# Physics 606, Quantum Mechanics, Final Exam

**Please show all your work on the separate sheets provided (and be sure to include your name).**

You are graded on your work on those pages, with partial credit where it is deserved.

All problems are, of course, nonrelativistic.

Vectors are marked with arrows, are in boldface, or are explicitly stated to be vectors.

$\hat{p}_x$ etc. are operators in either Hilbert space or the coordinate representation, depending on the context.

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Some potentially useful equations:

$$\hat{L}_x = \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right) \quad , \quad \hat{L}_y = \frac{1}{2i}\left(\hat{L}_+ - \hat{L}_-\right)$$

$$\int_b^a k(x)\,dx = \left(n + \frac{1}{2}\right)\pi$$

$$\int_{-1}^{1}\left(1-u^2\right)^{1/2} du = \frac{\pi}{2}$$ [although you should be able to do this integral!]

$$\left[\hat{L}_i, \hat{x}_j\right] = i\hbar\varepsilon_{ijk}\hat{x}_k \quad , \quad \left[\hat{L}_i, \hat{p}_j\right] = i\hbar\varepsilon_{ijk}\hat{p}_k$$

1. At low temperature, where vibrations can be neglected, a diatomic molecule like $O_2$ or $N_2$ can be treated as a rigid rotor. Let us consider a general symmetric rotor with the Hamiltonian

$$\widehat{H} = \frac{\hat{L}_x^2}{2I_x} + \frac{\hat{L}_y^2}{2I_y} + \frac{\hat{L}_z^2}{2I_z} \quad , \quad I_y = I_x \neq I_z$$

where $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ are the angular momentum operators in the (principal axes) body-axis frame, and the moments of inertia $I_x$ etc. are constants.

(a) (5) Rewrite the Hamiltonian in terms of $\hat{L}^2$, $\hat{L}_z^2$, $I_x$, and $I_z$.

(b) (5) Calculate the expectation values $\left\langle \hat{L}^2 \right\rangle$, $\left\langle \hat{L}_z \right\rangle$, and $\left\langle \widehat{H} \right\rangle$ in an angular momentum eigenstate $\left| \ell m \right\rangle$, with the usual notation for the quantum numbers.

(c) (5) Calculate the expectation value of $\left\langle \widehat{H} \right\rangle$ in a more general state $\left| \psi \right\rangle = \sum_{\ell m} \psi_{\ell m} \left| \ell m \right\rangle$ (in terms of the coefficients $\psi_{\ell m}$, the quantum numbers $\ell$ and $m$, and constants).

(d) (5) Suppose that the state at time $t = 0$ is $\left| \ell = 3, m = 0 \right\rangle$.

Determine the expectation value of $L_x$ at time $t = 4\pi I_x / \hbar$ .

(e) (3) For a real diatomic molecule, rotations about the molecular z axis are omitted from consideration. Make a very rough estimate of $I_z$ for $O_2$ and use it to justify the neglect of these rotations.

(As always, your argument, however brief, needs to be explicit, complete, clear, and convincing.)

2. (20) Using the WKB approximation, calculate the energy eigenvalues $E_n$ for the harmonic oscillator, with classical Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2$$

in terms of the angular frequency $\omega = \sqrt{K/m}$.

3. Consider a harmonic oscillator, with the quantized version of the Hamiltonian in Problem 2.

   (a) (10) For a trial wavefunction with the form

$$\psi(x) = A\,x\,e^{-\alpha x^2}$$

   use the variational method to calculate $\alpha$.

   (b) (10) Calculate the energy $E$ for this state.

   (c) (2) Can the variational method ever be used to treat excited states? Explain.

4. Let us consider a simplistic model of the shifts in energy for electrons when an electric field is applied: a box with cube edge $a$, in which the wavefunctions for the electrons must vanish at the sides of the cube.

   The energy eigenvalues are then

$$E\left(n_x, n_y, n_z\right) = \frac{\hbar^2\pi^2}{2ma^2}\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right)$$

   since $n\frac{\lambda}{2} = a$ , $\lambda = h / p = 2\pi\hbar / p$ , $E = \frac{p^2}{2m}$ for each direction. The states are labeled $\left|n_x, n_y, n_z\right\rangle$.

   The box extends from $0$ to $a$ along each axis; e.g., from $z = 0$ to $z = a$ .

   A weak electric field is applied in the $z$ direction with strength $\mathcal{E}$. Let us take this to mean that the perturbation is $e\mathcal{E}z$.

   A particular electron lies in a state with an energy $3\frac{\hbar^2\pi^2}{ma^2}$ before the electric field is applied.

   (a) (5) List the 3 degenerate states with this energy.

   (b) (15) Calculate the shifts $\Delta E$ in the energies for these states.

5. (15) Consider the unitary operator

$$\widehat{U} = e^{i\widehat{\mathbf{L}}\cdot\omega t/\hbar}$$

where $\widehat{\mathbf{L}}$ is the usual angular momentum operator, $\omega$ is the angular velocity of a rotating coordinate system, and $t$ is the time.

The $x, y, z$ coordinate system below rotates about the $z$ axis.

I.e., the vector $\omega$ points along the $z$ axis.

Define

$$\hat{x}_{stat}(t) = \widehat{U}\,\hat{x}\,\widehat{U}^{\dagger} \quad , \quad \hat{y}_{stat}(t) = \widehat{U}\,\hat{y}\,\widehat{U}^{\dagger} \quad , \quad \hat{z}_{stat}(t) = \widehat{U}\,\hat{z}\,\widehat{U}^{\dagger} \quad .$$

Using the commutation relations involving $\widehat{L}_i$ and $\hat{x}_i$, obtain simple expressions for $\hat{x}_{stat}(t), \hat{y}_{stat}(t), \hat{z}_{stat}(t)$ .

Interpret your result.

**Happy Holidays!**