Leo Radzihovsky, Fall 2015

PHYS 5250: Quantum Mechanics - I

Homework Set 7

Issued November 9, 2015
Due December 4, 2015

Reading Assignment: Shankar, Ch. 13, 14, 15; Sakurai: 3.5-3.8, 3.10, Appendix A.4, A.5, A.6.

1. Three-dimensional spherical square well potential with $V(r) = -V_0$, for $r < d$ and 0, for $r > d$.

   (a) For the bound states ($E < 0$):

      i. Find the eigenfunctions with angular momentum ℓ and a matching condition determining the corresponding coefficients of the radial part of the wavefunction. Express your answer in terms of special functions, but do not try to solve the transcendental equations for the matching coefficients. Argue based on this general structure of the solution that the spectrum must be discrete. Hint: note that at large r the spherical Henkel function of $h_\ell^{(1)}(kr) = j_\ell(kr) + in_\ell(kr) \sim e^{ikr}/(kr)$.

      ii. Specializing to $\ell = 0$, use above general result to explicitly find eigenfunctions in terms of elementary functions and greatly simplified transcendental matching equation. Formulate the transcendental equation graphically.

      iii. What is the critical value $V_{0c}^{(n)}$ at which nth bound level appears? Use this result to find the minimum value V_0^c of the potential depth V_0 below which an $\ell = 0$ bound state is impossible. Compare your answer with that of a 1d square well potential from an earlier homework assignment. Explain the connection and why here (in contrast to that earlier true 1d problem) a bound state only appears if the potential well is sufficiently deep, i.e., $V_0 > V_0^c$.

      iv. Study the problem for a very deep well and arbitrary ℓ. For states with energy $|E_{n,\ell}|$ comparable to V_0 (i.e., very deeply lying low energy bound states), determine the order in which these appear; use the $|n, \ell\rangle$ notation or the spectroscopic notation 1s, 1p, 2f, etc...to list the lowest 10 states.
      Hint: In this last case a considerable simplification takes place, but the eigenvalues must still be computed numerically.

   (b) For the continuum states ($E > 0$):

i. Write down the appropriate wavefunctions for inside and outside regions and the corresponding matching condition. Based on this make an argument that the eigenenergies form a continuum (rather than a discrete set).

ii. Write down large r asymptotic form of these wavefunctions and use it to relate the coefficients B and C of the outer solution to the (so-called) scattering phase shift $\delta_\ell(k)$, latter defined by the asymptotic form of the wavefunction $R(r \to \infty) \sim (kr)^{-1} \sin(kr - \frac{\pi}{2}\ell + \delta_\ell)$.

iii. Use above results to approximately compute $\delta_0(k)$ for the special case of $\ell = 0$, showing that at low energies (small k) $k \cot \delta_0(k) \approx -a^{-1} + \frac{1}{2} r_0 k^2$, and giving explicit expressions for parameters a (scattering length) and r_0 (effective range).

iv. Show that in $V_0 \to \infty$ limit, a reduces to the potential range d.

v. Using your results above, demonstrate a general result that $\delta_\ell(k) \to 0$ as $k \to 0$, and derive how rapidly (with k) it approaches zero for a given ℓ.

2. Hydrogen atom

(a) An electron in the Coulomb field of a proton is in a state described by a wave function $\psi(r) = Ae^{-r/r_0}$. What is the probability that (while in this state right before the measurement) it will be found in (i) a state with angular momentum $\ell \neq 0$ and $m \neq 0$? (ii) its ground state; for the latter, compute and sketch $P(r_0/a_0)$ and show that it is maximized at 1 for $r_0 = a_0$. Why? (a_0 is Bohr radius).

(b) Show that eigenfunctions of a spherically symmetric Hamiltonian are also eigenstates of parity with eigenvalue $P = (-1)^\ell$ determined only by the angular momentum quantum number ℓ.

3. Angular momentum

(a) Derive Pauli matrices $\vec{\sigma}$ by explicitly computing matrix elements of angular momentum components $\vec{J}$ for the $j = 1/2$ representation and using $\vec{J} = \frac{1}{2}\hbar\vec{\sigma}$.

(b) Using their commutation and anticommutation relations derive Pauli matrices identities:

i. $\mathrm{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$, also verifying it by explicit matrices found above.

ii. $(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = \vec{a} \cdot \vec{b} I + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}$. ($I$ is an identify matrix.)

iii. Use above identities to show that a square of the 2D Dirac Hamiltonian $H_D = c(\vec{p} - e\vec{A}/c) \cdot \vec{\sigma} + mc^2 \sigma_z$ (describing a spin 1/2 particle; $\vec{p} = (p_x, p_y)$) gives the Klein-Gordon Hamiltonian $H_{KG} = H_D^2 = (\vec{p} - e\vec{A}/c)^2 c^2 + m^2 c^4 - 2ce\vec{B} \cdot \vec{S}$ (describing a spin zero particle). Taylor expand the square-root of the latter to lowest order in $(\vec{p} - e\vec{A}/c)^2/m^2c^2$ to show that (upto a constant, that is the rest energy mc^2) one gets the Hamiltonian for the nonrelativistic Schrodinger's

equation, $H_{Sch} = \sqrt{H_{KG}} - mc^2$, with an additional "anomalous" Zeeman term $-2\mu_B \vec{B} \cdot \vec{S}$ term. Now you know how spin and its interaction with the magnetic field automatically emerge from the Dirac equation!
Hint: For the last part, (1) to warm up please first try doing it with $\vec{A} = 0$, (2) for convenience use the transverse gauge where $\vec{\nabla} \cdot \vec{A} = 0$, (3) be very careful with the order of $\vec{p}$ and $\vec{A}$, noting that in e.g., an expression like $\vec{p} \cdot \vec{A}$, $\vec{p}$ is an operator that is acting on both $\vec{A}$ and the wavefunction (that you have to imagine is actually there, as in $H\psi$), and hence $\vec{p} \cdot \vec{A}$ is actually $(\vec{p} \cdot \vec{A}) + \vec{A} \cdot \vec{p}$ (where now in the first term $\vec{p}$ is now only acting on $\vec{A}$).

(c) By explicitly diagonalizing matrix $\hat{n} \cdot \vec{\sigma}$ (with $\hat{\vec{n}}$ a unit vector defined by polar and azimuthal angles θ and ϕ) find its eigenvectors $\psi^{\hat{n}}_{\pm,\sigma}$ and the corresponding eigenvalues. Show that your result for eigenvectors is nothing more than an SU(2) rotation by a matrix $U_{\vec{\theta}} = e^{-i\vec{\theta}\cdot\vec{\sigma}/2}$ of spinors $\psi^{\hat{z}}_{+,\sigma} = (1, 0)$, $\psi^{\hat{z}}_{-,\sigma} = (0, 1)$ (eigenstates of σ_z) by angle θ about axis $\hat{\theta} = \hat{z} \times \hat{n}/|\hat{z} \times \hat{n}|$. Show formally why this is the case.

(d) i. What are the eigenvalues and eigenvectors of the operator $S_x + S_z$ for a spin $\hbar/2$ system? Answer the question by direct diagonalization and checking your answer by using the general result found above.

ii. Consider an electron that is measured to be in a spin state $+1/2$ using a Stern-Gerlach apparatus with the axis of magnetic field along $\hat{n} = (\hat{x} + \hat{z})/\sqrt{2}$. What is the probability that a subsequent measurement using a Stern-Gerlach apparatus with the axis of magnetic field along $\hat{z}$ finds an electron in $+1/2$ spin state?

(e) Spin precession:

i. Derive a Heisenberg equation of motion for a localized electron spin operator $\vec{S}(t)$ subjected to a magnetic field $\vec{B}$, expressing your answer in terms of the Bohr magneton $\mu_B = e\hbar/(2mc)$ and electron gyromagnetic ratio $g \approx 2$. Show that it corresponds to precession of the spin around the magnetic field. What is the precessional frequency? Solve this equation explicitly for the case of $\vec{B}$ along $\hat{z}$ in terms of $\vec{S}(0)$.

ii. Consider an $s = 1/2$ spin system in the presence of a $\vec{B} = B_z\hat{z}$ magnetic field that at $t = 0$ starts out in its up eigenstate. Derive the time evolution of this state, following a turning on of an *additional* constant magnetic field $B_x\hat{x}$, expressing your answer in terms of basis with a quantization axis along $\hat{z}$. Compute the probability $P_\uparrow(t)$ of finding the spin in the spin up eigenstate (defined with respect to the basis with quantization axis along $\hat{z}$). Show that it $P_\uparrow(t)$ oscillates in time and find the frequency and the amplitude of oscillation.
Hint: (a) Check simple limits ((i) $B_x = 0$, (ii) $B_z = 0$, (iii) $t = 0$, ...) of your expressions, making sure your intermediate answers make sense. (b) This

problem can be either solved using spin evolution operator, or equivalently by decomposing the initial noneigenstate into a linear combination of eigenstates, and then evolving the latter in time via their simple oscillatory phase factors.

(f) Prove that all the wavefunctions belonging to the *maximum* eigenvalue of the square of the total spin operator of a system of N electrons are symmetric in the spin coordinate of the individual electrons.

(g) Derive the spectrum and corresponding eigenstates of the dipole-dipole magnetic interaction energy $H_d = [\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_2 \cdot \hat{r})]/r^3$ of a proton and an antiproton at a fixed distance $r = a$ ($\hat{r}$ is a unit vector connecting them).

Hint: The total spin commutes with this Hamiltonian.

4. Consider a charged spinless particle moving in 3D, in a uniform constant magnetic field $\vec{B} = B\hat{z}$.

(a) Working in a symmetric gauge (where the vector potential is given by $\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B}$), show that the dynamics reduces to an effective 2D problem of a particle in a harmonic potential $\frac{1}{2}m\omega_0 r_\perp^2$ with an effective oscillator frequency ω_0 proportional to B, together with an orbital Zeeman term $-\Omega L_z$, linear in B. Write down explicitly the effective harmonic potential frequency ω_0 and the effective rotational frequency Ω.

(b) Recall your result (from last homework) for the spectrum of a 2D harmonic oscillator solved in polar coordinates in the presence of a rotation (orbital Zeeman term) $-\Omega L_z$. Use that information to construct the spectrum for this problem (of a particle in a uniform magnetic field), noticing a very special relation here between ω_0 and Ω.

Hint: From an even earlier homework assignment for a particle in a uniform magnetic field, solved in Cartesian coordinates and using a Landau gauge ($A = B(-y, 0, 0)$), you should know that the spectrum is that of macroscopically degenerate Landau levels.

(c) Estimate the ratio of the quadratic in B (diamagnetic) term to the linear in B term for a Hydrogenic electron in a uniform B field, finding the value of the magnetic field when these two terms become comparable. By plugging in typical values for an atom, show that the diamagnetic (quadratic in B) term is completely negligible under standard conditions in an atomic context.