Problem set #1

1.1. Second order perturbation theory and the speed of light in a dielectric material

In a dielectric material, by applying an electric field $E$, atoms in the material will polarize, resulting in an electric dipole moment. In E&M, we learned that the total energy for such a dipole $P$ in electric field $E$ is

$$U = -V P E$$  \hspace{1cm} (1.1)$$

where $V$ is the volume of the system, $P$ is dielectric polarization density and $E$ is the field strength. (Note, in principle, $P$ and $E$ should be vectors, and the product here should be a dot product. Here, because $P$ and $E$ are parallel to each other, we can ignore their directions and treat them as scalars). From this equation, we noticed that

$$P = -\frac{1}{V} \frac{dU}{dE}$$  \hspace{1cm} (1.2)$$
i.e., the polarization density is the first order derivative of the energy $U$ to the electric field strength $E$ (then divided by volume $V$). In this problem, we will study polarization effect using quantum mechanics. The problem can be solved exactly and/or using perturbation theory. We will use both methods and show that they agree with each other. In addition, we will use the perturbation theory to show that the speed of light in such a medium must be slower than the speed of light in vacuum (cannot be faster), consistent with the special relativity.

In quantum mechanics, this polarization effect can be studied by treating an atom as a harmonic oscillator. Because a nucleon is much heavier than an electron, we will ignore the motion of nucleons, i.e. assuming the position of a nucleon is fixed at the origin. An electron is oscillating around this nucleon. For small oscillations, we can approximate treat the system as a harmonic oscillator. For simplicity, we can treat the atom as a 1D system, because we only care about the motion along the direction of the external field $E$. So the following Hamiltonian will be used:

$$H_0 = \frac{\hat{p}^2}{2\mu} + \frac{1}{2} k x^2$$  \hspace{1cm} (1.3)$$

where $\hat{p} = -i \hbar \hat{\partial}_x$ is the momentum of the electron. $\mu$ is the electron mass. $k$ is the spring constant and $x$ is the position of the electron (relative to the nucleon). Without an external field, the eigenstates and eigenenergies of $H_0$ is known (i.e. a harmonic oscillator, see textbook section 2.3.2 for details). The eigenenergies are

$$E_n = \left( n + \frac{1}{2} \right) \hbar \omega$$  \hspace{1cm} (1.4)$$

where $n = 0, 1, 2, \ldots$ and $\omega = \sqrt{k/\mu}$ is the frequency of the oscillator. The corresponding eigenwavefunctions are

$$\psi_n(x) = \left( \frac{\mu \omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$  \hspace{1cm} (1.5)$$

where $\xi = \sqrt{\mu \omega / \hbar} \ x$ and $H_n(\xi)$ are Hermite polynomials [Eq. 2.85 in the textbook].
Consider a uniform electric field $E$. The electric potential energy for such a particle with charge $q$ is $V(x) = -q E x$, where $x$ is the position of the particle. This potential energy introduces an extra term to the Hamiltonian

$$H = H_0 - H' = H_0 - q E x \quad (1.6)$$

If $E$ is weak (small), the second term can be treated as a perturbation.

### 1.1.1. Preparation

Here, we first prove a very useful and important conclusion. Consider a Hamiltonian $H_0 = \frac{\mu^2}{2} + V(x)$. We assume that the potential is an even function $V(x) = V(-x)$, we will prove that any eigenwavefunctions of $H_0$ is either an odd function of $x$ or an even function of $x$. (more precisely, if an eigenwavefunction is NOT an even or odd function of $x$, we can always make it an even or odd function using the following procedure, as long as $V(x)$ is an even function).

1. **Prove that if $\psi(x)$ is an eigenstate, then $\psi(-x)$ is also an eigenstate with the same eigenvalue, i.e., if**

   $$\frac{\hbar^2}{2 \mu} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \quad (1.7)$$

   **then**

   $$\frac{\hbar^2}{2 \mu} \frac{d^2 \psi(-x)}{dx^2} + V(x) \psi(-x) = E \psi(-x) \quad (1.8)$$

2. **Using conclusions from (1), prove that $\psi_+(x) = \frac{\psi(x) + \psi(-x)}{\sqrt{2}}$ and $\psi_-(x) = \frac{\psi(x) - \psi(-x)}{\sqrt{2}}$ are also eigenstates of $H_0$ with the same eigenvalue $E$ [same as the eigenenergy of $\psi(x)$]**, i.e.

   $$\frac{\hbar^2}{2 \mu} \frac{d^2 \psi_+(x)}{dx^2} + V(x) \psi_+(x) = E \psi_+(x) \quad (1.9)$$

   and

   $$\frac{\hbar^2}{2 \mu} \frac{d^2 \psi_-(x)}{dx^2} + V(x) \psi_-(x) = E \psi_-(x) \quad (1.10)$$

3. **Since $\psi_+(x)$ and $\psi_-(x)$ are also eigenstates of $H_0$ with the same eigenvalue, here we will use $\psi_+(x)$ and $\psi_-(x)$ to represent eigenstates of $H_0$, instead of $\psi(x)$ or $\psi(-x)$**. Prove that $\psi_+(x)$ is an even function of $x$, while $\psi_-(x)$ is an odd function of $x$.

This conclusion is very important and worthwhile to memorize. For most of the potentials that we have studied in QMI, they are even functions of $x$ (e.g. harmonic oscillators, $1/r$ potential, square well, etc.), and if you look at any eigenwavefunction there, it is either an even or an odd function.

### 1.1.2. First order perturbation

According to the perturbation theory, the first order correction to the eigenenergy is

$$E_n^{(1)} = \langle \psi_0^0 | -q E x | \psi_n^0 \rangle = -q E \int \psi_0^0(x) \psi_n^0(x) * x \psi_n^0(x) \, dx \quad (1.11)$$

1. **Show that the function inside the integral, $\left[ \psi_n^0(x) \right] * x \psi_n^0(x)$, is an odd function of $x$**

   Hint: as shown in the previous part, $\psi_n^0(x)$ is either an even or odd function, same is true for $\left[ \psi_n^0(x) \right]^*$. 

2. **Show that $\int_{-\infty}^{\infty} f(x) \, dx = 0$, if $f(x)$ is an odd function**.

   Conclusions from (1) and (2) implies immediately that $E_n^{(1)} = 0$, i.e., the first order correction to the energy is zero.

### 1.1.3. Sign of the second order perturbation

Since the first correction is zero, we need to go to the second order. In this part, we will NOT do any calculations (which will be done in latter part). Instead, without any calculation, we can already obtain a lot of information and intuition about a dielectric material.
At low temperature, all the atoms are in their ground states, and thus the total energy of the system (if we ignore interactions between atoms),

\[ U = N E_0 \]  

where \( N \) is the number of atoms in the system and \( E_0 \) is the energy for each atom. As shown above, the polarization is

\[ P = \frac{1}{V} \frac{dU}{dE} = -N \frac{dE_0}{dE} = -N \frac{dE_0}{dE} \]  

where \( n = N/V \) is the particle density. Because the first order correction is zero, the correction to the eigenenergy is dominated by the second order term. As discussed in class, the second order perturbation always reduce the energy of the ground state, i.e. \( E_0(E) \) must decrease monotonically as \( E \) increases from 0. This means that the sign of \( \frac{dE_0}{dE} \) is fixed.

(1) Is \( \frac{dE_0}{dE} \) positive or negative?

(2) Is \( P > 0 \) or \( P < 0 \)?

(3) What is the sign of \( P/E \)? (For the whole problem we assume \( E > 0 \). One can prove that the same conclusion is found, if we assume \( E < 0 \) from the beginning).

1.1.4. the speed of light

The speed of light in a (linear) medium is

\[ c = \frac{c_0}{\sqrt{\epsilon \mu}} \]  

where \( \epsilon \) is the dielectric constant (also known as relative permittivity) and \( \mu \) is the magnetic permeability. \( c_0 \) is the speed of light in vacuum. For most media, \( \mu \approx 1 \). So here, we will treat \( \mu \) as identity for simplicity.

\[ c \approx \frac{c_0}{\sqrt{1 + \chi}} \]  

Here we used the fact that the dielectric constant is \( \epsilon = 1 + \chi \), where \( \chi \) is the electric susceptibility. For weak electric field \( E \), \( \chi \) is defined as

\[ \chi = \frac{P}{E} \]  

In the previous problem, we have shown that because second order perturbation reduces the energy of the ground state, \( P/E > 0 \). Therefore \( \chi > 0 \).

(1) Show that \( c < c_0 \), i.e. the speed of light in this medium must be smaller than the speed of light in vacuum. This conclusion is a direct consequence of the second order perturbation theory. And this conclusion must be true, if we don’t want to violate special relativity.

(NOTE: here we treat \( \mu = 1 \) for simplicity. In fact, one can use exactly the same procedure to show that \( \mu > 1 \) and thus even if we consider corrections to \( \mu \), \( c \) is still smaller than \( c_0 \))

(2) Does the conclusion rely on the sign of the charge \( q \)? Can the same conclusion hold for arbitrary potential \( V(x) \) [we will still assume \( V(x) \) being an even function of \( x \)]?

1.1.5. Second order perturbation

In this part, we compute the second order correction to the energy.

(1) Show that

\[ \int_{-\infty}^{+\infty} H_n(\xi) H_m(\xi) \ e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} \delta_{nm} \]  

Hint: we know that for eigenstates of an harmonic oscillator, \( \langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm} \); i.e., the eigenstates are orthonormal. So

\[ \delta_{nm} = \langle \psi_n^0 | \psi_m^0 \rangle = \int_{-\infty}^{+\infty} dx [\psi_n^0(x)]^\dagger \psi_m^0(x) \]  

Wave-functions \( \psi_n^0(x) \) contains Hermite polynomials [see textbook section 2.3.2 or Eq. (1.5) above]. This orthonormal condition [Eq. (1.14)] directly implies the relation that we want to prove.
(2) Prove that

$$\langle \psi_m^0 | H' | \psi_n^0 \rangle = \int_{-\infty}^{\infty} dx \left[ \psi_m^0(x) \right]^* H' \psi_n^0(x) = -q E \left( \sqrt{\frac{n+1}{2}} \delta_{m,n+1} + \sqrt{\frac{n}{2}} \delta_{m,n-1} \right) \sqrt{\frac{\hbar}{\mu \omega}}$$

(1.19)

Hint: Here we will need to use the following relation, i.e., Eq. [2.87] in the textbook

$$\xi H_n(\xi) = \frac{1}{2} H_{n+1}(\xi) + n H_{n-1}(\xi)$$

(1.20)

In addition, we will need to use Eq. (1.17) from part (1)

(3) Prove that the second order correction $E_{n}^{(2)} = -q^2 E^2 / (2 \mu \omega^2)$. For ground state ($n = 0$), the correction is indeed negative as we found above without doing any calculations.

(4) Ignore higher order corrections. Compute $\chi$, $\epsilon$ and $c$. Show that the speed of light $c$ in this medium is smaller than $c_0$.

1.1.6. Exact solution

It turns out that the eigenstates of this Hamiltonian $H$ can be solved exactly.

$$H = H_0 + H' = -\frac{\hbar^2}{\mu} \frac{d}{dx^2} + \frac{1}{2} k x^2 - q E x$$

(1.21)

(1) Show that by redefine $x$ as $y = x - a$, we can rewrite the Hamiltonian as

$$H = -\frac{\hbar^2}{2 \mu} \frac{d}{dy^2} + \frac{1}{2} k y^2 + \Delta$$

(1.22)

where $\Delta$ is a constant independent of $y$. Find $a$ and the $\Delta$.

Therefore, we find that after applying the field $E$, the Hamiltonian is still a harmonic oscillator with the same mass and the same spring constant. But this new harmonic oscillator is oscillating around a new equilibrium position (around $x = a$, instead of the origin anymore). In addition, the energy of this new oscillator is shifted by a constant $\Delta$.

Note: this conclusion is exactly the same as a classical harmonic oscillator. There, if we apply a constant force to a classical harmonic oscillator, we will only change the equilibrium position (and shift the total energy by a constant).

(2) Because the energy of the oscillator is shifted by $\Delta$, the eigenenergies (after applying the field $E$) will become

$$E_n = \hbar \omega \left( n + \frac{1}{2} \right) + \Delta.$$  

(1.23)

Compare it with the second order perturbation result that we find early one

$$E_n = E_n^0 + E_n^1 + E_n^2 + O(E^3)$$

(1.24)

and prove that the second order perturbation theory full agrees with the exactly solution.

1.1.7. Higher order perturbation

Since second order perturbation calculation has already recovered the exact solution. Higher order corrections must be zero. (in general this is not true for a general quantum Hamiltonian problem, but it happens to be the case for this problem).

(1) Show that the third order perturbation is zero.