Phys 451 – sec 1, Fall 2010
Quantum Mechanics **CID______________**
Instructor: Karine Chesnel

Final test

Th Dec 16, 11am-2pm

This test is time limited to 3 hours. The test is closed book and closed notes, but useful formulae and integrals are provided below. Please write your CID on each sheet of your work. When you are done, make sure to put your work in order and staple it. This test includes 5 problems equally weighted. Each problem will count toward your final score. I encourage you to first read through all questions in order to have a general idea of the test. Each of the five problems is focusing on specific topic of the course. You may answer the questions in the order you wish. Explain your reasoning as much as possible. Good luck!

Useful formulae and integrals

Schrödinger equation: $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi+V\Psi$

Operator momentum $\vec{p}=-i\hbar\vec{\nabla}$; $p_x=-i\hbar\frac{\partial}{\partial x}$; $[x,p_x]=i\hbar$; $\langle p\rangle=m\frac{d\langle x\rangle}{dt}$

General wave function in terms of stationary states: $\Psi(x,t)=\sum_n c_n\psi_n e^{-iE_nt/\hbar}$

Normalization $\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,dx=1$

Generalized uncertainty principle: $\sigma_A^2\sigma_B^2\geq\left|\frac{\langle[A,B]\rangle}{2i}\right|^2$

Heisenberg equation of motion $\frac{d\langle Q\rangle}{dt}=\frac{i}{\hbar}\langle[H,Q]\rangle+\left\langle\frac{\partial Q}{\partial t}\right\rangle$

<u>Harmonic oscillator</u> $V(x)=\frac{1}{2}m\omega^2x^2$; stationary states ψ_n , $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$

Ladder operators $a_\pm=\frac{1}{\sqrt{2m\hbar\omega}}(\mp ip+m\omega x)=\frac{1}{\sqrt{2m\hbar\omega}}\left(\pm\hbar\frac{\partial}{\partial x}+m\omega x\right)$

$x=\sqrt{\frac{\hbar}{2m\omega}}(a_++a_-)$; $p=i\sqrt{\frac{m\omega\hbar}{2}}(a_+-a_-)$; $a_+\psi_n=\sqrt{n+1}\psi_{n+1}$; $a_-\psi_n=\sqrt{n}\psi_{n-1}$

<u>Angular momentum</u>

$|lm\rangle=Y_l^m(\theta,\phi)$; $L_z|lm\rangle=\hbar m|lm\rangle$; $L^2|lm\rangle=\hbar^2l(l+1)|lm\rangle$; $\vec{J}=\vec{L}+\vec{S}$

$L_\pm|1m\rangle=\hbar\sqrt{l(l+1)-m(m\pm1)}\,|1(m\pm1)\rangle$

Electron spin

Pauli matrices: $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Hydrogen atom: $V = -\frac{e^2}{4\pi\varepsilon_0 r}$ and Bohr radius: $a = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$ Wavevector: $k = \sqrt{-2mE} / \hbar$

Rydberg formula: $\frac{1}{\lambda} = R\left|\frac{1}{n_f^2} - \frac{1}{n_i^2}\right|$ with $R = 1.097\times10^7\, m^{-1}$; $E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = -13.6 eV$

Solids: Fermi energy $E_F = \frac{\hbar^2}{2m}\left(3\rho\pi^2\right)^{2/3}$ with free electron density $\rho = \frac{qN}{V}$; $1eV = 1.6\times10^{-19} J$

Constants: $\hbar = 1.05\times10^{-34} J.s$; $m_e = 9.11\times10^{-31} kg$; $N_A = 6.02\times10^{23}$; $k_B = 1.38\times10^{-23} J / K$

Potentially useful integrals:

$$\int_0^a \sin^2(n\pi\frac{x}{a})dx = \frac{a}{2}$$

$$\int_0^a x\sin^2(n\pi\frac{x}{a})dx = \frac{a^2}{4}$$

$$\int_0^a x^2\sin^2(n\pi\frac{x}{a})dx = a^3\left(\frac{1}{6} - \frac{1}{4n^2\pi^2}\right)$$

$$\int x\sin(\alpha x)\, dx = \left[\frac{\sin(\alpha x)}{\alpha^2} - \frac{x\cos(\alpha x)}{\alpha}\right]$$

$$\int x^2\sin(\alpha x)\, dx = \left[\frac{2x\sin(\alpha x)}{\alpha^2} + \left(\frac{2}{\alpha^3} - \frac{x^2}{\alpha}\right)\cos(\alpha x)\right]$$

$$\int x^2 e^{\alpha x}dx = \left[\frac{e^{\alpha x}}{\alpha}\left(x^2 - \frac{2x}{\alpha} + \frac{2}{\alpha^2}\right)\right]$$

$$\int_0^\infty e^{-\alpha u^2}du = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$$

$$\int_0^\infty u e^{-\alpha u^2}du = \frac{1}{2\alpha}$$

$$\int_{-\infty}^\infty u^2 e^{-\alpha u^2}du = \frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}}$$

$$\sum_{n=1,3,5,...}^{\infty}\frac{1}{n^4} = \frac{\pi^4}{96}$$

Fourier series expansion: $f(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{a}\right)$ where $c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi x}{a}\right) f(x)\, dx$

1. Schrödinger equation, wave function, expectation values

Consider the wave function: $\Psi(x,t) = Ae^{-\lambda|x|}e^{-i\omega t}$

where A, λ and ω are positive real constants.

a) Normalize Ψ.

b) Does Ψ correspond to a stationary state? If so, what is its associated energy E?

c) Calculate the expectation values $\langle x \rangle$, $\langle x^2 \rangle$ and the standard deviation σ_x

d) Calculate $\langle p \rangle$, $\langle p^2 \rangle$ and σ_p. Check the uncertainty principle.

2. The infinite square well

Let's consider an infinite square well of size a : $V = 0$ for $0 < x < a$ and $V = \infty$ outside

a) Solve the Schrödinger equation for this potential and find out the stationary states ψ_n, with their corresponding energies E_n

b) A particle, in this infinite square well, has the initial wave function:

$\Psi(x,0) = Ax(a-x)$ for $0 < x < a$ *and* $\Psi(x,0) = 0$ elsewhere

Sketch $\Psi(x,0)$. Can we express $\Psi(x,0)$ as a linear combination of the eigenstates ψ_n ?

If so, find the corresponding coefficients c_n

c) When measuring the energy of this particle, what is the probability of finding E_n ?

d) What is the expectation value $\langle H \rangle$ of the Hamiltonian for this particle?

e) What is the wave function $\Psi(x,t)$ at later times?

3. Harmonic oscillator

Let's consider a particle in the harmonic oscillator: $V = \frac{1}{2}m\omega^2 x^2$

The initial wave function is $\Psi(x,0) = \frac{1}{\sqrt{5}}(\psi_0 + 2\psi_1)$

where ψ_n are the eigenstates of the Hamiltonian

a) What is the wave function $\Psi(x,t)$ at later time?

b) Calculate $\langle x \rangle$ and $\langle p \rangle$ a time t. Do they depend on time?

c) Check the Ehrenfest theorem for this particle: $\frac{d\langle p \rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle$

d) Show that in general $[f(x), p] = i\hbar\frac{df}{dx}$

e) Use the equation of motion for the operator p to confirm the Ehrenfest theorem.

4. Hydrogen atom: spherical harmonics, energy, and angular momentum

The stationary states of the electron in the hydrogen atom are described by the wave function $\psi_{nlm}(r,\theta,\phi)$ in spherical coordinates.

a) What are the respective names of the quantum numbers *n, l*, and *m*?

b) $\psi_{nlm}(r,\theta,\phi)$ is an eigenstate for three different operators. What are these operators and the corresponding eigenvalues, in terms of *n, l, m* and the ground state energy E_1?

c) Using table 4.3 and 4.7 write the wave function $\psi_{421}(r,\theta,\phi)$

d) What is the energy of the particle and what is its associated degeneracy? (explain)

e) If the electron would transit from the energy level E_4 to ground state E_1, what would be the wavelength of the light emitted? Where in the electromagnetic spectrum would it fall?

f) What do we get when applying L^2, L_z, L_+, L_-, L_x and L_y on ψ_{421}?

(Express your result in terms of ψ_{nlm})

5. Electron's spin angular momentum, atoms and solids

An electron is in the spin state $\chi = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\2i\end{pmatrix}$ in the basis (χ_+,χ_-) (eigenspinors of S_z)

a) Using Pauli matrices, find the expectation values $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$. When measuring the spin S_x along *x*, what is the probability of measuring ($+\hbar/2$)?

b) If the electron is brought in the presence of a uniform field applied in the z-direction, the Hamiltonian becomes $\hat{H} = -\gamma B_0 \hat{S}_z$. What are the possible values for the energy of the particle? What are the probabilities of finding the respective energies?

c) Explain the three Hund's rules for finding the electronic configuration of the elements.
The Oxygen atom has 8 electrons. Find its electronic configuration. What is the value of global angular momentum L and global spin S? What are the possible values for $\vec{J} = \vec{L} + \vec{S}$? What is the corresponding spectroscopic symbol ${}^{2S+1}L_J$?

d) In a solid, what are the "valence electrons"? What does the Fermi energy represent?
Using the free electron gas model, calculate the Fermi energy for copper, in eV.
Data: for Cu, use q = 1.2 free electrons per atom,
density 8.96 g/cm^3 and atomic weight 63.5 g/mol.