D18d **Principles of Quantum Mechanics: Sheet 4** Michaelmas 2016

1. The quantum-mechanical observable Q has just three eigenstates, $|1\rangle$, $|2\rangle$, $|3\rangle$ which are orthogonal and correspond to eigenvalues 2, 1, 1 respectively. The operator Q' is defined by $Q' = Q + \epsilon T$, where
$$\langle j|T|i\rangle = \begin{pmatrix} 3 & 1 & 0 \\ 1 & 2 & \sqrt{6} \\ 0 & \sqrt{6} & 1 \end{pmatrix} .$$
Deriving the necessary formulae from first principles, apply perturbation theory to find two of the eigenvalues of Q' correct to order ϵ and the third correct to order ϵ^2.

2. Two harmonic oscillators of frequency ω and mass m interact through a potential $m\omega^2\lambda x_1 x_2$ where x_1 and x_2 are the displacements of the oscillators. Use perturbation theory to calculate the ground state energy of the system correct to second order in powers of λ by adding the interaction potential on to the Hamiltonian. Find the energies of the first two excited states, working to lowest non-trivial order in perturbation theory.

   Verify your results by using the change of variables $\sqrt{2}\, q_1 = x_1 + x_2$, $\sqrt{2}\, q_2 = x_1 - x_2$ to obtain an exact expression for the energy eigenvalues.

3. The first excited energy level of the hydrogen atom is four-fold degenerate (ignoring electron spin). The four wave functions may be taken to be
$$\psi_0(\mathbf{x}) = \frac{1}{(8\pi a^3)^{\frac{1}{2}}}\left(1 - \frac{r}{2a}\right) e^{-r/2a}, \quad \psi_i(\mathbf{x}) = \frac{1}{(32\pi a^5)^{\frac{1}{2}}} x_i\, e^{-r/2a}, \qquad a = \frac{4\pi\epsilon_0\hbar^2}{e^2 m},$$
where x_i are the Cartesian components of the vector $\mathbf{x}$. The atom is perturbed by a weak electric field $\mathcal{E}$ parallel to the 3-axis. Show that the only non zero matrix elements of the perturbation H' are $\langle\psi_0|H'|\psi_3\rangle$ and $\langle\psi_3|H'|\psi_0\rangle$. Calculate the new energy levels to first order in $\mathcal{E}$.

4. The Hamiltonian for a quantum mechanical system is $H_0 + V(t)$, where H_0 has no explicit time dependence. At $t = 0$ the system is in an eigenstate $|a\rangle$ of H_0. Show that the probability that a measurement at time t yields a result corresponding to an eigenstate $|a'\rangle$ of H_0 is $|\langle a'|T(t)|a\rangle|^2$, where $T(t)$ satisfies the integral equation
$$T(t) = 1 - \frac{i}{\hbar}\int_0^t \bar{V}(t')T(t')\,\mathrm{d}t', \qquad \bar{V}(t) = e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}.$$
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 time-independent matrix representation
$$\begin{pmatrix} E & V \\ V & E \end{pmatrix} .$$
Show that, to lowest order in V, the probability of a transition from state $|1\rangle$ to state $|2\rangle$ in the time interval t is $V^2t^2/\hbar^2$. By comparing this with the exact result, state the conditions for such an approximation to be good.

5. 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.

6. A harmonic oscillator, with angular frequency ω, is acted on by the time-dependent perturbation
$$-\frac{ex}{\sqrt{\pi}\tau}\exp(-t^2/\tau^2) \qquad \text{for all } t\,.$$
Show that in first order perturbation theory the only allowed transition from the ground state is to the first excited state and find the probability that this takes place to first order in e^2 if the perturbation acts from very early times to very late times.

7. (a) Recall that the trace of an operator A on a space of states V is defined by $\mathrm{Tr}_V A = \sum_n \langle n|A|n\rangle$ where $\{|n\rangle\}$ is any orthonormal basis for V. Show that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ and hence $\mathrm{Tr}([A,B]) = 0$ (assuming all relevant sums converge). Use this to demonstrate that for an operator $\rho(t)$
$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho = [H,\rho] \qquad \Rightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}(\rho^n) = 0\ .$$
Verify that the first of these equations is satisfied if $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ provided the states $|\psi_i\rangle$ obey the time-dependent Schrödinger equation and the p_i are constants. Given that $|\psi_i\rangle$ are also orthonormal, calculate $\mathrm{Tr}(\rho^n)$ explicitly in terms of p_i.

(b) Consider a normalised state in $V \otimes W$ of the form
$$|\Psi\rangle \ = \ \lambda_1|\psi_1\rangle|\phi_1\rangle \ + \ \mu_1|\psi_1\rangle|\phi_2\rangle \ + \ \lambda_2|\psi_2\rangle|\phi_1\rangle \ + \ \mu_2|\psi_2\rangle|\phi_2\rangle \text{ with } \lambda_1\lambda_2^* + \mu_1\mu_2^* = 0\ ,$$
where $|\psi_i\rangle$ are orthonormal states in V, as in part (a) above, and $|\phi_i\rangle$ are orthonormal states in W. If A acts only on V and not on W, show that $\langle\Psi|A|\Psi\rangle = \mathrm{Tr}_V(\rho A)$ where the (reduced) density operator is $\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$, for p_1 and p_2 to be determined. Verify that $\mathrm{Tr}_V\rho = 1$. If, in addition, $\mathrm{Tr}_V\rho^2 = 1$, prove that either p_1 or p_2 must be zero. Is $|\Psi\rangle$ an entangled state in this case?

8. A spin-half system has space of states V and spin operators given by the Pauli matrices σ_x, σ_y, σ_z. What are the states obtained by applying σ_x, σ_y to the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ of σ_z?

A combination of three such systems has states belonging to $V^{(1)} \otimes V^{(2)} \otimes V^{(3)}$ and spin operators acting on each subsystem denoted by $\sigma_x^{(i)}$, $\sigma_y^{(i)}$ with $i = 1,2,3$. Show that the state
$$|\Psi\rangle = \frac{1}{\sqrt{2}}[\ |\uparrow\rangle_1|\uparrow\rangle_2|\uparrow\rangle_3 \ - \ |\downarrow\rangle_1|\downarrow\rangle_2|\downarrow\rangle_3\,]$$
satisfies
$$\sigma_x^{(1)}\sigma_y^{(2)}\sigma_y^{(3)}|\Psi\rangle \ = \ \sigma_y^{(1)}\sigma_x^{(2)}\sigma_y^{(3)}|\Psi\rangle \ = \ \sigma_y^{(1)}\sigma_y^{(2)}\sigma_x^{(3)}|\Psi\rangle \ = \ |\Psi\rangle \text{ and } \sigma_x^{(1)}\sigma_x^{(2)}\sigma_x^{(3)}|\Psi\rangle \ = \ -|\Psi\rangle\,.$$
Consider now whether these outcomes for measurements of particular combinations of the operators $\sigma_x^{(i)}$, $\sigma_y^{(i)}$ in the state $|\Psi\rangle$ could be reproduced by replacing the spin operators with classical variables $s_x^{(i)}$, $s_y^{(i)}$ which take values ±1 according to some probabilities. To agree with the results above for $\sigma_x^{(1)}\sigma_y^{(2)}\sigma_y^{(3)}$, $\sigma_y^{(1)}\sigma_x^{(2)}\sigma_y^{(3)}$, $\sigma_y^{(1)}\sigma_y^{(2)}\sigma_x^{(3)}$ on $|\Psi\rangle$,
$$s_x^{(1)}s_y^{(2)}s_y^{(3)} \ = \ s_y^{(1)}s_x^{(2)}s_y^{(3)} \ = \ s_y^{(1)}s_y^{(2)}s_x^{(3)} \ = \ 1\ .$$
Show that classically, this implies
$$s_x^{(1)}s_x^{(2)}s_x^{(3)} \ = \ 1\ ,$$
which does *not* agree with the quantum measurement of $\sigma_x^{(1)}\sigma_x^{(2)}\sigma_x^{(3)}$ in the state $|\Psi\rangle$.