Principles of Quantum Mechanics: Example Sheet 3

1. A harmonic oscillator of mass m, frequency ω and electric charge e is perturbed by a constant electric field of strength $\mathcal{E}$, resulting in a new term $H' = -e\mathcal{E}\mathbf{x}$ in the Hamiltonian. Calculate the change in the energy levels to order $\mathcal{E}^2$ and compare with the exact result.

2. A particle of spin $\frac{1}{2}$ is at rest in a magnetic field B parallel to the z-axis. A small additional magnetic field B' is then switched on parallel to the x-axis, so that the Hamiltonian becomes

$$H = -\tfrac{1}{2}\hbar\mu(B\sigma_3 + B'\sigma_1)$$

where μ is a constant.

Starting from the energy levels and eigenstates when $B' = 0$, use perturbation theory to calculate the corrections to the energies to order B'^2 and compare with the exact answer.

3a. Using a non-Gaussian trial wavefunction of your choice, estimate the ground state energy of the quartic oscillator with Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^4$$

and compare your result with that obtained with a Gaussian wavefunction. What motivated your choice?

[*Suggestions:* You could try $\psi = \cos(\pi x/2\alpha)$ or $\psi = (\alpha^2 - x^2)$ for $|x| < \alpha$ and vanishing outside this interval.]

b. Use the Gaussian-type wavefunction $\psi(x) = xe^{-\alpha x^2/2}$ to obtain an estimate of the energy of the first excited state of the quartic oscillator

[*Hint*: A handy way to do the integrals is to define $I_n = \int_{-\infty}^{\infty} dx\ x^{2n} e^{-\alpha x^2}$ and to show that $I_{n+1} = -\frac{d}{d\alpha} I_n$.]

4. A Hamiltonian takes the form $H = T + V$, with T the kinetic energy and V the potential energy. Assuming a discrete energy spectrum, $E_0 < E_1 < E_2 < ...$, show that the quantity $\langle\psi|H|\psi\rangle$, where $|\psi\rangle$ is normalized but otherwise arbitrary, is stationary whenever $|\psi\rangle$ is an energy eigenstate of H.

Suppose now that V is a homogeneous potential, satisfying $V(\lambda\mathbf{x}) = \lambda^n V(\mathbf{x})$. Show that the virial theorem $2\langle\psi|T|\psi\rangle = n\langle\psi|V|\psi\rangle$ holds for any energy eigenstate of H.

Show that there can be no localised states for $n < -3$.

5a. The Hamiltonian for a single electron orbiting a nucleus of charge Z is

$$H = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r}$$

Use the variational method with the trial wavefunction $\psi_\alpha(\mathbf{r}) = e^{-\alpha r/a_0}$ where α is a variational parameter and $a_0 = 4\pi\epsilon_0\hbar^2/me^2$ is the Bohr radius. Show that the minimum energy using this ansatz is

$$E_0 = -\frac{\hbar^2}{2m}\frac{Z^2}{a_0^2}$$

Compare this to the true ground state energy.

b. The Hamiltonian for two electrons orbiting a nucleus of charge Z is

$$H = \frac{\mathbf{p}_1^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_1} + \frac{\mathbf{p}_2^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Use the variational method with ansatz $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_\alpha(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)$ to estimate the ground state energy. What physical effect underlies the new minimum value of α?

Hint: You will need the following integral

$$\int d^3r_1 d^3r_2 \, \frac{|\psi_\alpha(\mathbf{r}_1)|^2|\psi_\alpha(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|^2} = \frac{5\pi^2}{8}\frac{a_0^5}{\alpha^5}$$

c. Derive this integral.

6. A covalent bond forms because two ions can lower their energy by sharing an electron. The simplest example occurs for the hydrogen molecule H_2^-. The Hamiltonian for a single electron, with position $\mathbf{r}$, orbiting two protons which are separated by distance $\mathbf{R}$ is given by

$$H = \frac{\mathbf{p}^2}{2m} + \frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{R} - \frac{1}{r} - \frac{1}{|\mathbf{r} - \mathbf{R}|}\right]$$

Use the un-normalised ansatz

$$\Psi = \psi(\mathbf{r}) + \psi(\mathbf{r} - \mathbf{R}) \qquad \text{with} \quad \psi = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/a_0}$$

and the integrals

$$\begin{aligned} u(R) &= \int d^3r\ \psi(\mathbf{r})\psi(\mathbf{r}-\mathbf{R}) = \left(1+\frac{R}{a_0}+\frac{R^2}{3a_0^2}\right)e^{-R/a_0} \\ v(R) &= \int d^3r\ \frac{\psi(\mathbf{r})\psi(\mathbf{r}-\mathbf{R})}{r} = \frac{1}{a_0}\left(1+\frac{R}{a_0}\right)e^{-R/a_0} \\ w(R) &= \int d^3r\ \frac{\psi(\mathbf{r})^2}{|\mathbf{r}-\mathbf{R}|} = \frac{1}{R}-\frac{1}{R}\left(1+\frac{R}{a_0}\right)e^{-2R/a_0} \end{aligned}$$

to show that the energy can be written as

$$\langle E\rangle - E_0 = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{R}-\frac{v(R)+w(R)}{1+u(R)}\right)$$

where E_0 is the ground state energy of hydrogen. Sketch $\langle E\rangle - E_0$ as a function of R (you may need to do this numerically) and comment on the implications for the binding of two protons.

7. Suppose a system has a basis of just two orthonormal states $|1\rangle$ and $|2\rangle$, with respect to which the total Hamiltonian has the matrix representation

$$\begin{pmatrix} E_1 & V_0 e^{i\omega t} \\ V_0 e^{-i\omega t} & E_2 \end{pmatrix}$$

where V_0 is independent of time. At $t = 0$, the system is in state $|1\rangle$. Show that the probability of a transition from state $|1\rangle$ to state $|2\rangle$ in time interval t is

$$P(t) = \frac{4V_0^2}{(E_1-E_2+\hbar\omega)^2}\sin^2\left(\frac{(E_1-E_2+\hbar\omega)t}{2\hbar}\right)+\mathcal{O}(V_0^4),$$

to lowest non–trivial order in V_0. Solve this two–state problem exactly to find the true value of $P(t)$ and hence state conditions necessary for the perturbative approach to be valid here.

8. A particle of mass m and charge e is contained within a cubical box of side a. Initially the particle is in the stationary state of energy $3\pi^2\hbar^2/2ma^2$. At time $t = 0$ a uniform electric field of strength E is switched on parallel to one of the edges of the cube. Obtain an expression to second order in e for the probability of measuring the particle to have energy $3\pi^2\hbar^2/ma^2$ at time t.

9. A harmonic oscillator of angular frequency ω is acted on by the time–dependent perturbation

$$\frac{q\mathcal{E}\hat{x}}{\sqrt{\pi}\tau}\exp\left(-\frac{t^2}{\tau^2}\right)$$

for all t, where $\hat{x}$ is the position operator and q, E and τ are constants. Show that in first–order perturbation theory, the only allowed transition from the ground state is to the first excited state. If the perturbation acts from very early times to very late times, find the probability that this transition takes place, correct to order $\mathcal{E}^2$.

By expanding $U_I(t)$ to second non–trivial order, calculate the corresponding probability for a transition from the ground state to the second excited state.

10. A particle travelling in one dimension with momentum $p = \hbar k > 0$ encounters the steep–sided potential well $V(x) = -V_0 < 0$ for $|x| < a$. Use Fermi's golden rule to show that the probability the particle will be reflected by the well is

$$P_{\text{reflect}} \approx \frac{V_0^2}{4E^2} \sin^2(2ka),$$

where $E = \frac{p^2}{2m}$. Show that in the limit $E \gg V_0$ this result is consistent with the exact result for the reflection probability. *[Hint: adopt periodic boundary conditions to normalise the wavefunctions of the initial and final states.]*

11. Consider the driven quantum harmonic oscillator with Hamiltonian

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \hbar\left(f^*(t)a + f(t)a^\dagger\right).$$

Taking H_0 to be the standard oscillator Hamiltonian, show that the perturbation in the interaction picture is

$$V_I(t) = \hbar\left(\tilde{f}^*(t)a + \tilde{f}(t)a^\dagger\right), \quad \text{where } \tilde{f}(t) = e^{i\omega t} f(t).$$

Show that $U(g) := e^{ga^\dagger - g^* a} = e^{-\frac{|g|^2}{2}} e^{ga^\dagger} e^{-g^* a}$ where $g = g(t)$. By taking the time–derivative of this expression, deduce that the time evolution operator in the interaction picture can be written as

$$U_I(t) = U(g) e^{-i\int_0^t \mathrm{Im}(\dot{g}^* g)\,\mathrm{d}t'} \quad \text{for the choice } g(t) = -i\int_0^t \tilde{f}(t')dt'.$$

At $t = 0$ the oscillator is initially in its ground state $|0\rangle$. In the case that $f(t) = e^{-i\omega t} f_0$ where f_0 is constant, show that at time t the oscillator is in the coherent state

$$|\psi_S(t)\rangle = e^{-|f_0|^2 t^2/2} e^{-i\omega t/2} e^{-itf(t)a^\dagger}|0\rangle$$

in the Schrödinger picture. Comment on the relevance of this model to the operation of a laser.