PHYS 4302
Homework 8

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May 2023

Problem 1

Consider a standard one-dimensional infinite square potential well for $0 < x < a$, where the stationary energy levels for a free particle of mass m are familiar

$$E_n^{(0)} = \frac{\hbar^2 \pi^2 n^2}{2ma^2},\ n = 1, 2, 3 \ldots \tag{1}$$

In this problem, the particle between the potential walls is however not free but exposed to the potential

$$V(x) = v \cos\left(\frac{\pi x}{a}\right), \tag{2}$$

where constant v defines the potential magnitude. Potential (2) modifies spectrum (1).

You are asked to find the resulting *small corrections* Δ_n to energy levels: $E_n = E_n^{(0)} + \Delta_n$, for quantum numbers n *sufficiently large* to satisfy *both* conditions of the semi-classical approximation and the smallness of the potential: $|v| \ll E_n$.

(a) Use the semi-classical equation for the problem at hand and apply it to find (first non-vanishing corrections) Δ_n in the specified limit (you do not need to solve the problem for large-magnitude potentials!) How does Δ_n depend on n?

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v\cos\left(\frac{\pi x}{a}\right)$$
$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m}$$
$$\frac{dp}{dt} = -\frac{\partial H}{\partial x} = -\frac{v\pi}{a}\sin\left(\frac{\pi x}{a}\right)$$

We now want to find the eigenfunctions and eigenvalues of the unperturbed Hamiltonian $\hat{H}_0$, given by

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

and $E_n^{(0)}$. Now, we find the perturbed energy levels E_n as

$$E_n = E_n^{(0)} + \Delta_n$$

For sufficiently large values of n, the corrections to the energy levels should become smaller and smaller, and the energy levels approach the unperturbed levels given by $E_n^{(0)}$.

(b) Also calculate (first non-vanishing) corrections Δ_n using the ordinary low-order perturbation theory with respect to perturbation (2) as appropriate. How do they compare to corrections in item (a)?

The low-order perturbation theory approach should result in a correction that is proportional to the strength of the perturbation $V(x)$, like the semi-classical approach in (a). However, the two approaches will differ more greatly at higher orders of n.

Problem 2

A quantum particle of mass m and charge q in three-dimensional space (vector of coordinates r) is subject to the isotropic harmonic potential

$$V(r) = \frac{m\omega^2 r^2}{2},\ r^2 = x^2 + y^2 + z^2, \tag{3}$$

and the spatially uniform electric field E. The system is in its ground state with the field directed along the z-axis:

$$E = E_1 = \mathscr{E}\hat{z}, \tag{4}$$

where $\mathscr{E}$ is the field magnitude and $\hat{z}$ the corresponding unit vector.

At some point in time, the field is made to *suddenly* (nearly instantaneously) change its direction and becomes

$$E = E_2 = \mathscr{E}\hat{s}, \tag{5}$$

the unit vector $\hat{s}$ specified with its Cartesian components s_x, s_y and s_z ($s_x^2 + s_y^2 + s_z^2 = 1$). The magnitude of the field and the change of its direction are *not* assumed small.

(a) Write down the generic system Hamiltonian with the account of field E and indicate its ground state wave function.

The system Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{H}',$$

where $\hat{H}_0$ is the Hamiltonian for the particle in the isotropic harmonic potential, given by

$$\hat{H}_0 = \frac{p^2}{2m} + \frac{m\omega^2 r^2}{2},$$

and $\hat{H}'$ is the Hamiltonian for the particle in the electric field potential, given by

$$\hat{H}' = -q\mathscr{E}z.$$

Therefore, the generic system Hamiltonian is

$$\boxed{\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2 r^2}{2} - q\mathscr{E}z.}$$

To find the ground state wave function of the system, we can find the ground state wave functions of both $\hat{H}_0$ and $\hat{H}'$ and perform a linear combination on them. The ground state wave functions of an isotropic harmonic oscillator and uniform electric field are given by

$$\psi_{0(\hat{H}_0)}(r) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{3}{4}} \exp\left(-\frac{m\omega}{2\hbar}r^2\right),$$
$$\psi_{0(\hat{H}')}(z) = C_0 \exp\left(-\frac{q\mathscr{E}}{2\hbar}z^2\right),$$

where C_0 is a normalization constant. We can now combine these to get

$$\boxed{\psi_0(r) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{3}{4}} \exp\left(-\frac{m\omega}{2\hbar}r^2\right) + C_0 \exp\left(-\frac{q\mathscr{E}}{2\hbar}(z_r)^2\right)}$$

(b) Find probability P that, after the change of the direction of E, the system will be found *not* in its ground state?

$$\begin{aligned} P_{0\to n} &= \frac{1}{\hbar^2}\left|\int_0^\infty dt\, \langle n|V(x)|0\rangle\, e^{i\omega t}\right|^2 \\ &= \frac{q^2\mathscr{E}^2}{\hbar^2}\left|\langle n|s|0\rangle\right|^2 \left|\int_0^\infty dt e^{i\omega t}\right|^2 \\ &= \frac{q^2\mathscr{E}^2}{\hbar^2}\left|\langle n|s|0\rangle\right|^2 \left|-i\omega e^{i\omega t}\right|^2 \\ &= \frac{q^2\mathscr{E}^2}{\hbar^2}\left|\langle n|s|0\rangle\right|^2 \omega^2 e^{2i\omega t} \end{aligned}$$

(c) How much work W has been done on the system during the change of the field direction?

The amount of work done is given by the change in potential and kinetic energy of the system. However, because the change in direction is almost instantaneous, the change in kinetic energy should be nearly 0. This is because if we use the classical definition of work $W = F \cdot d$, where F is the force on the particle due to the electric field and d is the displacement of the particle given by the kinematic equation

$$d(t) = x_0 + v_0 t + \frac{at^2}{2} = 0 + 0t + \frac{at^2}{2} = \frac{at^2}{2},$$

$t \simeq 0$ due to the instantaneous change, so $d \simeq 0$, so $W \simeq F \cdot 0$.

Therefore, the total work can be reduced to the change in potential energy, given by

$$W = \Delta U = \boxed{-q\mathscr{E}(s - z).}$$

Problem 3

A one-dimensional parabolic well with the *single-particle* potential energy

$$U(x) = \frac{m\omega^2 x^2}{2} \tag{6}$$

contains *two* identical spin-$\frac{1}{2}$ fermions of mass m each. These fermions also experience a mutual repulsion described by the interaction energy $V(x_1 - x_2)$ depending on the inter-particle distance $|x_1 - x_2|$. This interaction is weak and can be treated as a small perturbation. Moreover, over a relevant range of inter-particle distances (these distances do not become too large for the states of our interest), the interaction can be approximated by the first terms of the Taylor expansion:

$$V(x_1 - x_2) = A - B|x_1 - x_2|, \tag{7}$$

where A and B, along with ω in (6), are given positive constants of appropriate dimensions. Equation (7) thus shows how the repulsion energy decreases with the distance within this (approximate) description. You are asked to evaluate the effect of repulsion (7) on the eigen energies of the system for both singlet and triplet *two-particle* states (singlet and triplet "sectors" of the system).

(a) Write down the full Hamiltonian $\hat{H}$ of this two-particle system.

$$\hat{H}_1 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} + \frac{m\omega^2 x_1^2}{2},$$
$$\hat{H}_2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{m\omega^2 x_2^2}{2},$$
$$\hat{H}_{\text{int}} = V(x_1 - x_2),$$
$$\hat{H} = \boxed{\hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}}.}$$

(b) Find 2 lowest-possible energies in the singlet sector.

We will first consider the system as if there were no interaction term, so $\hat{H} = \hat{H}_1 + \hat{H}_2$. The eigenstates of $\hat{H}_0$ are given by the product of single-particle ground states:

$$\psi_n(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\phi_n(x_1)\phi_0(x_2) \pm \phi_0(x_1)\phi_n(x_2)\right),$$

where $\phi_n(x)$ are the eigenfunctions of a harmonic oscillator:

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} \exp\left(-\frac{x^2}{2}\right) \hat{H}_n(x),$$

where $n = 0, 1, 2, \ldots$ is the principal quantum number. The eigenvalues for ψ_n are

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

Now we combine the single-particle wave functions:

$$\psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2).$$

We can use perturbation theory to find the energy eigenvalues and eigenfunctions of this two-particle system because the interaction is small at sufficient distance. The first-order perturbation energy correction is given by:

$$\begin{aligned}
\Delta E_{n_1,n_2} &= \langle \psi_{n_1}(x_1)\,\psi_{n_2}(x_2) \,|\, \left(A - B\,|x_1 - x_2|\right) |\psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\rangle \\
&= A\,\langle \psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\,|\psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\rangle - B\,\langle \psi_{n_1}(x_1)\,\psi_{n_2}(x_2) \,|\, \left(|x_1 - x_2|\right) |\psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\rangle \\
&= A - B\,\langle \psi_{n_1}(x_1)\,\psi_{n_2}(x_2) \,|\, \left(|x_1 - x_2|\right) |\psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\rangle \\
&= A - B\left(\int\int \psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\,|x_1 - x_2|\,\psi_{n_1}(x_1)\,\psi_{n_2}(x_2)\,dx_1 dx_2\right)
\end{aligned}$$

(c) Find 1 lowest-possible energy in the triplet sector.
