943 QUANTUM MECHANICS - Final Exam Due: Tuesday, May 18, 2004, 1pm

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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.

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1. This problem is about the spherical tensor operators, $\hat{T}^{(\ell)}_m$, and their relationship with the carthesian tensor operators $\hat{T}_{i_n \ldots i_n}$.

   (a) Let $\hat{A}^{(\ell_1)}$ and $\hat{B}^{(\ell_2)}$ be spherical tensor operators. Show that their product decomposes into a sum of spherical tensors:

$$\hat{A}^{(\ell_1)}_{m_1} \, \hat{B}^{(\ell_2)}_{m_2} = \sum_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \hat{C}^{(\ell)}_{m=m_1+m_2} \langle \ell_1, \ell_2; \ell, m | \ell_1, \ell_2; m_1, m_2 \rangle \ , \tag{1}$$

   where the coefficients $\langle \ell_1, \ell_2; \ell, m | \ell_1, \ell_2; m_1, m_2 \rangle$ are ordinary Clebsch-Gordan coefficients for adding angular momenta ℓ_1 and ℓ_2.

   (b) An operator $\hat{A}$ is a scalar iff $[\hat{J}_i, \hat{A}] = 0$ while a set of three operators $\hat{B}_i$ is a vector iff $[\hat{J}_i, \hat{B}_j] = i\hbar \epsilon_{ijk} \hat{B}_k$.
   Derive a similar condition for the carthesian n-index operators $\hat{T}_{i_n \ldots i_n}$.

   (c) Prove that a set of $2\ell + 1$ operators $\hat{T}^{(\ell)}_m$ constitutes a spherical tensor of rank ℓ iff

$$[\hat{J}_z, \hat{T}^{(\ell)}_m] = \hbar m \hat{T}^{(\ell)}_m \quad , \quad [\hat{J}_\pm, \hat{T}^{(\ell)}_m] = \hbar \sqrt{(\ell \mp m)(\ell + 1 \pm m)} \hat{T}^{(\ell)}_{m\pm 1} \ . \tag{2}$$

   (d) When $\ell = 0$, $\hat{T}^{(0)}$ is simply a scalar. Show that for $\ell = 1$, $\hat{T}^{(1)}$ is equivalent to a vector. That is, identify

$$\hat{A}^{(1)}_0 \equiv \hat{A}_z \qquad \hat{A}^{(1)}_{\pm 1} \equiv \frac{\mp 1}{\sqrt{2}} (\hat{A}_x \pm i \hat{A}_y) \tag{3}$$

   and prove that $\hat{A}^{(1)}$ is a spherical tensor of rank 1 iff $\hat{A}_i$ is a vector.
   (Hint: use eq. (2).)

   (e) For two vector operators $\hat{A}_i$ and $\hat{B}_i$, their tensor product $\hat{A}_i \hat{B}_j$ clearly constitutes a 2-index carthesian tensor (a dyadic). On the other hand, the product $\hat{A}^{(1)}_{m_1} \hat{B}^{(1)}_{m_2}$ decomposes into a sum of spherical tensor operators $\hat{C}^{(\ell)}_m$ for $\ell = 0, 1, 2$. This suggests that *any* 2-index carthesian tensor operator $\hat{C}_{ij}$ is equivalent to a set of spherical tensors $\hat{C}^{(0)}$, $\hat{C}^{(1)}$ and $\hat{C}^{(2)}$, the identification being

$$\begin{aligned}
\hat{C}^{(0)}_0 &= \frac{1}{\sqrt{6}} (\hat{C}_{xx} + \hat{C}_{yy} + \hat{C}_{zz}) \ , \qquad & \hat{C}^{(2)}_0 &= \frac{1}{\sqrt{6}} (2\hat{C}_{zz} - \hat{C}_{xx} - \hat{C}_{yy}) \ , \\
\hat{C}^{(1)}_0 &= \frac{1}{\sqrt{2}} (\hat{C}_{xy} - \hat{C}_{yx}) \ , & \hat{C}^{(2)}_{\pm 1} &= \frac{1}{2} (\hat{C}_{zx} + \hat{C}_{xz} \pm i\hat{C}_{yz} \pm i\hat{C}_{zy}) \ , \\
\hat{C}^{(1)}_{\pm 1} &= \frac{1}{2} (\hat{C}_{zy} - \hat{C}_{yz} \pm i\hat{C}_{xz} \mp i\hat{C}_{zx}) \ , & \hat{C}^{(2)}_{\pm 2} &= \frac{1}{2} (\hat{C}_{xx} - \hat{C}_{yy} \pm i\hat{C}_{xy} \pm i\hat{C}_{yx}) .
\end{aligned} \tag{4}$$

Prove that this identification indeed makes $\hat{C}_{ij}$ a 2-index carthesian tensor when and only when $\hat{C}^{(\ell)}_m$ are spherical tensors of appropriate rank.

(Note that $\hat{C}^{(0)}_0 \propto \mathrm{tr}\ \hat{C}$, $\hat{C}^{(1)}_m$ are related to the antisymmetric components of $\hat{C}_{ij}$, while $\hat{C}^{(2)}_m$ are related to the traceless symmetric part of $\hat{C}_{ij}$, as discussed in class.)

2. This problem is about the Wigner-Eckart theorem, which here we will write as,

$$\langle j', m', \alpha' | \hat{T}^{(\ell)}_\mu | j, m, \alpha \rangle \;=\; \langle j', \alpha' || \hat{T}^{(\ell)} || j, \alpha \rangle \cdot \langle \ell, j; j', m' | \ell, j; \mu, m \rangle \tag{5}$$

and its application to matrix elements of vector operators.

(a) Use the Wigner-Eckart theorem to show that for $j' = j$ and for any vector operator $\hat{A}_i$,

$$\langle j, m', \alpha' | \hat{A}_i | j, m, \alpha \rangle \;=\; \langle j, \alpha' || \hat{A}^{(1)} || j, \alpha \rangle \cdot \frac{\langle j, m' | \hat{J}_i | j, m \rangle}{\langle j || \hat{J}^{(1)} || j \rangle} \;. \tag{6}$$

(b) Show that the matrix elements of the scalar product $\hat{A}_i \hat{J}_i$ are related to the reduced matrix elements of $\hat{A}^{(1)}$ via

$$\langle j, m, \alpha' | \hat{A}_i \hat{J}_i | j, m, \alpha \rangle \;=\; C_j \langle j, \alpha' || \hat{A}^{(1)} || j, \alpha \rangle \;, \tag{7}$$

where the coefficient C_j depends only on j and is the same for all vector operators $\hat{A}_i$ and all rotationally-invariant quantum numbers α, α'.

(c) Combine eqs. (6) and (7) and the fact that $\hat{J}_i$ is itself a vector operator to prove that

$$\langle j, m', \alpha' | \hat{A}_i | j, m, \alpha \rangle \;=\; \frac{1}{\hbar^2 j(j+1)} \langle j, m, \alpha' | \hat{A}_j \hat{J}_j | j, m, \alpha \rangle \cdot \langle j, m' | \hat{J}_i | j, m \rangle \;. \tag{8}$$

This formula, which we discussed in class, is often called *the projection theorem.*

(d) The magnetic moment of an electron is $\hat{\mu}_i = \frac{-e}{2M_e c}(\hat{L}_i + \hbar \hat{\sigma}_i)$. Hence, the magnetic moment of an atom is $\hat{\mu}_i = \frac{-e}{2M_e c}(\hat{L}_i + 2\hat{S}_i)$, where $\hat{L}_i$ is the combined orbital angular momentum of the atom's electrons and $\hat{S}_i$ is their combined spin.

The ground states of atoms usually have well-defined values of ℓ_{tot} and s_{tot} as well as j_{tot} and m_j (the so-called LS coupling). Show that the matrix elements of the magnetic moment between such states are:

$$\langle \ell, s, j, m', \mathrm{rad} | \hat{\mu}_i | \ell, s, j, m, \mathrm{rad} \rangle \;=\; \frac{-e}{2M_e c}\, g\, \langle j, m' | \hat{J}_i | j, m \rangle \;, \tag{9}$$

(Lande's formula) and compute the *gyromagnetic factor* g in terms of ℓ, s and j.

3. 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 not accidental but 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.

   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

$$\mathbf{K} \equiv \mathbf{p} \times \mathbf{L} - e^2ZM\mathbf{n}_r \tag{10}$$

   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. (10) implies that $\mathbf{x} \cdot \mathbf{K} = \mathbf{L}^2 - e^2ZMr$ and hence $r = \mathbf{L}^2/(|\mathbf{K}|\cos\phi + e^2ZM)$ 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 $\epsilon = \mathbf{K}/e^2ZM$; 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

$$\hat{\mathbf{K}} \equiv \frac{1}{2}(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}) - e^2ZM\hat{\mathbf{x}}\hat{r}^{-1} . \tag{11}$$

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

$$\hat{H} = \frac{1}{2M}\hat{\mathbf{p}}^2 - e^2Z\hat{r}^{-1} . \tag{12}$$

   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

$$[\,\hat{K}_i, \hat{L}_j\,] = i\hbar\epsilon_{ijk}\hat{K}_k \qquad [\,\hat{K}_i, \hat{K}_j\,] = -2M\hat{H} \cdot i\hbar\epsilon_{ijk}\hat{L}_k . \tag{13}$$

   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 $\hat{\mathbf{Q}}_-$:

$$\hat{\mathbf{Q}}_\pm \equiv \frac{\hat{\mathbf{L}}}{2} \pm \frac{\hat{\mathbf{K}}}{\sqrt{-8M\hat{H}}} . \tag{14}$$

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

$$[\,\hat{Q}^i_+, \hat{Q}^j_+\,] \;=\; i\hbar\epsilon^{ijk}\hat{Q}^k_+\,, \qquad [\,\hat{Q}^i_-, \hat{Q}^j_-\,] \;=\; i\hbar\epsilon^{ijk}\hat{Q}^k_-\,, \qquad [\,\hat{Q}^i_+, \hat{Q}^j_-\,] \;=\; 0\,. \tag{15}$$

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

$$\hat{\mathbf{K}}^2 \;=\; (e^2 ZM)^2 \;+\; 2M\hat{H}(\hat{\mathbf{L}}^2 + \hbar^2) \tag{16}$$

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

(g) Second, use eqs. (14) and (16) to derive

$$2\hat{\mathbf{Q}}^2_+ \;+\; 2\hat{\mathbf{Q}}^2_- \;+\; \hbar^2 \;=\; \frac{(e^2ZM)^2}{-2M\hat{H}}\,. \tag{17}$$

(h) And, finally, use eqs. (17) to show that the energy of the $|q, m_+, m_-\rangle$ bound state is

$$E_N \;=\; -\frac{M(e^2Z)^2}{2\hbar^2(2q+1)^2} \;\equiv\; -\frac{M(e^2Z)^2}{2\hbar^2 N^2} \tag{18}$$

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.