Quantum Mechanics (II): Homework 5
Due: May 27, 9 AM (hand-in box of Room 514 Physics Dept.), 2022

Ex. 1
(a) 10 If we assume that there exists a solution ψ_0 to the time-independent Schrodinger equation such that ψ_0 is real and never vanishes in the whole domain, show that ψ_0 is the ground state wavefunction. Hint: show that any other solution has higher energy.
(b) Consider a particle of mass m in the double-well potential

$$V(x) = \frac{1}{2}m\omega^2(|x| - a)^2.$$

(i) 10 Let $u_n(x)$ be the normalized eigenfunction for a harmonic potential centered at $x = 0$, $\frac{1}{2}m\omega^2 x^2$. Let $\psi_n(x)$ be the variational trial wavefunction for the nth level of $V(x)$

$$\psi_n(x) = c_1 u_n(x - a) + c_2 u_n(x + a),$$

where c_1 and c_2 are real parameters. By treating c_1 and c_2 as variational parameters, find the variational energies E_n (there are two of them) in terms of the following integrals:

$$A_n = \int_{-\infty}^{\infty} u_n(x - a)\hat{H}u_n(x - a),$$

$$B_n = \int_{-\infty}^{\infty} u_n(x + a)\hat{H}u_n(x - a),$$

$$C_n = \int_{-\infty}^{\infty} u_n(x - a)u_n(x + a),$$

where $\hat{H} = \frac{p^2}{2m} + V(x)$. What are the corresponding forms of the variational eigenfunctions?
(ii) 10 Consider the $n = 0$ states. There are two energies: $E_0^{\pm}$. For a much larger than the ground state width, show that $\Delta E = E_0^- - E_0^+ \approx 2\hbar\omega\sqrt{\frac{2V_0}{\pi\hbar\omega}}e^{-2V_0/\hbar\omega}$ where $V_0 = m\omega^2 a^2/2$. This is known as tunneling splitting. Explain why?
Ex 2 20 Exercise 17.3.4.
Ex 3 Fine Structure of Hydrogen atoms
The Coulomb potential $-e^2/r$ does not account for all interactions between the electron and the proton. There are so-called fine-structure corrections to this basic interaction. Two of them are relativistic in origin. One is the *correction to the kinetic energy* $p^2/2m$. The other is the *spin-orbit interaction*. Consider these two interactions as perturbations to $H = p^2/2m - e^2/r$.
(a) 5 Find the leading correction to the kinetic energy in terms of p ($\equiv \Delta T$).
(b) 10 Using Ex 2, calculate the energy shifts to first order in ΔT and show that they are $O(\alpha^2)$, where α is the *fine-structure constant*.
(c) 10 The spin-orbit interaction is given by

$$V = \frac{e^2}{2m^2c^2r^3}\mathbf{S} \cdot \mathbf{L}$$

 Calculate the energy shifts to first order in V and show that they are also $O(\alpha^2)$.
(d) 10 In addition to the above corrections, another possible correction is due to finite size of nucleus. Now consider the correction only due to finite size of nucleus by assuming that charge is uniformly distributed over a sphere of radius R. Let Bohr radius be a_0 and we shall assume $R \ll a_0$. Find the correction of the ground state energy of the hydrogen atom to leading order of R/a_0.
Ex 4 10 Show that the Green's function is given by

$$G(\mathbf{r}, \mathbf{r}') \equiv \langle\mathbf{r}|\frac{1}{E - \hat{H}_0 \pm i\varepsilon}|\mathbf{r}'\rangle = -\frac{2m}{\hbar^2}\frac{e^{\pm ik|\mathbf{r} - \mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}$$

 where $E = \hbar^2 k^2/2m$ and $\hat{H}_0 = \hat{p}^2/2m$ (finish the contour integrals).
Ex 5 10 Exercise 17.2.4.(1)
Ex 6 10 Exercise 17.2.1.(1)
Ex 7 10 Exercise 16.1.2.

Ex 8 15 Exercise 17.3.2.

Ex 9 15 An operator Λ_0 has non-degenerate eigenvalues and eigenkets λ_n and $|n\rangle$ such that

$$\Lambda_0 |n\rangle = \lambda_n |n\rangle.$$

Consider an operator function $F(\Lambda_0 + \epsilon \Lambda_1)$ with $\epsilon \ll 1$, show that

$$\langle n|F(\Lambda_0 + \epsilon \Lambda_1)|m\rangle = \delta_{nm} F(\lambda_n) + \epsilon \langle n|\Lambda_1|m\rangle \frac{F(\lambda_n) - F(\lambda_m)}{\lambda_n - \lambda_m} + O(\epsilon^2).$$

Ex. 10 10 Prove the following equality

$$\mathrm{P}\frac{1}{x - x_0} = \frac{1}{x - x_0 \pm \varepsilon} \pm i\pi\delta(x - x_0).$$

Ex. 11 10 The Hohenberg-Kohn theorem A widely used method in obtaining the band structure in the solid state physics is the density functional theory. This theory is based on the Hohenberg-Kohn theorem which says that given a Hamiltonian

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2m} + \mathrm{V}(\mathbf{r}),$$

the density distribution of the *ground state* $n(\mathbf{r}) \equiv \psi_0^*(\mathbf{r})\psi_0(\mathbf{r})$ *uniquely* determines the potential $\mathrm{V}(\mathbf{r})$ and $\psi_0(r)$. It therefore appears that one does not need to know the phase of ψ_0. To prove it, one assumes that two different sets $\mathrm{V}(\mathbf{r})$, $\psi_0(r)$ and $\mathrm{V}'(\mathbf{r})$ and $\psi_0'(r)$ gives the same density $n(\mathbf{r})$. Show that this leads to a contradiction.

Ex. 12 The Van der Walls interactions Consider the interaction of two atoms in a vacuum. Let us fix the centers of atoms at $\mathbf{r} = 0$ and $\mathbf{R}$. For simplicity, we shall assume that each atom has only one electron, e.g., the Hydrogen atoms (but in principle, the Van der Walls interaction exists between other atoms in ground state)

(a) 5 For fixed centers of atoms ($\mathbf{r} = 0$ and $\mathbf{R}$), if $R < c/\omega$ where ω is a typical atomic frequency, we can neglect retarded effect. If the we denote the positions of the electrons by $\mathbf{r}_1$ and $\mathbf{r}_2$, find the lowest order terms of the Hamiltonian for the two electrons with mass m in the limit $r_1, r_2 \ll R$.

(b) 10 Treat the part of the potential in (a) that depends on $\mathbf{R}$ as a perturbation, show that to the second order, the shift for the ground state energy ($= -2 \times 13.6$ eV for two H atoms before perturbation) of nonpolar atoms (i.e., atoms with spherical symmetry) $\Delta E(R)$ is always negative and decays as $1/R^6$. This interaction is known as the Van der Walls interaction.

(c) 5 Explain the dependence $1/R^6$ in terms of the dipole-dipole interaction.

(d) 10 Show that for H atoms,

$$\Delta E(R) \geq -\frac{8e^2 a_0^5}{R^6},$$

where a_0 is the Bohr radius.

Ex. 13 Canonical transformation Consider a Hamiltonian $\mathrm{H} = \mathrm{H}_0 + \mathrm{V}$ and assume that to every eigenket $|n_0\rangle$ of H_0 with eigenvalue E_n^0, there is an eigenket $|n\rangle$ of H with eigenvalue E_n. Sometimes, it is more convenient to eliminate (hide) V in the linear level by the so-called canonical transformation

$$\bar{\mathrm{H}} = e^S \mathrm{H} e^{-S},$$

where S is some operator that needs to be found such that $\bar{\mathrm{H}} = \mathrm{H}_0 + O(\mathrm{V}^2)$. Usually S can be chosen to be anti-Hermitian: $S^\dagger = -S$.

(a) 10 Show that if S satisfies $[S, \mathrm{H}_0] + \mathrm{V} = 0$, $\bar{\mathrm{H}} = \mathrm{H}_0 + O(\mathrm{V}^2)$ can be satisfied. More specifically, show that now

$$\bar{\mathrm{H}} = \mathrm{H}_0 + \frac{1}{2}[S, \mathrm{V}] + \frac{1}{3}[S, [S, \mathrm{V}]] + ... + \frac{n}{(n+1)!}[S, [S, [S, ..., [S, \mathrm{V}]]]] + ...$$

(b) 5 If we solve $\bar{\mathrm{H}}$ perturbatively, we find that to the zeroth order of V, the eigenket $|\bar{n}\rangle = |n_0\rangle$ and $\bar{E}_n = E_n^0$. The effect of V is entirely hidden. Show that if S is anti-Hermitian, the eigenvalues will be the same if one sums to all orders in V.

(c) 5 Verify that the lowest correction to E_n^0 in $\bar{E}_n$ is the same as the 2nd order correction to E_n^0 in E_n.

(d) 10 Do ex. 17.2.7. to find Ω (our S is the same as Ω in that problem).

Ex. 14 A hydrogen atom is subject to a uniform electric field E. We shall assume that the electric field is sufficiently weak and can thus be treated as a perturbation.

(a)10 Calculate the energy eigenvalue corrections for the first excited level (n = 2).

(b) 10 Find an expression for the induced electric dipole moment of the ground state to the lowest non-trivial order. Estimate an upper bound for the polarizability of the atom.

Ex. 15 (a) 5 Consider a system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2\alpha}(1 - e^{-\alpha x^2}).$$

Find the ground state energy to $O(\alpha)$.

(b) 10 A spin-1/2 particle of mass m moves in a spherical harmonic oscillator potential $U = 1/2m\omega^2 r^2$ and is subject to the interaction $V = \lambda\vec{\sigma} \cdot \vec{r}$. Here $\vec{S} = \hbar\vec{\sigma}/2$ is the spin operator of the particle. Find the shift of the ground state energy to $O(\lambda^2)$.

Ex. 16 10 Consider a particle of mass m confined in a two dimensional box, locating in the range $-a/2 \leq x \leq a/2$ and $-a/2 \leq y \leq a/2$. Inside the box, the potential that acts on the particle is $V(x, y) = -\lambda xy$ with $\lambda > 0$. Use the perturbation theory to calculate the energy shifts for the degenerate first excited states to first order of λ. What are the first order wave functions?