944 QUANTUM MECHANICS - Final Exam Due: Thursday, 20 December, 2007

No collaboration permitted on the final exam. You may freely use the literature, but with diligent referencing. Do not include rough notes or programming efforts; give only your final logical development in legible handwriting. Presentation will be a primary factor in grading.

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1. This problem is about the Bogoliubov transformation. A common tool in studying many-body quantum systems is the operator transform. Suppose the particle creation and annihilation operators $a_i^\dagger$ and a_i can be algebraically expressed in terms of a new set of operators $b_i^\dagger$ and b_i that obey the same canonical commutation relations:

$$[b_i, b_j] \;=\; [b_i^\dagger, b_j^\dagger] \;=\; 0 \qquad [b_i, b_j^\dagger] \;=\; \delta_{ij}\ . \tag{1}$$

The operators $b_i^\dagger$ and b_i are often said to create/annihilate quasiparticles. The commutation relations, Eq. (1), imply that there is a unique state $|B\rangle$ that is annihilated by all b_i; this state is usually referred to as the quasiparticle vacuum, the states of the form $b_i^\dagger\,|B\rangle$ are the one-quasiparticle states, *etc.* Whenever the quasiparticles can be labeled by the same quantum numbers (e.g. $\vec{k}$) as the original bosonic particles of the theory, it is often convenient to make a unitary operator transform:

$$b_i \;=\; U a_i U^\dagger, \qquad b_i^\dagger \;=\; U a_i^\dagger U^\dagger\ , \tag{2}$$

where U is a unitary operator in the Fock space, usually of the form $\exp(X)$ for some anti-hermitian polynomial X in a_i and $a_i^\dagger$.

   (a) Show that the unitarity of U automatically guarantees that b_n and $b_n^\dagger$ satisfy Eq. (1), and that the quasiparticle state $|B\rangle = U\,|0\rangle$ is the quasiparticle vacuum.

   (b) Verify that for $X = \sum_n (c_n a_n^\dagger - c_n^* a_n)$, $\exp(X) a_n \exp(-X) = a_n - c_n$. This transform is a c-number shift.

   (c) Now let $X = \sum_n \frac{1}{2}\eta_n (e^{i\lambda_n}(a_n^\dagger)^2 - e^{-i\lambda_n}(a_n)^2)$ (η_n and λ_n are real). Show that for this $U = \exp(X)$, Eqs. (2) define a diagonal canonical transform:

$$b_i \;=\; a_i \cosh\eta_i \;-\; e^{i\lambda_i} a_i^\dagger \sinh\eta_i, \qquad b_i^\dagger \;=\; \cosh\eta_i a_i^\dagger \;-\; e^{-i\lambda_i}\sinh\eta_i a_i\ . \tag{3}$$

   (d) In order to see the utility of the Bogoliubov transformation, consider the simple case of one creation/annihilation operator pair with $\lambda = \pi$. We then have

$$b \;=\; a\cosh\eta \;+\; a^\dagger \sinh\eta\ . \tag{4}$$

   Use this transformation to obtain the eigenvalues of the following Hamiltonian:

$$H \;=\; \hbar\omega a^\dagger a \;+\; \frac{1}{2}V(aa + a^\dagger a^\dagger)\ . \tag{5}$$

   Also give the upper limit on V for which this can be done.

   (e) Write down the ground state of the Hamiltonian above in terms of the number states $a^\dagger a\,|n\rangle = n\,|n\rangle$.

2. This problem is about Pauli's method of solving the hydrogen atom. For all spherically-symmetric potentials, discrete spectra of bound state energies have $(2l+1)$-fold degeneracy mandated by the $SO(3)$ symmetry — all states $|l, m, n_r\rangle$ with the same l and n_r but different m have the same energy $E(l, n_r)$. For most potentials, there is no further degeneracy — different combinations of l and n_r give different energies. However, there are two "accidentally degenerate" exceptions to that rule: the spherically-symmetric harmonic oscillator potential $\hat{V} = \frac{1}{2}M\omega^2\hat{r}^2$, and the Coulomb potential $\hat{V} = -e^2Z/\hat{r}$. In both cases the extra degeneracy is due to non-obvious conservation laws leading to unexpected enlargement of the symmetry group from the rotations-only $SO(3)$ to $SU(3)$ in the harmonic case and to $SO(3) \times SO(3)$ in the Coulomb case. (We saw this in problem 1 of HW 3 for the case of the two-dimensional harmonic oscillator where $SO(2)$ is enlarged to $SU(2) \sim SO(3)$.)

   The unexpected conservation law in the Coulomb case is the Laplace-Runge-Lenz theorem generalized from classical to quantum mechanics. Classically, we define the Runge-Lenz vector $\mathbf{K}$ as

$$\mathbf{K} \;\equiv\; \mathbf{p} \times \mathbf{L} \;-\; e^2 ZM\mathbf{n}_r \tag{6}$$

   where M is the particle's mass, $\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}$ is its angular momentum and $\mathbf{n}_r \equiv \mathbf{x}/r$ is a unit vector pointing towards the particle. The Laplace-Runge-Lenz theorem states that for the Coulomb (Newton) potential, $\mathbf{K}$ is a conserved quantity, *i.e.*, does not change with time.

   (a) Prove the classical Laplace-Runge-Lenz theorem.

   The definition, Eq. (6) implies that $\mathbf{x} \cdot \mathbf{K} = \mathbf{L}^2 - e^2 ZMr$ and hence $r = \mathbf{L}^2/(|\mathbf{K}|\cos\phi + e^2 ZM)$ where ϕ is the angle between $\mathbf{K}$ and $\mathbf{x}$. Therefore, constancy of the Runge-Lenz vector implies that the classical orbits are conical sections of eccentricity $\epsilon = \mathbf{K}/e^2 ZM$; for $\epsilon < 1$ the orbit is a closed ellipse whose pericenter lies in the direction pointed to by $\mathbf{K}$.

   In quantum mechanics we define the Runge-Lenz vector operator

$$\hat{\mathbf{K}} \;\equiv\; \frac{1}{2}(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}) \;-\; e^2 ZM\hat{\mathbf{x}}\hat{r}^{-1}\,. \tag{7}$$

   (b) Verify that each of the component operators $\hat{K}_i$ is hermitian and is conserved, *i.e.* commutes with the Hamiltonian

$$\hat{H} \;=\; \frac{1}{2M}\hat{\mathbf{p}}^2 \;-\; e^2 Z\hat{r}^{-1}\,. \tag{8}$$

   To find out the Lie algebra generated by the conserved operators $\hat{L}_i$ and $\hat{K}_i$, we need their commutation relations. We know that $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$.

   (c) Show that

$$[\,\hat{K}_i, \hat{L}_j\,] \;=\; i\hbar\epsilon_{ijk}\hat{K}_k \qquad [\,\hat{K}_i, \hat{K}_j\,] \;=\; -2M\hat{H} \cdot i\hbar\epsilon_{ijk}\hat{L}_k\,. \tag{9}$$

   Now consider the subspace of the Hilbert space spanned by the bound states of the Hamiltonian. On this subspace let us define two vector operators $\hat{\mathbf{Q}}_+$ and $\hat{\mathbf{Q}}_-$:

$$\hat{\mathbf{Q}}_\pm \;\equiv\; \frac{\hat{\mathbf{L}}}{2} \;\pm\; \frac{\hat{\mathbf{K}}}{\sqrt{-8M\hat{H}}}\,. \tag{10}$$

(d) Show that the six operators $\hat{Q}^i_\pm$ are hermitian, conserved and obey the $SO(3) \times SO(3)$ commutation relations:

$$[\,\hat{Q}^i_+, \hat{Q}^j_+\,] \;=\; i\hbar\epsilon^{ijk}\hat{Q}^k_+\,, \qquad [\,\hat{Q}^i_-, \hat{Q}^j_-\,] \;=\; i\hbar\epsilon^{ijk}\hat{Q}^k_-\,, \qquad [\,\hat{Q}^i_+, \hat{Q}^j_-\,] \;=\; 0\,. \tag{11}$$

This $SO(3) \times SO(3)$ Lie algebra can be used to describe all bound states as $|q_+, m_+, q_-, m_-\rangle$ — simultaneous eigenstates of the $\hat{\mathbf{Q}}^2_\pm$ and $\hat{Q}^z_\pm$ operators. However, this description is somewhat redundant:

(e) Verify that $\hat{\mathbf{K}} \cdot \hat{\mathbf{L}} = \hat{\mathbf{L}} \cdot \hat{\mathbf{K}} = 0$ and use this fact to show that all bound states have $\hat{\mathbf{Q}}^2_+ = \hat{\mathbf{Q}}^2_-$ and hence $q_+ = q_-$.

Therefore we can label the bound states of the Coulomb potential as $|q, m_+, m_-\rangle$; their energies depend only on q and thus are $(2q+1)^2$-fold degenerate. To compute these energies:

(f) First, show that

$$\hat{\mathbf{K}}^2 \;=\; (e^2ZM)^2 \;+\; 2M\hat{H}(\hat{\mathbf{L}}^2 + \hbar^2) \tag{12}$$

(in classical mechanics, $\mathbf{K}^2 \;=\; (e^2ZM)^2 \;+\; 2ME\mathbf{L}^2$.)

(g) Second, use Eqs. (10) and (12) to derive

$$2\hat{\mathbf{Q}}^2_+ \;+\; 2\hat{\mathbf{Q}}^2_- \;+\; \hbar^2 \;=\; \frac{(e^2ZM)^2}{-2M\hat{H}}\,. \tag{13}$$

(h) And, finally, use Eqs. (13) to show that the energy of the $|q, m_+, m_-\rangle$ bound state is

$$E_N \;=\; -\frac{M(e^2Z)^2}{2\hbar^2(2q+1)^2} \;\equiv\; -\frac{M(e^2Z)^2}{2\hbar^2N^2} \tag{14}$$

where $N \equiv 2q+1$ is a positive integer, usually called the *principal quantum number* of the bound state.

(i) Show that for each value of the principal quantum number N, the orbital quantum number l takes all integer values between zero and $N-1$.
(Hint: Use $\hat{\mathbf{L}} = \hat{\mathbf{Q}}_+ + \hat{\mathbf{Q}}_-$.)

Also, argue that this means that in terms of l and the radial quantum number n_r, $N = l + n_r + 1$, which implies that the spectrum of N consists of *all* positive integers.

3. This problem is about time-dependent perturbation theory and its relation with time-independent perturbation theory.

   (a) When the potential V is time-independent, work out $\langle s|\,\tilde{T}(t,0)\,|s\rangle$ to second order and identify $\Delta^{(1)}$, $\Delta^{(2)}$ and the "wave-function renormalization" Z_i in the expansion of

$$\begin{aligned}\langle s|\,\tilde{T}(t,0)\,|s\rangle \;&=\; Z_i\, e^{-i\Delta E t/\hbar} \;+\; \textit{rapidly oscillating terms} \\ &=\; Z_i \;-\; \frac{i}{\hbar}\left(\Delta_i^{(1)}+\Delta_i^{(2)}\right)t \;+\; \frac{1}{2!}\left(-\frac{i}{\hbar}\Delta_i^{(1)}t\right)^2 \;+\; \vartheta(V^3)\end{aligned} \quad (15)$$

   and show that they agree with the results from time-independent perturbation theory, Eqs. (5.1.42), (5.1.44) and (5.1.48b) in Sakurai. Note that this identification is done in the $t \to \infty$ limit where rapidly oscillating terms are dropped. Explain why this identification works.

   (b) Now consider a harmonic perturbation $V = V_0 \cos\omega t$. Work out the second-order energy shift. Does your expression recover the result from time-independent perturbation theory in the limit $\omega \to 0$? Explain your answer.

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4. This problem is about scattering in one dimension. The Lippmann-Schwinger formalism can be applied to a one-dimensional transmission-reflection problem with a finite range potential, $V(x) \neq 0$ for $0 < |x| < a$ only.

   (a) Suppose that we have an incident wave coming from the left: $\langle x|\phi\rangle = e^{ikx}/\sqrt{2\pi}$. How must we handle the singular $1/(E - H_0)$ operator if we are to have a transmitted wave only for $x > a$ and a reflected wave and the original wave for $x < -a$? Is the $E \to E + i\epsilon$ prescription still correct? Obtain an expression for the appropriate Green's function and write an integral equation for $\langle x|\psi^{(+)}\rangle$.

   (b) Consider the special case of an attractive δ-function potential

$$V \;=\; -\left(\frac{\gamma\hbar^2}{2m}\right)\,\delta(x), \qquad (\gamma > 0)\;. \quad (16)$$

   Solve the integral equation to obtain the transmission and reflection amplitudes.

   (c) The one-dimensional δ-function potential with $\gamma > 0$ admits one and only one bound state for any value of γ. Show that the transmission and reflection amplitudes you computed have bound-state poles at the expected positions when k is regarded as a complex variable.