13. Consider an electron in a weak one-dimensional periodic potential ("lattice") $V(x) = V(x+d)$. Assume the lattice has a size $L = Nd$, and that we the have a periodic boundary condition on our wave functions: $\psi(x) = \psi(x+L)$. With this boundary condition, the unperturbed wave functions are plane waves, $\psi_p(x) = \frac{1}{\sqrt{L}} e^{ipx}$, where $p = 2\pi n/L$, $n =$ integer, and the unperturbed eigenenergies are $\varepsilon_n = \frac{p^2}{2m} = \left(\frac{2\pi n}{L}\right)^2 \frac{1}{2m}$. We expand the potential in a Fourier series:

$$V(x) = \sum_{n=-\infty}^{\infty} e^{in2\pi x/d} V_n. \qquad (1)$$

(a) If we label our eigenfunctions by $|p\rangle = \frac{1}{\sqrt{L}} e^{2\pi i n_p x/L}$, determine all nonvanishing matrix elements of V :

$$\langle q|V|p\rangle$$

Express your answer in terms of V_n, and a condition involving p and q or equivalently on $n_p = Lp/2\pi$ and $n_q = Lq/2\pi$.

(b) Suppose ε_{n_p} and ε_{n_q} are not close to each other $\forall n_q (\neq n_p)$, given some n_p. Calculate the perturbed wave function in ordinary first order perturbation theory corresponding to unperturbed wave function $\psi_p(x)$. Also, calculate the energy to 2$^{\text{nd}}$ order. Express your answer in terms of V_n.

72 hr extension

$$\frac{L}{d} = N$$

a.)
$$\langle q|V|p\rangle = \frac{1}{L}\sum_{n=-\infty}^{\infty} V_n \int_0^L e^{-iqx} e^{in2\pi x/d} e^{ipx}\, dx$$

$$= \frac{1}{L}\sum_{n=-\infty}^{\infty} V_n \int_0^L \underbrace{\exp\left[i2\pi \frac{x}{L}(n_p + Nn - n_q)\right]}_{e^{\alpha x}} dx$$

Notice this integral is nonzero only if $\alpha = 0$. To prove this, suppose $\alpha \neq 0 \rightarrow n_p + Nn - n_q \equiv n' \neq 0$. Then we have that the integral is equivalent to

$$\int_0^L e^{i2\pi x \cdot \frac{n'}{L}} dx \; ; n' \in \mathbb{Z}$$

$$\propto \int_0^1 e^{i2\pi n' z} dz$$

$$= \frac{1}{i2\pi n'}\left(e^{i2\pi n'} - 1\right) = 0$$

$$\int_0^1 e^{i\alpha x} dx$$
$$= \frac{1}{i\alpha} e^{i\alpha x}\Big|_0^1$$
$$= \frac{1}{i\alpha}(e^{i\alpha} - 1)$$
$$e^{i\alpha} \neq 1 \Rightarrow \int \neq 0$$
$$\alpha \neq 2\pi n$$

Thus, we must have

$$n_p + Nn - n_q \equiv n' = 0 \Rightarrow n = \frac{n_q - n_p}{N}$$

In this case, the integral is

$$\int_0^L e^0\, dx = \int_0^L 1\, dx = L$$

$$\int_0^L e^0 \, dx = \int_0^L 1 \, dx = L$$

Thus,

$$\langle q|V|p\rangle = \frac{1}{L} V_n \cdot L = V_n \quad , \quad n = \frac{n_q - n_p}{N}$$

Since $n \in \mathbb{Z}$,

$$\boxed{\langle q|V|p\rangle = V_n \; ; \; n = \frac{n_q - n_p}{N} \quad \text{if } n \in \mathbb{Z} \text{ and zero otherwise}}$$

b.) The perturbed wave function can be calculated to first order using the formula below:

Then we have original 1st order PT results:

$$|N_i'\rangle = |n_i'\rangle + \sum_{m \notin [n_i]} |m\rangle \frac{\langle m|V|n_i'\rangle}{E_n - E_m} + \dots$$

$$\rightarrow |P\rangle = |p\rangle + \sum_{m \neq n_i} |m\rangle \frac{\langle m|V|p\rangle}{E_{n_p} - E_m}$$

$$\rightarrow |P\rangle = |p\rangle + \sum_{m:\, m' \in \mathbb{Z}} |m\rangle \frac{V_{m'}}{E_{n_p} - E_m}$$

momentum state; m is not the same as n_m.

$$\text{with} \quad m' = \frac{\left(\frac{L}{2\pi}\right)m - n_p}{N} \in \mathbb{Z}$$

$$\rightarrow \left(\frac{L}{2\pi}\right)m - n_p = N m' \quad \rightarrow \quad m = (N m' + n_p)\frac{2\pi}{L}$$

$$\Rightarrow |P\rangle = |p\rangle + \sum_{m'=-\infty}^{\infty} \left|\frac{2\pi}{L}(N m' + n_p)\right\rangle \frac{V_{m'}}{E_{n_p} - E_{N m' + n_p}}$$

$\neq 0$

The second-order perturbed energy is given by

The second-order perturbed energy is given by

$$E_{n_p} = \varepsilon_{n_p} + \underbrace{\langle n_p | V | n_p \rangle}_{= V_{\frac{n_p - n_p}{N}} \to V_0} + \sum_{m \neq n} \frac{|\langle m | V | n \rangle|^2}{\varepsilon_{n_p} - \varepsilon_m}$$

$$\to \boxed{E_{n_p} = \varepsilon_{n_p} + V_0 + \sum_{m'=-\infty}^{\infty} \frac{|V_{m'}|^2}{\varepsilon_{n_p} - \varepsilon_{m'+n_p}}}$$

$m' \neq 0$

14. It may happen that we encounter a situation where two eigenvalues of H_0, call them ε_n and ε_m, are nearly, but not quite equal. In this case, we don't seem to be able to use degenerate perturbation theory, and ordinary perturbation theory is likely to converge slowly. Let us try to deal with such a situation: Suppose the two eigenstates $|n\rangle$ and $|m\rangle$ of H_0 have nearly the same energy (and all other eigenstates don't suffer this disease, for simplicity). Let $H = H_0 + V$, and write

$$V = \sum_{i,j} |i\rangle\langle i|V|j\rangle\langle j| \tag{2}$$

$$H_0|i\rangle = \varepsilon_i|i\rangle, \tag{3}$$

where

$$\langle i|j\rangle = \delta_{ij}. \tag{4}$$

Let

$$V = V_1 + V_2, \tag{5}$$

with

$$V_1 = |m\rangle\langle m|V|m\rangle\langle m| + |n\rangle\langle n|V|n\rangle\langle n| + \tag{6}$$

$$+|m\rangle\langle m|V|n\rangle\langle n| + |n\rangle\langle n|V|m\rangle\langle m| \tag{7}$$

and V_2 is everything else.

If we can solve exactly the problem with $H_1 = H_0 + V_1$, then the troublesome $1/(\varepsilon_n - \varepsilon_m)$ terms are avoided by the exact treatment, and we may treat V_2 as a perturbation in ordinary perturbation theory (since $\langle i|V_2|j\rangle = 0$ for $i, j = n, m$). All states $|i\rangle$, $i \neq n, m$, are eigenstates of H_1, since $V_1|i\rangle = 0$ in this case. However, $|n\rangle$ and $|m\rangle$ are not in general eigenstates of H_1.

(a) Solve exactly for the eigenstates and eigenvalues of H_1, in the subspace spanned by $|n\rangle$, $|m\rangle$. Express your answer in terms of

$$\varepsilon_n, \varepsilon_m, \langle m|V|n\rangle, \langle n|V|n\rangle, \langle m|V|m\rangle.$$

(You may also use the shorthand

$$E^{(1)}_{n,m} = \varepsilon_{n,m} + \langle n, m|V|n, m\rangle$$

if you find it convenient.)

(b) Now consider the periodic potential of problem 13. What is the condition on n_p (and hence on p) so that $|p\rangle$ will be nearly degenerate in energy with another eigenstate of H_0? You might find it convenient to define the "reciprocal lattice constant" $K \equiv 2\pi/d$.

(c) Assume that the condition in part (b) is satisfied, and use part (a) to solve this "almost degenerate" case for the eigenenergies. Try to make a sketch of the energy as a function of momentum ("dispersion relation"). Fig. 1 gives a start for momenta less than π/d.

a.) Notice that the matrix representation of H_1 in the subspace spanned by $|n\rangle$ and $|m\rangle$ is

$$H_1 = H_0 + V_1 = \begin{pmatrix} \varepsilon_n & 0 \\ 0 & \varepsilon_m \end{pmatrix} + \begin{pmatrix} V_{nn} & V_{nm} \\ V_{mn} & V_{mm} \end{pmatrix}$$

where $|n\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|m\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$; $V_{ij} = \langle i|V|j\rangle$.

$$\Rightarrow H_1 = \begin{pmatrix} \varepsilon_n + V_{nn} & V_{nm} \\ V_{mn} & \varepsilon_m + V_{mm} \end{pmatrix} = \begin{pmatrix} E_n & b \\ c & E_m \end{pmatrix}$$

$$\rightarrow (H_1 - \lambda I)|n\rangle_1 = 0$$

$$\Rightarrow \det(H_1 - \lambda I) = 0 \rightarrow \begin{vmatrix} E_n - \lambda & b \\ c & E_m - \lambda \end{vmatrix} = 0$$

Let $a = E_n$, $d = E_m$, let $x = -\lambda$

$$\rightarrow (x+a)(x+d) - bc = 0$$

$$\Rightarrow x^2 + (a+d)x + ad - bc = 0$$

$$\Rightarrow x = \frac{-(a+d) \pm \sqrt{(a+d)^2 - 4(ad-bc)}}{2}$$

$$\Rightarrow \lambda_{1,2} = \frac{(E_n + E_m) \pm \sqrt{(E_n+E_m)^2 - 4(E_nE_m - V_{nm}V_{mn})}}{2}$$

$V_{nm} = V_{mn}^*$

$$\Rightarrow \boxed{\lambda_{1,2} = \frac{(E_n + E_m) \pm \sqrt{(E_n - E_m)^2 + |V_{nm}|^2}}{2}}$$

Eigenvectors:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ k \end{pmatrix} = \lambda \begin{pmatrix} 1 \\ k \end{pmatrix}$$

$$\rightarrow a + bk = \lambda$$

$\rightarrow \quad a + bk = \lambda$

$c + dk = \lambda k \rightarrow k_{1,2} = \dfrac{c}{\lambda_{1,2} - d}$

$$\cancel{\Rightarrow \quad k_{1,2} = \frac{\lambda_{1,2} - a}{b} = \frac{\lambda_{1,2} - E_n}{V_{nm}}}$$

$$\boxed{\Rightarrow \text{The eigenvectors are } \begin{pmatrix} 1 \\ k_1 \end{pmatrix}; \begin{pmatrix} 1 \\ k_2 \end{pmatrix} \quad \text{with} \quad k_{1,2} = \frac{V_{mn}}{\lambda_{1,2} - E_m}}$$

6.) Notice that $\varepsilon_p = \varepsilon_{-p}$

Moreover

$$E_p = \varepsilon_p + V_0 + \sum_{m'=-\infty}^{\infty} \frac{|V_{m'}|^2}{\varepsilon_p - \varepsilon_{Nm'+n_p}}$$

$$= \varepsilon_p + V_0 + \sum_{m'=\infty}^{-\infty} \frac{|V_{-m'}|^2}{\varepsilon_p - \varepsilon_{-Nm'+n_p}}$$

Notice that $n_{-p} = -n_p$ and $V_{-m'} = V_{m'}^*$

(also $\varepsilon_p = \varepsilon_{-p}$)

Thus,

$$E_{-p} = \varepsilon_{-p} + V_0 + \sum^{\infty} \frac{|V_{m'}|^2}{\quad}$$

Thus,

$$E_p = \varepsilon_{-p} + V_0 + \sum_{m'=-\infty}^{\infty} \frac{|V_{m'}|^2}{\varepsilon_p - \varepsilon_{Nm'+n_p}}$$

$$= E_{-p}$$

Thus the condition is

$$\boxed{\begin{gathered} n_q = n_{-p} = -n_p \\ \text{or} \quad q = -p \end{gathered}}$$

c.) Letting $m = -n$ in our formula in part (a), we see that the eigen energies are

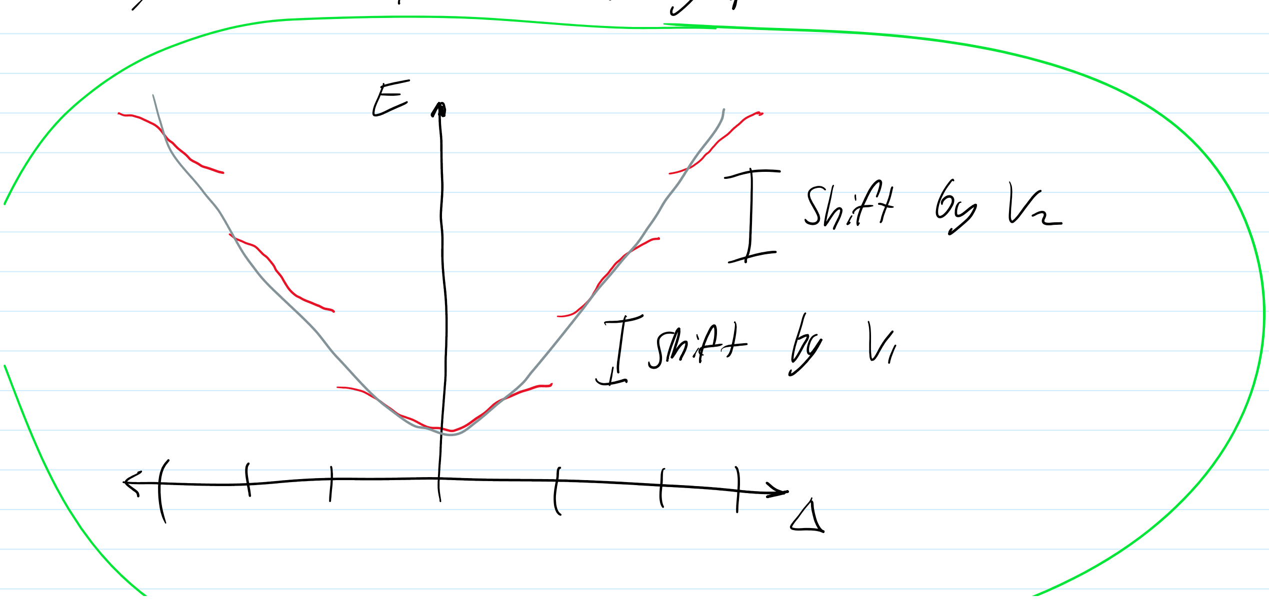
$$\lambda = \varepsilon_n + V_0 \pm \sqrt{0 + V_{2n_p}^2}$$

$$\rightarrow \boxed{\lambda = \varepsilon_n + V_0 \pm V_{2n_p}}$$

Write p as

$$p(\Delta) = \frac{2\pi}{L}(1+\Delta).$$

Then, plotting E as a function of Δ, we produce this graph:



15. When we calculate the density of states for a free particle, we use a "box" of length L (here, we consider one dimension), and impose periodic boundary conditions to ensure no net flux of particles into or out of the box. We have in mind that we can eventually let $L \to \infty$, and are really interested in quantities per unit length (or volume). However, we should really demonstrate our conclusion. So, let us justify more carefully the use of periodic boundary conditions, *i.e.*, we wish to carefully convince ourselves that the intuitive rationale given above is in fact correct. To do this, consider a free particle in a one-dimensional "box" from $-L/2$ to $L/2$. Remembering that the Hilbert space of allowed states is a linear space, show that the periodic boundary condition:

$$\psi(-L/2) = \psi(L/2), \quad (8)$$
$$\psi'(-L/2) = \psi'(L/2) \quad (9)$$

gives acceptable wave functions. "Acceptable" here includes that the probability to find a particle in the box must be constant. Are there other acceptable choices?

Notice that we can calculate the probability density as

$$j = \frac{\hbar}{2mi}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right) = \frac{\hbar}{m}\Re\left\{\Psi^* \frac{1}{i}\frac{\partial \Psi}{\partial x}\right\} = \frac{\hbar}{m}\Im\left\{\Psi^* \frac{\partial \Psi}{\partial x}\right\},$$

In order for the wave function to be acceptable, we must have its probability current density equal at both boundary points:

$$j(-L/2) = j(L/2)$$

at $-L/2$ — at $L/2$

$$\Rightarrow \mathrm{Re}\left[\psi^* \frac{1}{i}\frac{\partial \psi}{\partial x}\right] = \mathrm{Re}\left[\psi^* \frac{1}{i}\frac{\partial \psi}{\partial x}\right]$$

and

$$\mathrm{Im}\left[\psi^* \frac{\partial \psi}{\partial x}\right] = \mathrm{Im}\left[\psi^* \frac{\partial \psi}{\partial x}\right]$$

$$\Rightarrow \psi^* \frac{\partial \psi}{\partial x}(-L/2) = \psi^* \frac{\partial \psi}{\partial x}(L/2)$$

Notice that a periodic function $\psi(x,t)$ of $\sin\left(\frac{2\pi n}{L}x\right)$, $\cos\left(\frac{2\pi n}{L}x\right)$ satisfies this.

Moreover, any function that is acceptable can be constructed from these because they form a complete set (via the fourier series). Therefore, the only functions that are acceptable are ones who are periodic and have periodic derivatives. There are no other acceptable choices

16. Note: I have posted a note reviewing complex variables in the module for week 4, in case it is helpful (to evaluate an integral).

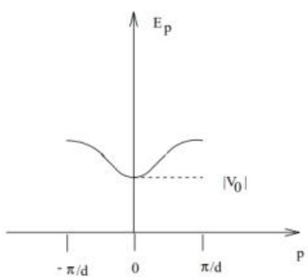


Figure 1: Energy versus momentum for the one-dimensional lattice problem.

Consider a proton (charge e) in a one dimensional harmonic oscillator potential with unperturbed Hamiltonian

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2. \tag{10}$$

We add a small time-dependent electric field so that $H = H_0 + V_t$ with

$$V_t = \frac{eEx}{1+(t/\tau)^2}, \quad -\infty < t < \infty. \tag{11}$$

If the system is initially in the ground state at $t = -\infty$, what is the probability to observe it in the first excited state after a long time ($t = \infty$)?

The ground state of the QHO is given by

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}.}$$

We note that

$$\langle n \,|\, \psi(t)\rangle = \frac{1}{i}\int_{t_0}^{t} \mathrm{d}t_1 e^{i(\varepsilon_n - \varepsilon_i)t_1} \left\langle n \,\middle|\, \hat{\mathrm{V}}_{t_1} \,\middle|\, i\right\rangle \tag{28}$$

Taking the magnitude and squaring it, we get the transition probability (with $t_0 = -\infty$ and $t = \infty$):

$$P(\psi_0 \to \psi_1) = \left| \frac{1}{i}\int_{-\infty}^{\infty} dt_1\, e^{i(\varepsilon_1 - \varepsilon_0)t_1} \langle \psi_1 | V_{t_1} | \psi_0 \rangle \right|^2$$

Notice

$$\psi_1(x) = A_1 \hat{a}_+ \psi_0 = \frac{A_1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$
$$= A_1\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\, x e^{-\frac{m\omega}{2\hbar}x^2}. \qquad A_1 = 1$$

$$\Rightarrow \langle \psi_1 | V_{t_1} | \psi_0 \rangle = \int_{-\infty}^{\infty} c_1 x e^{-\frac{\alpha}{2}x^2} \cdot c_v(t_1) \cdot x \cdot c_0 e^{-\frac{\alpha}{2}x^2} dx$$

$$= c_1 c_0 c_v(t_1) \underbrace{\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx}$$

— learned this in Ph 12b

$$= \frac{\sqrt{\pi}}{2\alpha^{3/2}} \cdot c_1 \cdot c_0 \cdot c_v(t_1)$$

$$\cdot\ c_1 \cdot c_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \sqrt{\frac{2m\omega}{\hbar}} = \sqrt{\frac{2}{\pi}} \cdot \frac{m\omega}{\hbar}$$

$$\cdot\ \alpha = \frac{m\omega}{\hbar}$$

$$\rightarrow \frac{\sqrt{\pi}}{2} c_1 c_0 = \frac{1}{\sqrt{2}} \cdot \left(\frac{\hbar}{m\omega}\right)^{1/2} \equiv c_2$$

$$\Rightarrow \mathbb{P}(\psi_0 \to \psi_1) = \left| \frac{c_2}{i} \int_{-\infty}^{\infty} e^{i(\varepsilon_1 - \varepsilon_0)t_1} \cdot c_v(t_1)\, dt_1 \right|^2$$

$$= \left| \frac{c_2}{i} \int_{-\infty}^{\infty} \frac{eE}{1+(t_1/\tau)^2} \cdot e^{i(\varepsilon_1 - \varepsilon_0)t_1} dt_1 \right|^2$$

$$= \left| \frac{eEc_2}{i} \underbrace{\int_{-\infty}^{\infty} \frac{e^{i\varepsilon t}}{1+(t/\tau)^2} dt_1}_{\equiv I_5} \right|^2$$

Recall what we learned in ACM 95a:

<u>Improper Integrals involving Trig Functions</u>

$I_1 = \text{P.V.} \int_{-\infty}^{\infty} f(x)\cos(\alpha x)\,dx$

$I_2 = \text{P.V.} \int_{-\infty}^{\infty} f(x)\sin(\alpha x)\,dx$

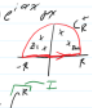
$I_3 = \text{P.V.} \int_{-\infty}^{\infty} f(x)\, e^{\pm i\alpha x}\,dx$

Conditions
- $\alpha > 0$
- $f(x)$ is a rational function and continuous on $\mathbb{R}$ and $\deg p \geq \deg q + 2$

<u>Remark</u>: $\boxed{I_1 = \text{Re}[I_3^{\pm}], \quad I_2 = \text{Im}[I_3^+] = -\text{Im}[I_3^-]}$

Two cases: I^+ vs I^-

$I_3^+ = \text{P.V.} \int_{-\infty}^{\infty} f(x) e^{i\alpha x} dx$



$$\underbrace{\int_C f(z) e^{i\alpha z} dz}_{\text{CRT}} = \int_{C_R^+} + \underbrace{\int_{-R}^{R}}_{I}$$

On C_R^+: $|f(z)e^{i\alpha z}| \leq \frac{k}{|z|^2} |e^{i\alpha Re^{i\theta}}|$

$$= \frac{k}{R^2} \left| e^{i\alpha R(\cos\theta + i\sin\theta)} \right| = \frac{k}{R^2} \underbrace{\left| e^{i\alpha R\cos\theta} \right|}_{1} \cdot \left| e^{-\overset{>0}{\alpha R\sin\theta}} \right| \leq \frac{k}{R^2}$$

$$\overset{ML}{\Rightarrow} \left| \int_{C_R^+} \right| \to 0$$

$I_3^- = \text{PV} \int_{-\infty}^{\infty} f(x) e^{-i\alpha x} dx$

$$I_3^+ = 2\pi i \sum_{k=1}^{n} \text{Res}(f(z) e^{i\alpha z}, z_k) \quad \text{Im}[z_k] > 0$$

$$I_3^- = -2\pi i \sum_{k=1}^{n} \text{Res}(f(z) e^{-i\alpha z}, z_k) \quad \text{Im}[z_k] < 0$$

$$\boxed{\begin{aligned} I_3^+ &= 2\pi i \sum_{k=1}^{n} \operatorname{Res}\left(f(z)\, e^{iqz}, \underbrace{z_k}_{\text{Im}[z_k]>0}\right) \\ I_3^- &= -2\pi i \sum_{k=1}^{n} \operatorname{Res}\left(f(z)\, e^{-iqz}, \underbrace{z_k}_{\text{Im}[z_k]<0}\right) \end{aligned}}$$

Since $\varepsilon > 0$ we see that

$$I_3 = 2\pi i \sum_{k=1}^{n'} \operatorname{Res}\left(\frac{e^{i\varepsilon t}}{1+(t/\tau)^2}, z_k\right)$$

with $\{z_k : \text{im}[z_k] > 0\} = \{t = +i\tau \equiv z_0\}$

and

$$f(t) = \frac{1}{1+(t/\tau)^2} \leftarrow (1 + it/\tau)(1 - it/\tau)$$

$$\frac{i}{\tau}\left(\frac{\tau}{i} + t\right) \quad \frac{i}{\tau}\left(\frac{\tau}{i} - t\right)$$

Notice

$$\operatorname{Res}\left(f(t)\, e^{i\varepsilon t}, z_0\right) = \lim_{t \to z_0} (\cancel{t - i\tau}) \frac{e^{i\varepsilon t}}{\frac{-1}{\tau^2}(\cancel{t - i\tau})(-t - i\tau)}$$

$$= \frac{e^{i\varepsilon(i\tau)}}{-\frac{1}{\tau^2}\,{-2(i\tau)}} = \frac{e^{-\varepsilon\tau}}{\frac{2i}{\tau}} = \frac{\tau e^{-\varepsilon\tau}}{2i}$$

$$\rightarrow I_3 = \pi \tau e^{-\varepsilon\tau}$$

$$\rightarrow \mathbb{P}(\psi_0 \to \psi_1) = \left|\frac{eEc_2}{i} \pi \tau e^{-\varepsilon\tau}\right|^2$$

$$= (eE c_2 \pi \tau)^2 e^{-2\varepsilon\tau}$$

$$= 2\left(\left(\frac{\hbar}{m\omega}\right)^{1/2}\right)^2 \cdot e^2 E^2 \pi^2 \tau^2 e^{-2\varepsilon\tau}$$

$$= \boxed{2\pi^2 \frac{\hbar}{m\omega} e^2 E^2 \tau^2 e^{-2\hbar\omega\tau}}$$