.$$

<sup>11</sup>Significant help received from my friend Tingran Wang.

Thus the distribution function above becomes,

$$\int D(E) dE = \iint \frac{-P_0}{E \sin \theta} E dE d\theta = \int \left[ \int_{\theta_0}^{\pi-\theta_0} \frac{-P_0}{\sin \theta} d\theta \right] dE,$$

where we see,

$$\theta_0 = \arcsin \left( \frac{\Delta_0}{E} \right).$$

The integral above then becomes,

$$\begin{aligned} -P_0 \int \left[ \int_{\theta_0}^{\pi-\theta_0} \csc \theta d\theta \right] dE &= -P_0 \int [\ln |\csc \theta - \cot \theta|] \Big|_{\theta_0}^{\pi-\theta_0} dE \\ &= - \int P_0 [\ln |\csc(\pi - \theta_0) - \cot(\pi - \theta_0)| - \ln |\csc(\theta_0) - \cot(\theta_0)|] dE \\ &= -P_0 \int \ln \left| \frac{\csc(\pi - \theta_0) - \cot(\pi - \theta_0)}{\csc(\theta_0) - \cot(\theta_0)} \right| dE = -P_0 \int \ln \left| \frac{\csc(\theta_0) + \cot(\theta_0)}{\csc(\theta_0) - \cot(\theta_0)} \right| dE \\ &= - \int P_0 \ln \left| \frac{\csc(\theta_0) + \cot(\theta_0)}{\csc(\theta_0) - \cot(\theta_0)} \right| dE = \int D(E) dE \end{aligned}$$

However, from the triangle above, we know that,

$$\csc \theta_0 = \frac{E}{\Delta_0}, \quad \cot \theta_0 = \frac{\sqrt{E^2 - \Delta_0^2}}{\Delta_0}$$

Thus, the above expression can be simplified as,

$$\int D(E) dE = - \int P_0 \ln \left[ \frac{E + \sqrt{E^2 - \Delta_0^2}}{E - \sqrt{E^2 - \Delta_0^2}} \right] dE$$

Therefore, we see that,

$$D(E) = -P_0 \ln \left| \frac{E + \sqrt{E^2 - \Delta_0^2}}{E - \sqrt{E^2 - \Delta_0^2}} \right|.$$

c. Fermi's golden rule states that the transition rate between a state  $i$  and  $f$  would be written as,

$$R_{i \rightarrow f} = \frac{2\pi}{\hbar^2} |\langle f | \hat{V} | i \rangle|^2 \delta(\omega_{f \leftarrow i} - \omega), \text{ where } \omega_{f \leftarrow i} = \frac{E_f - E_i}{\hbar}$$

However, since there are multiple possible transition energies  $E$  that gives the tunnelling energy  $\Delta$ , we in effect will have to integrate over all  $\Delta$ s to find that,

$$R_{i \rightarrow f}^{\text{total}} = \int_{\text{all } \Delta} \frac{2\pi}{\hbar} |\langle f | \hat{V} | i \rangle|^2 \delta(\omega_{f \leftarrow i} - \omega) = \frac{2\pi}{\hbar} |\langle f | \hat{V} | i \rangle|^2 D(E')$$

where  $D(E')$  is the density of states of the final states. Even though we are interested in the decay of the SC qubit from the excited state to the ground state, we know that a decay of the SC qubit from the high state to the ground state will imply a raise of the TLS from the low state to a high state. Therefore, to find the transition rate of the SC qubit we can simply find the transition rate of the TLS. Moreover, we know that the matrix element  $\langle \text{ground} | \hat{H} | \text{excited} \rangle$  are given to be  $J_{\text{TLS}}$ . Substituting the results from here above, we yield the transition rate from the excited state to the

ground state of the SC qubit, equivalent to the transition rate from the low to excited state of the TLS, since  $E$  is the energy gained from the low to excited state of the TLS, would be,

$$R_{i \rightarrow f}^{\text{total}} = \frac{2\pi J_{\text{TLS}}^2}{\hbar^2} D(E) = \frac{2\pi J_{\text{TLS}}^2}{\hbar^2} \left( P_0 \ln \left| \frac{E + \sqrt{E^2 - \Delta_0^2}}{E - \sqrt{E^2 - \Delta_0^2}} \right| \right).$$