PROBLEMS:

READING: Section 18.3 and 18.4 in Shankar on time-dependent perturbation theory and on electromagnetic interactions.

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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:

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

(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 :

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

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

1.1

The matrix elements of V are given by the integral:

$$\langle q|V|p\rangle = \int_0^L \mathrm{d}x \frac{1}{\sqrt{L}} e^{-2\pi i n_q x/L} V(x) \frac{1}{\sqrt{L}} e^{2\pi i n_p x/L} \tag{1}$$

We can plug in the Fourier series for $V(x)$ into the above equation:

$$\langle q|V|p\rangle = \int_0^L \mathrm{d}x \frac{1}{\sqrt{L}} e^{-2\pi i n_q x/L} \sum_{n=-\infty}^{\infty} e^{in2\pi x/d} V_n \frac{1}{\sqrt{L}} e^{2\pi i n_p x/L} \tag{2}$$

Bringing the sum and coefficients outside the integral:

$$\langle q|V|p\rangle = \frac{1}{L} \sum_{n=-\infty}^{\infty} V_n \int_0^L \mathrm{d}x e^{-2\pi i n_q x/L} e^{in2\pi x/d} e^{2\pi i n_p x/L} \tag{3}$$

We can use the expression we are given for d to combine the exponentials:

$$\begin{aligned} &= \frac{1}{L} \sum_{n=-\infty}^{\infty} V_n \int_0^L \mathrm{d}x e^{-2\pi i n_q x/L} e^{in2\pi x/(L/N)} e^{2\pi i n_p x/L} \\ &= \frac{1}{L} \sum_{n=-\infty}^{\infty} V_n \int_0^L \mathrm{d}x e^{\frac{2\pi i x}{L}(nN+n_p-n_q)} \end{aligned} \tag{4}$$

This integral evaluates to L when $nN + n_p - n_q = 0$, leading to the condition for non-zero contributions:

$$nN + n_p - n_q = 0 \tag{5}$$

where n is an integer. We can thus express the matrix element as:

$$\langle q|V|p\rangle = \sum_{n=-\infty}^{\infty} V_n \delta_{n_p, n_q+nN} \tag{6}$$

Most of the terms in the sum will be zero, as the Kronecker delta will only be non-zero when $n_p - nq$ is a multiple of N:

$$\langle q|V|p\rangle = V_{\frac{n_p-n_q}{N}} \tag{7}$$

1.2

(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^{nd} order. Express your answer in terms of V_n.

We may consider the projection of the unperturbed wave function $\langle q|$ onto the perturbed wave function $\left|N^{(1)}\right\rangle$:

$$\left\langle q\middle|N^{(1)}\right\rangle = \frac{1}{\varepsilon_{n_p} - \varepsilon_{n_q}} \langle q| V |p\rangle \tag{8}$$

Using the expression for the matrix elements of V we derived in part (a), we can write the above equation as:

$$\left\langle q\middle|N^{(1)}\right\rangle = \frac{1}{\varepsilon_{n_p} - \varepsilon_{n_q}} V_{\frac{n_p - n_q}{N}} \tag{9}$$

To first order, the perturbed wave function is:

$$\left|N^{(1)}\right\rangle = |p\rangle + \sum_{n_q \neq n_p} \frac{1}{\varepsilon_{n_p} - \varepsilon_{n_q}} V_{\frac{n_p - n_q}{N}} |q\rangle \tag{10}$$

where we earlier stated that n_q has to be an integer multiple away from n_p. The energy to second order consists of the unperturbed energy plus the first order correction plus the second order correction:

$$\varepsilon_{n_p} \approx \varepsilon_{n_p}^{(0)} + \langle n| V |n\rangle + \sum_{n_q \neq n_p} \frac{|\langle q| V |p\rangle|^2}{\varepsilon_{n_p} - \varepsilon_{n_q}} \tag{11}$$

where n is an unperturbed eigenstate. We can simplify to:

$$\varepsilon_{n_p} \approx \varepsilon_{n_p}^{(0)} + V_0 + \sum_{n_q \neq n_p} \frac{|V_n|^2}{\varepsilon_{n_p} - \varepsilon_{n_q}} \tag{12}$$

where we again have that n_q has to be an integer multiple away from n_p.

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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

$$V = \sum_{i,j} |i\rangle\langle i|V|j\rangle\langle j|$$
$$H_0|i\rangle = \varepsilon_i|i\rangle,$$

where

$$\langle i \mid j\rangle = \delta_{ij}.$$

Let

$$V = V_1 + V_2$$

with

$$\begin{aligned} V_1 \equiv & |m\rangle\langle m|V|m\rangle\langle m| + |n\rangle\langle n|V|n\rangle\langle n| + \\ & + |m\rangle\langle m|V|n\rangle\langle n| + |n\rangle\langle n|V|m\rangle\langle m| \end{aligned}$$

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.)

2.1

We want to diagonalize the matrix representation of H_1 in the subspace spanned by $|n\rangle$ and $|m\rangle$. We have:

$$H_1 = \begin{pmatrix} \varepsilon_n + \langle n|V_1|n\rangle & \langle n|V_1|m\rangle \\ \langle m|V_1|n\rangle & \varepsilon_m + \langle m|V_1|m\rangle \end{pmatrix} \tag{13}$$

since we have that $H_1 \equiv H_0 + V_1$. Diagonalizing this matrix in SymPy gives the eigensystem:

$$\lambda_1 = \frac{-V_{mm} + V_{nn} - \epsilon_m + \epsilon_n - \sqrt{V_{mm}^2 - 2V_{mm}V_{nn} + 2V_{mm}\epsilon_m - 2V_{mm}\epsilon_n + 4V_{mn}V_{nm} + V_{nn}^2 - 2V_{nn}\epsilon_m}}{2V_{mn}} \tag{14}$$

with the corresponding eigenvector:

$$|\lambda_1\rangle = \frac{V_{mm}}{2} + \frac{V_{nn}}{2} + \frac{\epsilon_m}{2} + \frac{\epsilon_n}{2} - \frac{\sqrt{V_{mm}^2 - 2V_{mm}V_{nn} + 2V_{mm}\epsilon_m - 2V_{mm}\epsilon_n + 4V_{mn}V_{nm} + V_{nn}^2 - 2V_{nn}}}{2} \tag{15}$$

2.2

(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.

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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:

$$\psi(-L/2) = \psi(L/2)$$
$$\psi'(-L/2) = \psi'(L/2)$$

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?

3.1

We may restate the condition of no net floods into or out of the box as:

$$0 = \frac{\partial}{\partial t} \int_{-L/2}^{L/2} |\psi(x,t)|^2 \, \mathrm{d}x \tag{16}$$

That is, the probability to find a particle in the box must not change with time. Now, if we have some acceptable wave function $\psi(x)$. And another acceptable function ϕ:

$$\phi(x) = e^{\frac{i2\pi^2 t}{mL^2}} \sin\left(\frac{2\pi x}{L}\right) \tag{17}$$

Any linear combination of $\psi(x)$ and $\phi(x)$ is also an acceptable wave function. So, we plug in the linear combination of $\psi(x)$ and $\phi(x)$ into the condition of no net floods into or out of the box:

$$\begin{aligned} 0 &= \frac{\partial}{\partial t} \int_{-L/2}^{L/2} |\psi(x) + \phi(x)|^2 \, \mathrm{d}x \\ &= \frac{\partial}{\partial t} \int_{-L/2}^{L/2} |\psi(x)|^2 \, \mathrm{d}x + \frac{\partial}{\partial t} \int_{-L/2}^{L/2} |\phi(x)|^2 \, \mathrm{d}x + \frac{\partial}{\partial t} \int_{-L/2}^{L/2} \psi^*(x)\phi(x) + \psi(x)\phi^*(x) \, \mathrm{d}x \end{aligned} \tag{18}$$

We know the first two terms are zero, as $\psi(x)$ and $\phi(x)$ are acceptable wave functions. So, we are left with:

$$0 = \frac{\partial}{\partial t} \left[\int_{-L/2}^{L/2} \psi^*(x)\phi(x) \, \mathrm{d}x + \int_{-L/2}^{L/2} \psi(x)\phi^*(x) \, \mathrm{d}x \right] \tag{19}$$

We can write the above equation as:

$$0 = \frac{\partial}{\partial t} \left[\int_{-L/2}^{L/2} \psi^*(x)\phi(x) \, \mathrm{d}x \right] + \frac{\partial}{\partial t} \left[\int_{-L/2}^{L/2} \psi(x)\phi^*(x) \, \mathrm{d}x \right] \tag{20}$$

Now, we can use the product rule to differentiate the above equation:

$$0 = \int_{-L/2}^{L/2} \frac{\partial}{\partial t} \left[\psi^*(x)\phi(x)\right] \mathrm{d}x + \int_{-L/2}^{L/2} \frac{\partial}{\partial t} \left[\psi(x)\phi^*(x)\right] \mathrm{d}x \tag{21}$$

We can write the above equation as:

$$0 = \int_{-L/2}^{L/2} \left[\frac{\partial}{\partial t}\psi^*(x)\right] \phi(x) + \psi^*(x) \left[\frac{\partial}{\partial t}\phi(x)\right] \mathrm{d}x + \int_{-L/2}^{L/2} \left[\frac{\partial}{\partial t}\psi(x)\right] \phi^*(x) + \psi(x) \left[\frac{\partial}{\partial t}\phi^*(x)\right] \mathrm{d}x \tag{22}$$

Rewriting the above equation to emphasize that the wave functions are time dependent

$$0 = \int_{-L/2}^{L/2} \left[\frac{\partial}{\partial t}\psi^*(x,t)\right] \phi(x,t) + \psi^*(x,t) \left[\frac{\partial}{\partial t}\phi(x,t)\right] \mathrm{d}x + \int_{-L/2}^{L/2} \left[\frac{\partial}{\partial t}\psi(x,t)\right] \phi^*(x,t) + \psi(x,t) \left[\frac{\partial}{\partial t}\phi^*(x,\right. \tag{23}$$

Now, the time dependent Schrödinger equation is:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t) \tag{24}$$

So, we can write the above equation as: Isolate the time derivative of the wave function

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{i\hbar}\hat{H}\psi(x,t) \tag{25}$$

Now, for the complex conjugate of the wave function:

$$\frac{\partial}{\partial t}\psi^*(x,t) = -\frac{1}{i\hbar}\hat{H}\psi^*(x,t) \tag{26}$$

We can plug in the time derivative of the wave function into the above equation:

$$0 = \int_{-L/2}^{L/2} \left[\frac{1}{i\hbar}\hat{H}\psi^*(x,t)\right] \phi(x,t) + \psi^*(x,t) \left[\frac{1}{i\hbar}\hat{H}\phi(x,t)\right] \mathrm{d}x + \int_{-L/2}^{L/2} \left[\frac{1}{i\hbar}\hat{H}\psi(x,t)\right] \phi^*(x,t) + \psi(x,t) \left[\frac{1}{i\hbar}\right. \tag{27}$$

The free-particle Hamiltonian is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{28}$$

So, we can plug in the Hamiltonian into the above equation:

$$0 = \int_{-L/2}^{L/2} \left[\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi^*(x,t) \right] \phi(x,t) + \psi^*(x,t) \left[\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \phi(x,t) \right] \mathrm{d}x$$
$$+ \int_{-L/2}^{L/2} \left[\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x,t) \right] \phi^*(x,t) + \psi(x,t) \left[\frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \phi^*(x,t) \right] \mathrm{d}x \tag{29}$$

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).

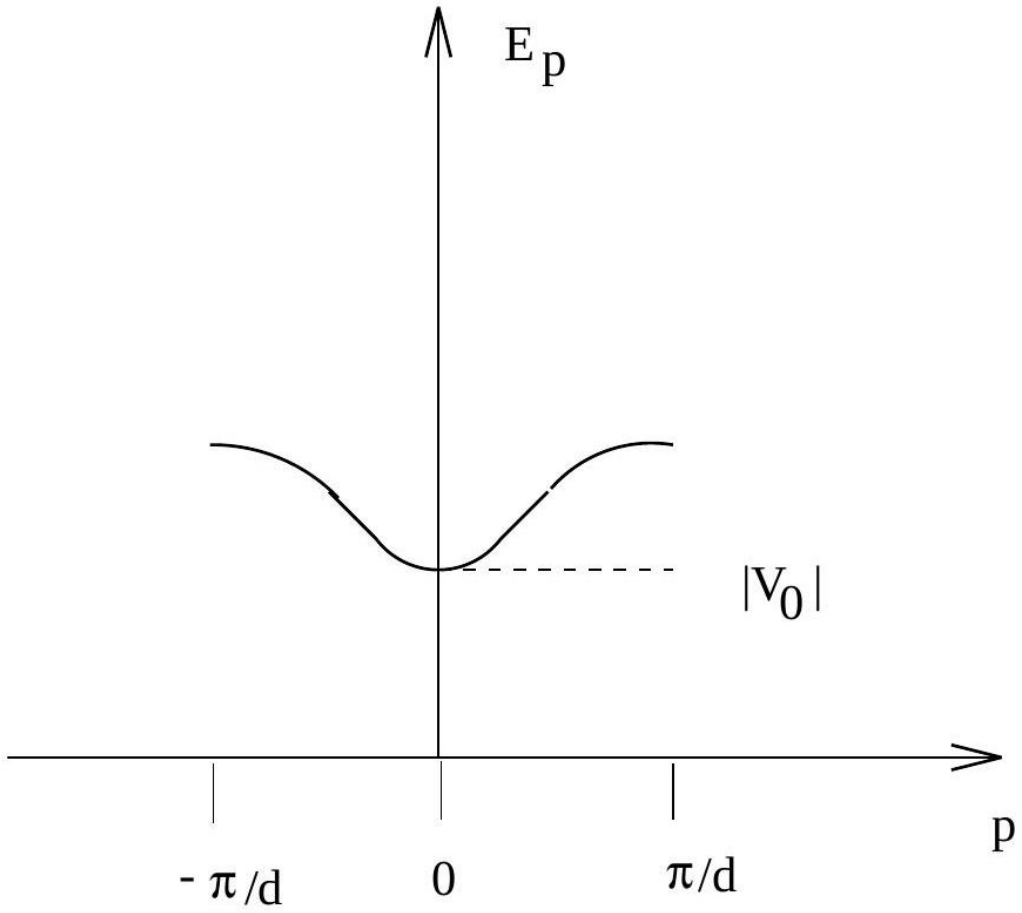

Figure 1: Energy versus momentum for the one-dimensional lattice problem.

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

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

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

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

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 ($t = \infty$) ?

Thus,

$${}_\infty\langle 1 \mid 0\rangle_{-\infty} = \frac{eE}{i}\pi\tau e^{-\omega\tau}\frac{1}{\sqrt{2m\omega}} = -\frac{i\pi\tau eE}{\sqrt{2m\omega}}e^{-\omega\tau}$$

Finally, the desired transition probability is

$$P(1) = \,|_\infty \langle 1 \mid 0\rangle_{-\infty}|^2 = -\frac{(\pi\tau eE)^2}{2m\omega}e^{-2\omega\tau}$$

3.2

We want to evaluate the desired transition probability using the formalism of time-dependent perturbation theory in the interaction picture. We have:

$$P_1 = -\frac{i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t \,\langle 1\,|V_t|\,0\rangle\, e^{i\omega_{1,0}t} \tag{30}$$