

# Physics 451: Introduction to Quantum Mechanics

## Final Exam

Thursday, December 11, 2014 / 08:00–11:00 / Room 2-228, Lewis Hall

Student's Name: \_\_\_\_\_

### Instructions

There are 18 questions, 15 in multiple choice format and 3 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
10		long answer	16
10			17
15			18
<b>50</b>	<b>points</b>		

## Trigonometric identities

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

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

## Linear algebra identities

a matrix  $M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

its inverse  $M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

its characteristic polynomial  $p_M(\lambda) = \det(M - \lambda I) = (a - \lambda)(d - \lambda) - bc$

## Occupation number formalism for the quantum harmonic oscillator

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{m\omega^2}{2} \hat{x}^2 = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right)$$

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} + \frac{i}{m\omega} \hat{p} \right)$$

$$1 = [a, a^\dagger] = aa^\dagger - a^\dagger a$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

$$a |0\rangle = 0$$

## Pauli matrices

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

$$\sigma_u \sigma_v = \delta_{uv} I + \sum_{w=x,y,z} i \epsilon_{uvw} \sigma_w$$

$$[\sigma_u, \sigma_v] = \sigma_u \sigma_v - \sigma_v \sigma_u = \sum_{w=x,y,z} 2i \epsilon_{uvw} \sigma_w$$

$$\{\sigma_u, \sigma_v\} = \sigma_u \sigma_v + \sigma_v \sigma_u = 2\delta_{uv} I$$

## Short answer questions (15 points)

1. Identify the correct form of the *time-independent* Schrödinger equation.

- (a)  $i\hbar\partial^2\psi/\partial t^2 = (\hbar^2/2m)\partial^2\psi/\partial x^2 + V\psi$
- (b)  $i\hbar\partial\psi/\partial t = (\hbar^2/2m)\partial^2\psi/\partial x^2 + V\psi$
- (c)  $i\hbar\partial^2\psi/\partial t^2 = (\hbar^2/2m)\partial\psi/\partial x + V\psi$
- (d)  $i\hbar\partial\psi/\partial t = (\hbar^2/2m)\partial\psi/\partial x + V\psi$

2. A quantum particle is repeatedly prepared in the state

$$|\psi\rangle = \int d^3r |\mathbf{r}\rangle\langle\mathbf{r}|\psi\rangle = \int d^3r \psi(\mathbf{r})|\mathbf{r}\rangle$$

and its position and momentum determined experimentally (not simultaneously, of course). The measurements reveal a narrow distribution of position values, sharply peaked around the point  $\mathbf{r} = \mathbf{r}_0$  and a wide distribution of momentum values, centred on  $\mathbf{p} = 0$ . Which of the following is not true.

- (a) The relationship above between the abstract state vector  $|\psi\rangle$  and the wave function  $\psi(\mathbf{r})$  was reached by acting on the ket with a representation of unity,  $\hat{1} = \int d^3r |\mathbf{r}\rangle\langle\mathbf{r}|$ .
- (b) The widths of the position and momentum distributions are inversely related, and their product exceeds  $\hbar/2$ .
- (c) If  $\psi(\mathbf{r})$  is properly normalized, then  $P(\mathbf{r}) = \mathbf{r}|\psi(\mathbf{r})|^2$  is the probability density for finding the particle at position  $\mathbf{r}$ .
- (d) A reasonable approximation for the wave function is  $\psi(\mathbf{r}) \approx \exp(-|\mathbf{r} - \mathbf{r}_0|^2/2\sigma^2)$ , where  $\sigma$  is the width of the observed position distribution.
- (e) The integral  $\int d^3r \psi(\mathbf{r})^* \nabla\psi(\mathbf{r})$  vanishes, at least within the experimental uncertainty (governed by the number of measurement trials).

3. The overlap between infinite square well eigenstates satisfies

$$\langle\phi_m|\phi_n\rangle = \frac{2}{L} \int_0^L dx \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) = \begin{cases} 1 & \text{if } m = n, \\ 0 & \text{otherwise.} \end{cases}$$

This is a statement of what?

- (a) orthogonality
- (b) orthonormality
- (c) completeness
- (d) duality
- (e) criticality

4. 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 incorrect 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 eigenstates are normalizable.
  - (c) The wave functions  $\{\psi_{n,l,m}(r, \theta, \phi)\}$  form a complete set, so long as the indices are taken to range over  $n = 1, 2, 3, \dots$ ;  $l = 0, 1, 2, \dots$ ; and  $m = -l, -l + 1, \dots, l$ .
  - (d)  $\psi_{n,l,m}(L, \theta, \phi) = 0$  for all angles  $\theta, \phi$  and for all allowed quantum numbers  $n, l, m$ .
  - (e) The radial function  $R_{n,l}(r)$  is perfectly sinusoidal in shape.
  - (f) The number of radial nodes (i.e., points where  $R_{n,l}(r) = 0$  with  $0 < r < L$  strictly inside the well) is equal to  $n - 1$ .
  - (g) Each energy level  $E_n$  is  $(2l + 1)$ -fold degenerate.
5. An electron feels an image charge potential that attracts it to a metallic surface. (The potential is zero when the electron is an infinite distance from the surface.) In class, we computed the energy levels for this system:  $E_n = -(0.85 \text{ eV})/n^2$  (with  $n = 1, 2, 3, \dots$ ). The ground state ( $n = 1$ ) wave function is  $\phi_1(z < 0) = 0$  and  $\phi_1(z > 0) \sim (z/a_B)e^{-z/a_B}$ . Which of the following is an incorrect statement?
- (a) In each mode  $n$ , the wave function  $\phi_n(z)$  vanishes at the metal surface ( $z = 0$ ).
  - (b) The wave function  $\phi_n(z)$  has  $n - 1$  nodes at positions  $z > 0$  away from the surface.
  - (c) The expectation value  $\langle \phi_1 | z | \phi_1 \rangle$  is greater than zero and has units of  $a_B$ .
  - (d) There is a countably infinite number of bound states.
  - (e) There is a continuum of positive-energy states with wave functions that behave like  $e^{ikz}$  at distances far from the surface.
  - (f) There is a finite number of states with energy  $E < 0$ .
6. Indicate with certainty which one of these people formulated the uncertainty principle.
- (a) Hamilton
  - (b) Heisenberg
  - (c) Hermite
  - (d) Hilbert

7. At time  $t = 0$ , an electron is described by a wave packet  $\phi(x, 0) \sim \exp[-(x/\sigma)^2 + ik_0x]$ . Which of the following is an incorrect statement.
- The expectation value  $\langle \phi(t) | \hat{x} | \phi(t) \rangle$  is zero for all time.
  - The corresponding  $k$ -space (or momentum-space) description of the wave packet is produced by Fourier transformation.
  - $k_0$  is a constant wave vector with units of inverse distance; the electron's momentum is proportional to  $\hbar k_0$ .
  - Because of the nonlinear dispersion relation (frequency  $\omega$  as a function of  $k$ ), the wave packet distorts as it propagates in time.
  - Measuring time in appropriately chosen units, we find that the effective width of the distribution  $|\phi(x, t)|^2$  evolves according to  $\sigma(t) = \sigma(0)\sqrt{1 + t^2}$ .
8. A flux of particles of energy  $E$  is incident on a single potential barrier of height  $V_0 > E$  and width  $a$ . Only some fraction of the particles manage to tunnel through the barrier. The transmission probability  $T$  is strictly less than 1, and it decreases with the width and height of the barrier:  $T \sim \exp(-2[2m(V_0 - E)/\hbar^2]^{1/2}a)$ . What's different about the double barrier system?
- For special values of  $E$ , the transmission probability can be as large as 1.
  - The well between the two barriers may be able to support bound states.
  - The double-barrier system may allow for resonant tunnelling.
  - All of the above are true.
9. A quantum object of mass  $m$  sits in a harmonic potential with natural frequencies  $\omega_x$  and  $\omega_y$  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?
- $\hat{H}|n_x, n_y\rangle = \hbar[\omega_x(n_x + 1/2) + \omega_y(n_y + 1/2)]|n_x, n_y\rangle$
  - $\hat{H}|n_x, n_y\rangle = \hbar[\omega_x(n_x + 1/2) + \omega_y(n_y + 1/2)]|n_x, n_y\rangle$
  - $\hat{H}|n_x, n_y\rangle = (\hbar/2)(\omega_x + \omega_y)(n_x + n_y + 1)|n_x, n_y\rangle$
  - $\hat{H}|n_x, n_y\rangle = \hbar(\omega_x\omega_y + 1)^{1/2}|n_x, n_y\rangle$
10. Which of the following statements about the Pauli matrices is incorrect?
- $\sigma_x\sigma_y\sigma_z = I$  (the  $2 \times 2$  identity matrix).
  - $\det \sigma_x = \det \sigma_y = \det \sigma_z = -1$
  - $\text{tr } \sigma_x = \text{tr } \sigma_y = \text{tr } \sigma_z = 0$
  - $(\mathbf{p} \cdot \boldsymbol{\sigma})(\mathbf{q} \cdot \boldsymbol{\sigma}) = I(\mathbf{p} \cdot \mathbf{q}) + i(\mathbf{p} \times \mathbf{q}) \cdot \boldsymbol{\sigma}$
  - $p \exp(\mathbf{p} \cdot \boldsymbol{\sigma}) = pI \cosh p + (\mathbf{p} \cdot \boldsymbol{\sigma}) \sinh p$  (with  $p = |\mathbf{p}|$ )

11. 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 incorrect statement about this system.

- (a) The  $\mu$  appearing in the Hamiltonian is the reduced mass,  $\mu = (m_1^{-1} + m_2^{-1})^{-1}$ .
- (b) The energy spectrum is  $0, E_1, 4E_1, 9E_1, 25E_1, \dots$ , 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.

12. 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 correct.

- (a) The centrifugal barrier has no effect on 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  $l$ .

13. The 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 throughout the region  $0 < x < L$ , it looks like  $V(x) = V_0 a \delta(x - L/2)$ . In other words, it's zero except for a strongly repulsive narrow spike at the centre of the well. 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)  $V_0$
- (b)  $-V_0$
- (c)  $V_0 \sqrt{a/L}$
- (d)  $2V_0 a/L$
- (e)  $2V_0 a/L$  for odd values of  $n$  and 0 otherwise.

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

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

What value of  $\kappa$  produces the most restrictive upper bound on the ground state energy?

- (a) The value that maximizes  $E[\kappa]$
  - (b) 0
  - (c)  $(V_0 m / \hbar^2 a)^{1/3}$
  - (d)  $(-2V_0 m / \hbar^2 a)^{1/3}$
  - (e)  $\infty$
15. In Assignment 5, you proved the Ehrenfest relation in the special case of the quantum harmonic oscillator. Identify it.

- (a)  $d\langle \hat{p} \rangle / dt = m d^2 \langle \hat{x} \rangle / dt^2$
- (b)  $d\langle \hat{x} \rangle / dt = \langle \hat{p} \rangle / m$
- (c)  $d\langle \hat{x}^2 \rangle / dt = \langle \hat{p}^2 \rangle / m$
- (d)  $d\langle \hat{p}^2 \rangle / dt = 0$

## Long answer questions (35 points)

16. When written in terms of the creation and annihilation operators,  $a^\dagger$  and  $a$ , the quantum harmonic oscillator Hamiltonian has this compact form:  $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$ .

(a) Its energy eigenstates  $\{|n\rangle : n = 1, 2, 3, \dots\}$  are simultaneous eigenstates of the Hamiltonian and the number operator  $\hat{N}$ ; i.e.,  $\hat{H}|n\rangle = E_n|n\rangle$  and  $\hat{N}|n\rangle = n|n\rangle$ . This follows from the fact that  $\hat{H}$  and  $\hat{N}$  commute with one another. Tell me the very simple reason why they commute.

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



- (c) Suppose that the system is prepared in a state  $|\psi\rangle = 3|0\rangle + 5i|1\rangle$ . Compute the expectation value of the operator  $\hat{x}$  with respect to  $|\psi\rangle$ .

(d) Using the same definition of  $|\psi\rangle$ , compute the expectation value of the operator  $\hat{p}^2$ .

17. Consider the isotropic quantum harmonic oscillator in spatial dimension higher than one:

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{m\omega^2}{2}\hat{\mathbf{r}}^2.$$

- (a) For the two-dimensional case, with  $\mathbf{r} = (x, y)$  and  $\mathbf{p} = (p_x, p_y)$ , complete the following table of eigenenergies and corresponding degeneracies. Be sure to fill in all five missing entries.

energy	degeneracy
$\hbar\omega$	—
$2\hbar\omega$	—
$3\hbar\omega$	—
—	—

- (b) Do the same for the three-dimensional case, with  $\mathbf{r} = (x, y, z)$  and  $\mathbf{p} = (p_x, p_y, p_z)$ . Fill in all six missing entries.

energy	degeneracy
—	1
—	3
—	6
—	10
—	—

- (c) Go back to the two-dimensional case, and think about what you expect to happen to the energy spectrum if the confining potential is distorted so that the spring constant is slightly stiffer in the x direction than in the y: i.e.,

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

for some  $\alpha < 1$ . Suppose that the energy eigenvalues are found to be  $0.99\hbar\omega$ ,  $1.97\hbar\omega$ ,  $1.99\hbar\omega$ ,  $2.95\hbar\omega$ ,  $2.97\hbar\omega$ ,  $2.99\hbar\omega$ ,  $\dots$ . What value of  $\alpha$  is consistent with this sequence? What is the lowest-energy pair of degenerate states?

18. The intrinsic angular momentum (“spin”) of an electron is specified as some linear superposition of the spin-up ( $|\uparrow\rangle$ ) and spin-down ( $|\downarrow\rangle$ ) configurations.

- (a) Suppose that the spin  $\hat{S}$  interacts with a magnetic field that has been applied in the z direction. The resulting Hamiltonian is

$$\hat{H} = -\frac{\mu_B g_S}{\hbar} (B \mathbf{e}_z) \cdot \hat{S} = -\frac{\mu_B g_S B}{\hbar} \hat{S}_z.$$

Here,  $\mu_B$  is the Bohr magneton, and  $g_S \doteq 2.0023192$  is the Landé g-factor. These are just constants—with the product  $\mu_B g_S B$  having units of energy. Consider the combination  $\hbar/(\mu_B g_S B)$ . What is the nature of its units (length? time? mass? ...), and what does it represent physically?

- (b) When expressed in terms of the basis  $\{|\uparrow\rangle, |\downarrow\rangle\}$ , the vector components of the spin operator are proportional to the Pauli matrices (given on page 2). Hence,

$$H = \begin{pmatrix} \langle \uparrow | \hat{H} | \uparrow \rangle & \langle \uparrow | \hat{H} | \downarrow \rangle \\ \langle \downarrow | \hat{H} | \uparrow \rangle & \langle \downarrow | \hat{H} | \downarrow \rangle \end{pmatrix} = -(\mu_B g_S / \hbar) (B \mathbf{e}_z) \cdot \frac{\hbar}{2} \boldsymbol{\sigma}.$$

Show explicitly that the column vectors

$$\chi_{\uparrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_{\downarrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

are eigenvectors of  $H$  with energies  $-\hbar\omega$  and  $\hbar\omega$ , where  $\omega = \mu_B g_S B / 2\hbar > 0$ .

- (c) The wave function at time  $t_0 = \pi/2\omega$  is the following linear superposition of spin up and spin down spinors:

$$\psi(t_0) = e^{-iHt_0/\hbar}\psi(0) = 2i\chi_{\uparrow} + 3\chi_{\downarrow}.$$

Compute  $\psi(0)$ .

- (d) Imagine that the original magnetic field is augmented by another one of strength  $B'$  applied in the x direction, so that

$$\mathbf{B}_{\text{net}} = B\mathbf{e}_z + B'\mathbf{e}_x.$$

Show that the modified Hamiltonian can be represented as

$$H = -\hbar\omega \begin{pmatrix} 1 & \beta \\ \beta & -1 \end{pmatrix},$$

where  $\beta = B'/B$ .

(e) Find the eigenenergies as a function of  $\beta$  and then show that they can be re-written as

$$E_+ = \mu_B g_S \sqrt{B^2 + (B')^2}$$

$$E_- = -\mu_B g_S \sqrt{B^2 + (B')^2}$$



- (f) Find the normalized eigenvectors as a function of  $\beta$ . Derive their  $\beta \rightarrow 0$  and  $\beta \rightarrow \infty$  limits and provide a physical interpretation of the results.

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