Final test
M Dec 12, 7am-10am

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 \( \hat{p} = -i\hbar \hat{\nabla} \); \( p_x = -i\hbar \frac{\partial}{\partial x} \); \( [x, p_x] = i\hbar \; \); \( \langle p \rangle = m \frac{d\langle x \rangle}{dt} \)

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

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

Generalized uncertainty principle: \( \sigma_x^2 \sigma_p^2 \geq \left| \frac{\langle [A, B] \rangle}{2i} \right| \)

Heisenberg equation of motion \( \frac{d\langle Q \rangle}{dt} = i\hbar \left[ H, Q \right] + \left\langle \frac{\partial Q}{\partial t} \right\rangle \); \( \left[ f(x), p \right] = i\hbar \frac{df}{dx} \)

Harmonic oscillator \( V(x) = \frac{1}{2} m\omega^2 x^2 \); stationary states \( \psi_n, E_n = \left( n + \frac{1}{2} \right) \hbar \omega \)

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

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

Angular momentum
\( |m\rangle = Y^m_{\ell}(\theta, \phi); \; L_z |m\rangle = \hbar m |m\rangle; \; L^2 |m\rangle = \hbar^2 \ell(\ell + 1) |m\rangle; \; \hat{J} = \hat{L} + \hat{S} \)

\( L_z |l\rangle = \hbar \sqrt{(l+1) - m(m+1)} |l \rangle \)
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 \( R = 1.097 \times 10^7 \text{ m}^{-1} \); \( E_i = -\frac{m}{2\hbar^2} \left( \frac{e^2}{4\pi\varepsilon_0} \right)^2 = -13.6 \text{ eV} \)

Solids: Fermi energy \( E_F = \frac{\hbar^2}{2m} \left( 3\rho \pi^2 \right)^{2/3} \) with free electron density \( \rho = \frac{qN}{V} \); \( 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J} \)

Constants: \( h = 1.05 \times 10^{-34} \text{ J s} \); \( m_e = 9.11 \times 10^{-31} \text{ kg} \); \( N_A = 6.02 \times 10^{23} \); \( k_B = 1.38 \times 10^{-23} \text{ J/K} \)

Potentially useful integrals:

\[
\int_0^a \sin^2 \left( \frac{n\pi x}{a} \right) dx = \frac{a}{2}
\]

\[
\int_0^a x \sin \left( \frac{n\pi x}{a} \right) dx = \frac{a^2}{4}
\]

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

\[
\int x \sin \left( ax \right) dx = \left[ \frac{\sin(ax)}{a^2} - \frac{x \cos(ax)}{a} \right]
\]

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

\[
\sum_{n=1,3,5,\ldots} \frac{1}{n^4} = \frac{\pi^4}{96}
\]

Fourier series expansion: \( f(x) = \sum_{n=1}^{\infty} c_n \sin \left( \frac{n\pi x}{a} \right) \) where \( c_n = \frac{2}{a} \int_0^a \sin \left( \frac{n\pi x}{a} \right) f(x) dx \)
TABLE 4.3: The first few spherical harmonics, $Y^m_l(\theta, \phi)$.

<table>
<thead>
<tr>
<th>l</th>
<th>Y^0_0</th>
<th>Y^0_2</th>
<th>Y^1_0</th>
<th>Y^1_2</th>
<th>Y^{1\pm}_3</th>
<th>Y^{3\pm}_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\frac{1}{\sqrt{4\pi}}$</td>
<td>$\frac{1}{\sqrt{8\pi}}$</td>
<td>$\frac{3}{4\pi}$</td>
<td>$\frac{1}{\sqrt{16\pi}}$</td>
<td>$\frac{7}{32\pi}$</td>
<td>$\frac{21}{64\pi}$</td>
</tr>
<tr>
<td>1</td>
<td>$\frac{3}{8\pi}$</td>
<td>$\frac{5}{16\pi}$</td>
<td>$\frac{15}{8\pi}$</td>
<td>$\frac{105}{32\pi}$</td>
<td>$\frac{35}{64\pi}$</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 4.7: The first few radial wave functions for hydrogen, $R_l(r)$.

<table>
<thead>
<tr>
<th>l</th>
<th>R_{10}</th>
<th>R_{20}</th>
<th>R_{21}</th>
<th>R_{30}</th>
<th>R_{31}</th>
<th>R_{32}</th>
<th>R_{40}</th>
<th>R_{41}</th>
<th>R_{42}</th>
<th>R_{43}</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$2a^{-3/2}\exp(-r/a)$</td>
<td>$\frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$</td>
<td>$\frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1</td>
<td>$\frac{2}{\sqrt{27}}a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$</td>
<td>$\frac{8}{27\sqrt{6}}a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\frac{r}{a}\exp(-r/3a)$</td>
<td>$\frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{4}a^{-3/2}\left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$</td>
<td>$\frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$</td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{64\sqrt{5}}a^{-3/2}\left(1 - \frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$</td>
<td>$\frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$</td>
<td></td>
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</tbody>
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TABLE 4.8: Clebsch-Gordan coefficients. (A square root sign is understood for every entry; the minus sign, if present, goes outside the radical.)

```
1/2 x 1/2
1 1/2 1
0 -1/2 -1/2
-1 -1/2 -1/2

1 x 1/2
1/2 1/2
1/2 1/2
1/2 -1/2 -1/2
1/2 -1/2 -1/2

2 x 1/2
3/2 1/2 3/2 1/2
3/2 1/2 3/2 1/2
3/2 -1/2 -3/2 -1/2
3/2 -1/2 -3/2 -1/2

3/2 x 1
5/2 1/2 5/2 1/2
5/2 1/2 5/2 1/2
5/2 -1/2 -5/2 -1/2
5/2 -1/2 -5/2 -1/2
```
1. Schrödinger equation, wave function, expectation values

A particle of mass \( m \) is in the state: 
\[ \Psi(x,t) = \left( \frac{2am}{\pi \hbar} \right)^{1/4} e^{-amx^2/\hbar} e^{-iat} \]

where \( a \) is a positive real constant.

a) Calculate the density of probability \( \rho(x,t) \)

b) Calculate the probability current \( J(x,t) = \frac{i\hbar}{2m} \left( \psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right) \)

Check that \( J(x,t) = \frac{d\rho}{dt} \)

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

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

2. 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 
\[ \Psi(x,0) = \frac{1}{\sqrt{10}} (\psi_1 + 3\psi_2) \]

where \( \psi_n \) are the eigenstates of the Hamiltonian

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

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

c) Calculate \( \langle H \rangle \). Does it depend on time? Explain why or why not

d) Check the Ehrenfest theorem for this particle: 
\[ \frac{d\langle p \rangle}{dt} = \langle -\frac{\partial V}{\partial x} \rangle \]

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

3. Finite square barrier and tunneling

Let’s consider a finite square barrier of size \( 2a \): \( V = V_0 \) for \(-a < x < a \) and \( V = 0 \) outside.
A free particle of energy \( E \), with \( 0 < E < V_0 \) is approaching the barrier from the negative side.

a) Write down the solutions to the Schrödinger equation in each of the three regions

\( (1) \ x < -a , \ (2) \ -a < x < a \) and \( (3) \ x > a \), using coefficients \( k = \frac{\sqrt{2mE}}{\hbar} \) and \( l = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \)

b) Write down the continuity conditions at boundaries \(-a\) and \(+a\)

c) Show that the transmission coefficient is 
\[ T = \left[ 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right) \right]^{-1} \]

d) Calculate \( T \) if the incident particle is an electron of energy \( E = 5eV \) and if the barrier height is \( V_0 = 20eV \) and width \( a = 2nm \)
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 \( \psi_{n\ell m}(r, \theta, \phi) \) in spherical coordinates.

a) Using table 4.3 and 4.7 write the wave function \( \psi_{4\ell 1}(r, \theta, \phi) \)

b) Work out the radial part \( R_{4\ell 1}(r) \) using the recursion formula (up to a normalization constant):

\[
R_{n}(r) = \frac{1}{r} (kr)^{\ell+1} e^{-kr} v(kr) \quad \text{where} \quad v(\rho) = \sum_{j=0}^{\infty} c_{j} \rho^{j} \quad \text{and} \quad c_{j+1} = \frac{2(j + 1 - n)}{(j + 1)(j + 2\ell + 2)} c_{j}
\]

(Express your answer in terms of the wavevector \( k, r \) and \( c_{0} \))

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

d) If the electron would transit from the energy level \( E_{4} \) down to \( E_{2} \), what would be the wavelength of the light emitted? Where in the electromagnetic spectrum would it fall?

e) What do we get when applying \( L^{2}, L_{z}, L_{+}, L_{-}, L_{x} \) and \( L_{y} \) on \( \psi_{4\ell 1} \)?

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

An electron is in the spin state \( \chi_{0} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 1+i \end{array} \right) \) in the basis \( \{ \chi_{s}, \chi_{s} \} \) (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 \( S_{z} \) along \( x \), what is the probability of measuring \( (-\hbar / 2) \)?

b) The electron is brought in the presence of an oscillating field applied in the z-direction.

The Hamiltonian becomes \( \hat{H} = -\gamma B_{0} \cos(\omega t) \hat{S}_{z} \).

Write down the equation of motion for the spinor \( \chi(t) \)

If the spin is initially in the state \( \chi_{0} \), find the state of the spin \( \chi(t) \) at later times.

c) Explain the three Hund’s rules for finding the electronic configuration of the elements.

The Fluorine atom (F) has 9 electrons. Find its electronic configuration.

What is the value of global angular momentum \( L \) and global spin \( S \)?

What are the possible values for \( \bar{J} = \bar{L} + \bar{S} \)?

What is the corresponding spectroscopic symbol \( ^{2S+1}L_{J} \)?

d) In a solid, what does the Fermi energy represent?

Using the free electron gas model, calculate the Fermi energy for iron, in eV.

**Data**: for Fe, use \( q = 1.9 \) free electrons per atom,

density 7.97 g/cm\(^3\) and atomic weight 55.84 g/mol.