33-756 Final Exam Tuesday, May 6, 2014

This exam has four problems of varying length. Some parts require explicit calculation (*e.g.* "calculate" or "determine"), while other parts request direct numerical or verbal answers (*e.g.* "what is?" or "state"). If you are unsure what is requested, please ask. Be aware that somtimes later parts of a question may be answered even if an earlier part has been missed.

1. (Harmonic oscillator in applied field)

A particle moves in a harmonic potential under the influence of an applied force F. The net potential energy is thus

$$U(x) = \frac{1}{2}m\omega^2 x^2 - Fx.$$

Recall that the normalized ground state wave function for F = 0 is

$$\psi_0(x) = \sqrt[4]{\frac{\alpha}{\pi}} e^{-\alpha x^2/2}$$

with $\alpha = m\omega/\hbar$.

(a) What is the ground state wavefunction $\psi_F(x)$ with F > 0?

(b) The oscillator is initially in its ground state ψ_0 with F = 0. The force is increased very slowly until it reaches some F > 0. What is the probability that the oscillator is in the F > 0 ground state ψ_F at this later time, in the limit of slow variation?

(c) Calculate the same probability as in (b), but for the case that the force is insantaneously increased to F > 0.

2. (Collisions of identical particles, adapted from Cohen-Tannoudji #14.4-5)

Recall the solution for single particle scattering takes the form

$$e^{ikz} + f(\theta)\frac{e^{ikr}}{r},$$

assuming the interaction potential V has rotational symmetry around the z axis.

(a) Consider two identical spin 0 particles traveling in the $\pm \hat{z}$ directions with center of mass at z = 0 and interacting with each other *via* the same potential V as above. Determine the cross section to detect a particle at angle θ relative to \hat{z} .

(b) Now let the identical particles have spin 1/2, both polarized up. Determine the cross section to detect a particle at angle θ , and comment on any noteworthy special angle.

(c) Finally, let the spin 1/2 particle traveling in the $+\hat{z}$ direction be spin up and the other be spin down. What is the cross section to detect a spin up particle at θ ?

3. (Hubbard model of H₂ molecule) Consider an LCAO model of the H₂ molecule. Electrons on different sites can be regarded as distinguishable, while electrons on the same site must be in the spin singlet $|\uparrow\downarrow\rangle$ state owing to the Pauli exclusion principle. Denote an empty site by $|0\rangle$. The Hilbert space for the two electrons is spanned by the basis set:

$$|\uparrow;\uparrow\rangle \quad |\uparrow;\downarrow\rangle \quad |\downarrow;\uparrow\rangle \quad |\downarrow;\downarrow\rangle \quad |0;\uparrow\downarrow\rangle \quad |\uparrow\downarrow;0\rangle$$

where the two components of the ket-vector refer to the two sites. The Hubbard model Hamltonian allows for electrons to hop between neighboring sites, with matrix element -t and charges a Coulomb energy penalty U > 0 when electrons share a single site. In the basis given, the Hamiltonian becomes a 6×6 matrix

where the + and - signs arise from the antisymmetry of the identical electrons.

(a) Construct spin singlet $|S = 0, M = 0\rangle$ and spin triplet $|S = 1, M = \pm 1, 0\rangle$ states out of the first four basis vectors. Note that the fifth and sixth basis vectors are already spin singlets.

(b) Verify that each of your spin triplets is an eigenvector of H and determine its energy eigenvalue.

(c) Since you have already determined the spin triplet eigenstates, it suffices to restrict further attention to the spin singlet subspace. Re-express H as a 3×3 matrix in the spin singlet subspace.

(d) Calculate the lowest spin singlet energy up to second order in perturbation theory for small t. Comment on the sign of the second order term.

(e) Does the H_2 molecule favor ferromagnetism (spins aligned) or antiferromagnetism (spins antialigned)? What is the physical mechanism by which this occurs?

4. (Adapted from 2010 Qualifying Exam) This problem concerns transitions from excited states of a hydrogen atom (2s and 2p) into the ground state (1s). Electron spin can be neglected for the purposes of this problem. While answering the questions you may encounter various matrix elements. Do not evaluate nontrivial matrix elements ! However, if a matrix element *is* trivial, this fact must be noted and the value reported.

(a) An atomic orbital couples to electromagnetic fields via

$$W = W_{DE} + W_{DM} + W_{QE} + \cdots$$

where

$$W_{DE} = -q\mathcal{E}Z, \quad W_{DM} = \frac{-q}{2m}\mathcal{B}L_x, \quad W_{QE} = \frac{-q}{2mc}\mathcal{E}(YP_z + ZP_y)$$

(i) For atomic transitions in general, which of the three terms is the most important, and why? (ii) For each interaction, indicate if it allows or forbids a $2s \rightarrow 1s$ transition and explain why. (iii) The interactions above omit the $q^2 |\mathbf{A}|^2$ term from the quantum Hamiltonian $(\mathbf{p} - q\mathbf{A})^2$. What is the physical significance of this term, why is it usually ignored and when might it be important? (b) Explain why the 2p level is relatively short lived (its lifetime τ is about 10^{-10} seconds).

(c) The wavefunction

$$\psi(t) = b_{\alpha}(t)e^{-iE_{\alpha}t/\hbar}|\alpha\rangle + b_{\beta}(t)e^{-iE_{\beta}t/\hbar}|\beta\rangle$$

represents a superposition of states $\alpha = 2s$ and $\beta = 2p$. Their amplitudes vary as

$$i\hbar \dot{b}_{lpha} = 0 \qquad i\hbar \dot{b}_{eta} = -\frac{i\hbar}{ au} b_{eta},$$

where we have used the long lifetime of 2s to approximate b_{α} as a constant, but we keep the short lifetime τ of 2p leading to decay of b_{β} . These equations represent the time-dependent Schrödinger equation in the subspace spanned by $\{\alpha, \beta\}$. Now apply a constant electric field $\tilde{\mathbf{E}} = E\hat{z}$ to the atom and derive the new equations for \dot{b}_{α} and \dot{b}_{β} . Note that \dot{b}_{α} becomes nonzero and explain how this leads to a new mechanism for decay of the 2s state. (d) Find the time constant for decay of 2s using your result of part (c). Since the energy difference $\Delta E_{\alpha\beta} = E_{\alpha} - E_{\beta}$ is rather small, you may simplify your calculations by setting $\Delta E_{\alpha\beta} = 0$. What is the 2s lifetime in the limit of strong applied electric field?

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