Physics 451: Introduction to Quantum Mechanics

Final Exam

Thursday, December 10, 2015 / 08:00–11:00 / Room 2-228, Lewis Hall

Student's Name: ____________________

Instructions

There are 17 questions, 15 in multiple choice format and 2 that require written answers or mathematical derivations. You should attempt all of them. Mark your response on the test paper in the space provided. Aids of any kind—including class notes, textbooks, cheat sheets, and calculators—are not permitted.

Good luck!

15	points	short answer	questions	1–15
15		long answer		16
10				17
40	**points**			

Trigonometric identities

$$2\cos\theta = e^{i\theta} + e^{-i\theta}$$
$$2i\sin\theta = e^{i\theta} - e^{-i\theta}$$

Linear algebra identities

$$\begin{aligned}
\text{a matrix} \qquad & M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \\
\text{its inverse} \qquad & M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \\
\text{its characteristic polynomial} \qquad & p_M(\lambda) = \det(M - \lambda I) = (a - \lambda)(d - \lambda) - bc
\end{aligned}$$

Occupation number formalism for the quantum harmonic oscillator

$$\begin{aligned}
\hat{H} &= \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{x}^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \\
a &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \\
1 &= [a, a^\dagger] = aa^\dagger - a^\dagger a \\
a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\
a|n\rangle &= \sqrt{n}|n-1\rangle \\
a|0\rangle &= 0
\end{aligned}$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

$$\begin{aligned}
\sigma_u\sigma_v &= \delta_{uv} I + \sum_{w=x,y,z} i\epsilon_{uvw}\sigma_w \\
[\sigma_u, \sigma_v] &= \sigma_u\sigma_v - \sigma_v\sigma_u = \sum_{w=x,y,z} 2i\epsilon_{uvw}\sigma_w \\
\{\sigma_u, \sigma_v\} &= \sigma_u\sigma_v + \sigma_v\sigma_u = 2\delta_{uv} I
\end{aligned}$$

Short answer questions (15 points)

1. The time evolution of a quantum state is given by

$$|\psi(t)\rangle = \exp\left[-i\hat{H}t/\hbar\right]|\psi(0)\rangle.$$

If we act with $i\hbar(\partial/\partial t)$ on both sides of this equation, what do we get?

(a) $i\hbar\partial|\psi(t)\rangle/\partial t = \hat{H}|\psi(t)\rangle$

(b) $i\hbar\partial|\psi(t)\rangle/\partial t = \hat{H}|\psi(0)\rangle$

(c) $i\hbar\partial|\psi(t)\rangle/\partial t = t\exp\left[-i\hat{H}t/\hbar\right]|\psi(0)\rangle$

(d) $i\hbar\partial|\psi(t)\rangle/\partial t = \int_0^t dt' \exp\left[-i\hat{H}t'/\hbar\right]|\psi(0)\rangle$

2. A quantum state $|\psi(t)\rangle$ is normalized at time zero (i.e., $\langle\psi(0)|\psi(0)\rangle = 1$). What is the normalization at future times?

(a) $\langle\psi(t)|\psi(t)\rangle > 1$

(b) $0 < \langle\psi(t)|\psi(t)\rangle < 1$

(c) $\langle\psi(t)|\psi(t)\rangle = 1$

(d) $\langle\psi(t)|\psi(t)\rangle = 0$

3. Because the Schrödinger equation is a linear equation, its solutions obey which of the following?

(a) completeness

(b) orthonormality

(c) superposition principle

(d) uncertainty principle

4. If A_1 and A_2 are the quantum probability amplitudes for two events, what is the probability of observing both events?

(a) $A_1 + A_2$

(b) $|A_1 - A_2|^2$

(c) $|A_1|^2 + |A_2|^2$

(d) $|A_1|^2 + 2\,\mathrm{Re}\,A_1A_2^* + |A_2|^2$

5. We studied the case of a single particle in three dimensions, constrained by an isotropic infinite square well potential; i.e. $V(x, y, z) = \infty$ if $x^2 + y^2 + z^2 > L^2$ and $V(x, y, z) = 0$ otherwise. Which of the following is an <u>incorrect</u> statement.

   (a) Each eigenstate has a wave function of product form $\psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi)$, where $Y_{l,m}$ are the spherical harmonics.

   (b) The wave functions $\{\psi_{n,l,m}(r, \theta, \phi)\}$ form a complete set, so long as the indices are taken to range over $n = 1, 2, 3, \ldots$; $l = 1, 2, 3, \ldots$; and $m = -l, -l + 1, \ldots, l$.

   (c) $\psi_{n,l,m}(L, \theta, \phi) = 0$ for all angles θ, ϕ and for all allowed quantum numbers n, l, m.

   (d) Each energy level E_n is $(2l + 1)$-fold degenerate.

6. At time $t = 0$, an electron is described by a wave packet $\phi(x, 0) \sim \exp\left[-(x/\sigma)^2 + ik_0 x\right]$. Which of the following is an <u>incorrect</u> statement.

   (a) The expectation value $\langle \phi(t)|\hat{x}|\phi(t)\rangle$ is zero for all time.

   (b) The corresponding k-space (or momentum-space) description of the wave packet is produced by Fourier transformation.

   (c) k_0 is a constant wave vector with units of inverse distance; the electron's momentum is proportional to $\hbar k_0$.

   (d) Because of the nonlinear dispersion relation (frequency ω as a function of k), the wave packet distorts as it propagates in time.

   (e) Measuring time in appropriately chosen units, we find that the effective width of the distribution $|\phi(x, t)|^2$ evolves according to $\sigma(t) = \sigma(0)\sqrt{1 + t^2}$.

7. A quantum object of mass m sits in a harmonic potential with natural frequencies ω_x and ω_y in the x and y directions. The energy eigenstates $\{|n_x, n_y\rangle\}$ are labelled by the corresponding numbers of vibrational quanta. Which of the following is the correct energy eigenvalue equation?

   (a) $\hat{H}|n_x, n_y\rangle = \hbar[\omega_x(n_x + 1/2) + \omega_y(n_y + 1/2)]|n_y, n_x\rangle$

   (b) $\hat{H}|n_x, n_y\rangle = \hbar[\omega_x(n_x + 1/2) + \omega_y(n_y + 1/2)]|n_x, n_y\rangle$

   (c) $\hat{H}|n_x, n_y\rangle = (\hbar/2)(\omega_x + \omega_y)(n_x + n_y + 1)|n_x, n_y\rangle$

   (d) $\hat{H}|n_x, n_y\rangle = \hbar(\omega_x \omega_y + 1)^{1/2}|n_x, n_y\rangle$

8. A diatomic molecule consists of two atoms of mass m_1 and m_2. The chemical bond is so stiff that, to good approximation, the molecule is a rigid rotor with bond length r_0. The resulting Hamiltonian is $\hat{H} = \hat{L}^2/2\mu r_0^2$. Which of the following is an <u>incorrect</u> statement about this system.

   (a) The μ appearing in the Hamiltonian is the average mass, $\mu = (m_1 + m_2)/2$.

   (b) The energy spectrum is $0, E_1, 3E_1, 6E_1, 10E_1, \ldots$, where $E_1 = \hbar^2/\mu r_0^2$

   (c) In this limit, the vibrational modes are at such high energies that they are irrelevant for determining the molecule's low-energy spectrum.

   (d) The propensity of the molecule to undergo quantum transitions by absorbing or emitting light scales up with the strength of its electric dipole moment.

9. Suppose instead that the diatomic molecule has low-lying vibrational modes. In that case, the wave function for the relative coordinate is of the form $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$, and the radial function satisfies the equation

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right]R(r) = ER(r).$$

   We sometimes group the "centrifugal barrier" term with the potential to form an effective potential $V_{\text{eff}}(r) = V(r) + \hbar^2 l(l+1)/2\mu r^2$. Which of the following statements is most <u>correct</u>.

   (a) The centrifugal barrier vanishes for s-wave orbitals.

   (b) Whatever divergence $V(r)$ has at the origin is overwhelmed by the centrifugal barrier term.

   (c) The $l = 0$ and $l = -1$ modes are energy degenerate.

   (d) The normalization condition $\int_0^\infty r^2 dr\, |R(r)|^2 = 1$ places an upper limit on the value of l.

10. The eigenstate wave functions of a particle confined to an infinite square-well potential of width L have the form $\psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$. Suppose that the potential is modified so that, instead of having the value zero across the bottom of the well, it looks like $V(x) = V_0$ for $0 < x < L/2$ and $V(x) = 0$ for $L/2 < x < L$. Following the prescription of perturbation theory, what is the first order energy shift, $\Delta E_n^{(1)} = \langle\psi_n|V|\psi_n\rangle$?

   (a) $V_0\int_0^{L/2} dx\, \psi_n(x)^*\psi_0(x)$

   (b) $V_0\int_0^{L/2} dx\, \psi_n(x)^*\psi_{n+1}(x)$

   (c) $(2V_0/L)\int_0^L dx\, \sin^2(n\pi x/L) = V_0$

   (d) $(2V_0/L)\int_0^{L/2} dx\, \sin^2(n\pi x/L) = V_0/2$

11. A trial state $|\psi[\kappa]\rangle$ with one free parameter κ is used as a guess for the ground state of a system described by $\hat{H}$. Evaluation of the energy expectation value yields

$$E[\kappa] = \frac{\langle\psi[\kappa]|\hat{H}|\psi[\kappa]\rangle}{\langle\psi[\kappa]|\psi[\kappa]\rangle} = \frac{\hbar^2\kappa^2}{2m} - V_0 \log \kappa a.$$

What value of κ produces the most restrictive upper bound on the ground state energy?

(a) The value that maximizes $E[\kappa]$

(b) 0

(c) $\sqrt{mV_0}/\hbar$

(d) $\sqrt{2mV_0}/\hbar$

(e) ∞

12. A quantum harmonic oscillator of mass m and natural frequency ω has eigenstates $\{|\phi_n\rangle\}$. The overlap between any two such states satisfies the following orthogonality relation:

$$\langle\phi_n|\phi_{n'}\rangle = \sqrt{\frac{m\omega}{2^{n+n'}n!(n')!\pi\hbar}} \int_{-\infty}^{\infty} dx\, e^{-m\omega x^2/\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) H_{n'}\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = \begin{cases} 1 & \text{if } n = n', \\ 0 & \text{otherwise.} \end{cases}$$

What does the symbol H_n represent here?

(a) Hermite polynomial

(b) Hildebrandt polynomial

(c) Hilbert space

(d) trace of the Hamiltonian, $\mathrm{tr}\,\hat{H}$

(e) expectation value of the Hamiltonian in the nth state, $\langle\phi_n|\hat{H}|\phi_n\rangle$

13. Consider the potential $V(x < 0) = 0$ and $V(x > 0) = V_0$, representing a step-edge barrier of height V_0. The wave function $\psi(x)$ describes the situation in which a flux of particles with energy E is incident from the negative-x side. Which of the following is an <u>incorrect</u> statement?

(a) In the case where $0 < E < V_0$, the probability $\int_0^\infty dx\,|\psi(x)|^2$ is greater than zero, even though there is *no* probability current in the region $x > 0$.

(b) In the case where $E > V_0$, the reflection probability is $R = [(k_+ - k_-)/(k_+ + k_-)]^2$, with k_- and k_+ denoting the wave vectors in the regions $x < 0$ and $x > 0$.

(c) In the case where $E > V_0$, the transmission probability is $T = (k_+^2 - k_-^2)/(k_+ + k_-)^2$.

14. Which of the following is an incorrect statement about the wave function $\psi(\mathbf{r}) \sim \exp(i\mathbf{k}\cdot\mathbf{r})$.

    (a) $\psi(\mathbf{r})$ is a plane wave state.

    (b) $\psi(\mathbf{r})$ represents a state of definite momentum $\mathbf{p} = \hbar\mathbf{k}$.

    (c) The wave function of an energy eigenstate can behave like $\psi(\mathbf{r}) \sim \exp(i\mathbf{k}\cdot\mathbf{r})$ only in regions where the potential is exactly zero.

    (d) The probability density $|\psi(\mathbf{r})|^2$ of finding the particle in the vicinity of $\mathbf{r}$ is uniform in space.

15. When written in terms of the creation and annihilation operators, $a^\dagger$ and a, the quantum harmonic oscillator Hamiltonian has this compact form: $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$. The energy eigenstates $\{|n\rangle : n = 1, 2, 3, \ldots\}$ are eigenstates of the number operator $\hat{N} = a^\dagger a$. Which two of the following expressions are incorrect. (Circle both.)

    (a) $a^\dagger a a^\dagger a|n\rangle = n^2|n\rangle$

    (b) $aa^\dagger + a^\dagger a = 1$

    (c) $|n\rangle = (1/\sqrt{n!})(a^\dagger)^n|0\rangle$

    (d) $a^\dagger|0\rangle = |1\rangle$

    (e) $a|1\rangle = |0\rangle$

    (f) $a|0\rangle = |-1\rangle$

Long answer questions (25 points)

16. Consider the Hamiltonian

$$\hat{H} = \hbar\omega a^\dagger a + \Gamma a^\dagger + \Gamma^* a + V a^\dagger a^\dagger a a.$$

As usual, $a^\dagger$ and a are the quantum harmonic oscillator creation and annihilation operators. $\hbar\omega$ and V are real constants with units of energy. Γ is a complex constant with units of energy.

(a) Compute $[\hat{H}, a]$ and $[\hat{H}, a^\dagger]$. You should accomplish this through repeated application of the commutation relation $[a, a^\dagger] = 1$.

(b) Provide the seven matrix elements $H_{mn} = \langle m|\hat{H}|n\rangle$ that are missing (marked "?") from the matrix below.

$$H = \begin{pmatrix} H_{00} & H_{01} & H_{02} & \cdots \\ H_{10} & H_{11} & & \\ H_{20} & & \ddots & \\ \vdots & & & \end{pmatrix} = \begin{pmatrix} 0 & \Gamma^* & 0 & 0 & \cdots \\ \Gamma & \hbar\omega & ? & ? & \\ 0 & ? & ? & ? & \\ 0 & ? & ? & 3\hbar\omega + 6V & \\ \vdots & & & & \ddots \end{pmatrix}.$$

(c) For the special case of $V = 0$, re-express $\hat{H} = \hbar\omega a^\dagger a + \Gamma a^\dagger + \Gamma^* a$ in terms of $\hat{x}$ and $\hat{p}$. Keep in mind that the position and momentum operators do not commute. You should be able to show that

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{\hbar\omega}{2} + \sqrt{\frac{2m\omega}{\hbar}}\big(\mathrm{Re}\,\Gamma\big)\hat{x} - \sqrt{\frac{2}{\hbar m\omega}}\big(\mathrm{Im}\,\Gamma\big)\hat{p}.$$

Explain why the last two terms above yield no first-order energy shift in perturbation theory with respect to the $\Gamma = 0$ ground state, $\phi_0(x) = \langle x|0\rangle = (m\omega/\pi\hbar)^{1/4}\exp(-(m\omega/2\hbar)x^2)$.

(d) Suppose that we truncate the Hilbert space to include only $\{|0\rangle, |1\rangle\}$, so that the Hamiltonian has the 2×2 matrix representation

$$H = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} = \begin{pmatrix} 0 & \Gamma^* \\ \Gamma & \hbar\omega \end{pmatrix}.$$

Find all the eigenvalue/eigenstate pairs. Then, express the eigenstates in Dirac notation as properly normalized kets.

17. Consider a quantum particle confined to an infinite well in two spatial dimensions:

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2m}\hat{p}_y^2 + V(x, y).$$

$V(x, y) = 0$ in the rectangle defined by $0 < x < L_x$ and $0 < y < L_y$; $V(x, y) = \infty$ otherwise.

(a) Solve the Schrödinger equation for this system in order to write down an expression for the normalized wave functions $\phi_{n_x,n_y}(x, y)$. Be sure to explain the presence of the quantum number labels n_x and n_y.

(b) Show that the energy eigenvalues are given by

$$E_{n_x,n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right).$$

Tabulate the energies (in units of $h^2/8mL_x^2$) and their degeneracies when $L_y = 2L_x$.

(c) Compute the variance $\langle \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}} \rangle - \langle \hat{\boldsymbol{r}} \rangle \cdot \langle \hat{\boldsymbol{r}} \rangle$ of the position vector $\hat{\boldsymbol{r}} = (\hat{x}, \hat{y})$ for the $(n_x = n_y = 0)$ ground state.

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