Quantum Mechanics Qualifying Exam

August 2019

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Possibly Useful Information

Handy Integrals:

$$\begin{aligned}
\int_0^\infty x^n e^{-\alpha x}\,dx &= \frac{n!}{\alpha^{n+1}} \\
\int_0^\infty e^{-\alpha x^2}\,dx &= \frac{1}{2}\sqrt{\frac{\pi}{\alpha}} \\
\int_0^\infty x\ e^{-\alpha x^2}\,dx &= \frac{1}{2\alpha} \\
\int_0^\infty x^2\ e^{-\alpha x^2}\,dx &= \frac{1}{4}\sqrt{\frac{\pi}{\alpha^3}} \\
\int_{-\infty}^\infty e^{i\,a\,x - b\,x^2}\ dx &= \sqrt{\frac{\pi}{b}} e^{-a^2/4b}
\end{aligned}$$

Spherical Harmonics

$$Y_0^0(\theta,\phi) = \frac{1}{2\sqrt{\pi}}$$

$$Y_1^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \qquad Y_1^{\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{3}{\pi}}\sin\theta e^{\pm i\phi} \qquad Y_1^{\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{3}{\pi}}\sin\theta e^{\pm i\phi}$$

$$Y_2^0(\theta,\phi) = \frac{1}{3}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) \qquad Y_2^{\pm1}(\theta,\phi) = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta e^{\pm i\phi} \qquad Y_2^{\pm2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{\pm 2i\phi}$$

Normalization:

$$\int_0^{2\pi} d\phi \int_0^{\pi} Y_\ell^m(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi)^* \sin\theta\, d\theta = \delta_{m,m'}\delta_{\ell,\ell'}$$

Physical Constants:

Coulomb constant $\mathrm{K} = 8.998 \times 10^9$ N-m$^2/C^2$
$\epsilon_0 = 8.85 \times 10^{-12}\mathrm{C}^2/\mathrm{N}\cdot\mathrm{m}^2$
$\mu_0 = 4\pi \times 10^{-7}$T m/A
electronic charge $e = 1.60 \times 10^{-19}$C
electronic mass $m_e = 9.11 \times 10^{-31}$kg
Atomic mass unit: 1.66×10^{-27}kg.
Boltzmann's constant: $k_B = 1.38 \times 10^{-23}$J/K
Planck's constant: $\hbar = 1.054 \times 10^{-34}\mathrm{m}^2\mathrm{kg/s}$
speed of light: $c = 3.00 \times 10^8$m/s
Ideal Gas Constant: $R = 0.0820\,\ell\mathrm{atm}\cdot\mathrm{mol}^{-1}\mathrm{K}^{-1}$
Gravitaional Constant: $6.67 \times 10^{-11}\mathrm{J}\cdot\mathrm{m}\cdot\mathrm{kg}^{-2}$

1. **One dimensional scattering**

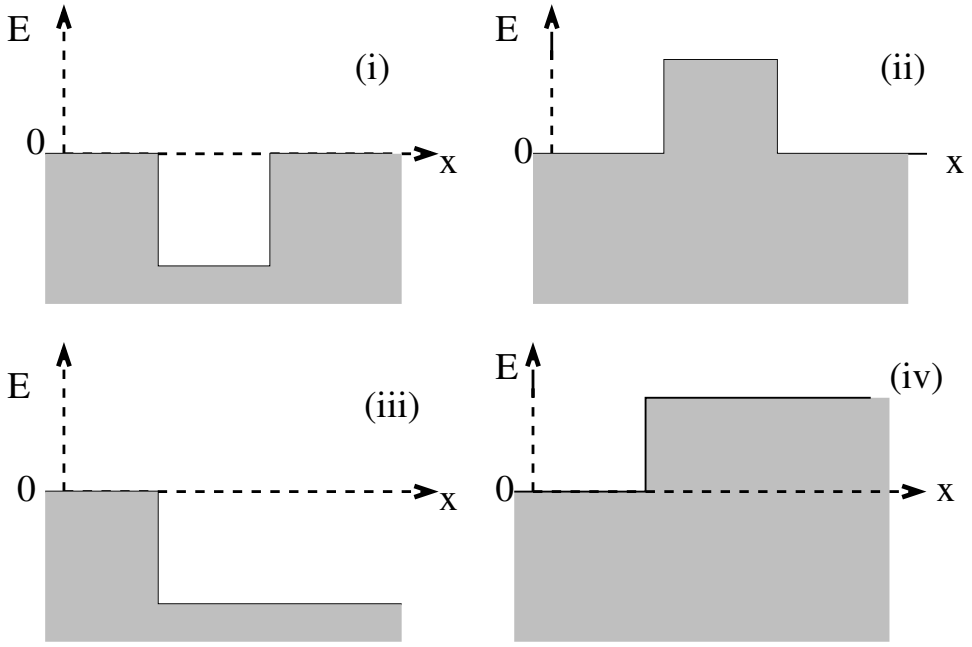

Figure 1: One dimensional potential energy functions.

Please answer the following questions about the figures above. All figures that you draw should be on your answer sheet and not on this page. In all cases we start with a plane wave beam of free, independent particles incident from the left with total energy $E_0 > 0$ and incident wavelength λ_0. For parts (a)-(c) in which you are asked to plot the wave function you should provide qualitatively accurate results and ignore scattering resonances. For parts (d)-(f) express your answers in terms of E_0 and λ_0.

(a) Sketch the real part of the wave function for the plane wave solution for the case (i), where the depth of the well is $-3E_0$ and its width is λ_0. (1 point)

(b) Sketch the real part of the wave function for the plane wave solution for the case (ii), where the height of the barrier is $E_0/2$ and its width is λ_0. (1 point)

(c) Sketch the real part of the wave function for the plane wave solution for the case (ii), where the height of the barrier is $3E_0$ and its width is λ_0. (1 point)

(d) For case (iii), what fraction of incident particles are found to the right of the step potential when the step height (down) is $-3E_0$? (3 points)

(e) For case (iv), what fraction of incident particles are found to the right of the step potential when the step height is $E_0/2$? (2 points)

(f) For case (iv) what is the square of the amplitude of the wave function to the right of the step (as a function of x) when the step height is $3E_0$? What does this quantity mean? (2 points)

2. **States of a Model Three Atom Molecule**

In this problem, we consider a model of a simple, co-linear, 3-atom molecule with one valence electron. We initially separate the atoms far apart so that the electron can be localized to the left atom, the center atom or the right atom. We will label the three states of the system $|L\rangle$, $|C\rangle$, and $|R\rangle$, respectively. Call this the LCR basis of states.

(a) First, we need to specify the eigenenergies of the different localized states before the atoms are brought together to form a molecule. In this model the eigenenergy of the states $|L\rangle$ and $|R\rangle$ is ϵ, and the eigenenergy of state $|C\rangle$ is equal to 0. Write down the Hamiltonian matrix (call it H_0) for the system in the LCR basis. (1 point)

(b) The Hamiltonian H_0 neglects all interactions that occur when the atoms are brought together to form the molecule. Assume that when the atoms are brought together, there is a nearest neighbor coupling interaction V between the states described by:

$$V|L\rangle = \gamma|C\rangle, \quad V|R\rangle = \gamma|C\rangle. \tag{1}$$

and

$$\langle i|V|i\rangle = 0 \tag{2}$$

for all three states $|i\rangle = LCR$.

Write down the matrix for this interaction in the LCR basis. Note that the interaction and total Hamiltonian are Observables. (1 point)

(c) What are the eigenenergies of the full Hamiltonian, $H_0 + V$? Show that your answer reduces to the correct result in the limit as $\gamma \to 0$. (3 points)

(d) Consider the case were the coupling between the atoms is of the same magnitude as H_0: $\gamma = \epsilon$. What are the energy eigenvalues of the full Hamiltonian? What are the eigenstates in the LCR basis? (3 points)

(e) For the case where $\gamma = \epsilon$, if the electron in the *coupled* system is initially prepared in the state $|C\rangle$ and the energy is measured, what are the possible outcomes of the measurement and their probabilities? Answer this same question for an electron initially prepared in the state $|R\rangle$. (2 points)

3. **Spin 1/2 systems**

Consider a spin half particle. The basis states for describing the wave function are denoted by $|+\rangle$ and $|-\rangle$ which are the spin up and spin down eigenstates of the spin along the $\hat{z}-$direction.

You build an apparatus that can measure the spin of the particle in any arbitrary direction $\hat{z'}$, where $\hat{z'}$ is a unit vector given by the usual polar and azimuthal angles $\hat{z'} = \sin\theta\cos\phi\hat{x} + \sin\theta\sin\phi\hat{y} + \cos\theta\hat{z}$.

(a) If your apparatus were to measure the spin along this arbitrary direction $\hat{z'}$, what range of values in units of $\hbar$ could you possibly obtain? Please provide an explicit derivation. (2 points)

(b) Suppose your apparatus now actually measures the spin along the $\hat{z'}$ direction and gives you an answer $+\hbar/2$. This act of measurement changes the state of the particle, putting it into a state $|\psi\rangle$. Express $|\psi\rangle$ in terms of $|+\rangle$ and $|-\rangle$. (6 points)

(c) Now the particle is in state $|\psi\rangle$. You ask your apparatus to measure the spin in the original $\hat{z}$ direction. What is the probability that the answer will be $+\hbar/2$? (2 points)

4. The Hamiltonian for an electron in a 3D hydrogen-like atom can be written as:

$$H\psi = \left\{ -\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{Ze^2}{r} \right\} \psi(\vec{r}) = E\,\psi(\vec{r})$$

where we have approximated the reduced mass by the electron mass, m. Performing separation of variables in spherical coordinates $\psi(\vec{r}) = R_{n\ell}(r)\,Y_\ell^m(\theta,\phi)$ yields the radial equation

$$\left\{ -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2} \right) - \frac{Ze^2}{r} \right\} R_{n\ell}(r) = E\,R_{n\ell}(r)$$

which has eigenenergies $E_n = -w_0 Z^2/n^2$ in which

$$w_0 = \frac{me^4}{2\hbar^2} = \frac{e^2}{2a_0}$$

is the groundstate energy of the hydrogen atom and a_0 is the Bohr radius. The normalized radial functions $R_{n\ell}(r)$ are given below.

Lithium has an atomic number $Z = 3$, so that doubly ionized lithium has a single electron and can be treated as a hydrogen-like atom. There is an unstable isotope of lithium that decays via the emission of a proton to helium. After the emission the nucleus has an atomic number $Z' = 2$. Assume this process happens instantaneously, and ignore both recoil and the change in the reduced mass. If a single electron starts in the groundstate of the lithium ion then:

(a) What is the probability that it ends up in the ground state of the helium ion? (2 points)

(b) What is the probability that it ends up in the $n = 2$ and $\ell = 1$ state of the helium ion? (2 points)

(c) What is the probability that it ends up in the $n = 2$ and $\ell = 0$ state of the helium ion? (2 points)

(d) What is the expectation value of the energy the instant after the transition? If it is the same as the energy before the transition, prove why it must be the same. If it is different, calculate this expectation value. (4 points).

$$\begin{aligned}
R_{1,0}(r) &= \left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0} \\
R_{2,0}(r) &= \left(\frac{Z}{2a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0} \\
R_{2,1}(r) &= \left(\frac{Z}{2a_0}\right)^{3/2} \frac{1}{\sqrt{3}} \frac{Zr}{a_0} e^{-Zr/2a_0}
\end{aligned}$$

5. **Half-harmonic oscillator:**

An electron is subject to the potential:

$$V(x) = \begin{cases} \frac{1}{2}\, k\, x^2 & \text{for } x > 0 \\ \\ \infty & \text{for } x \leq 0 \end{cases}$$

The time-independent Schrodinger equation:

$$H\psi(x) = \left\{ -\frac{\hbar^2}{2m}\, \frac{\partial^2}{\partial x^2} \, + V(x) \right\} \psi(x) = E\, \psi(x)$$

can be written in terms of the dimensionless variable, $s = x\sqrt{m\omega/\hbar}$

$$h\psi(s) = \left\{ -\frac{1}{2}\, \frac{\partial^2}{\partial s^2} \, + v(s) \right\} \psi(s) = \epsilon\, \psi(s)$$

where $\epsilon = E/(\hbar\omega)$, and $\omega = \sqrt{k/m}$. The potential $v(s)$ is

$$v(s) = \begin{cases} \frac{1}{2}\, s^2 & \text{for } s > 0 \\ \\ \infty & \text{for } s \leq 0 \end{cases}$$

We will try a variational guess at the ground state,

$$\phi(x; a) = c\, s\, e^{-a\, s/2}$$

where a is a variational parameter and c is a normalization constant.

(a) Prove that *in general* any variational wave function $\phi(x; a)$ will have an energy bounded below by the true ground state energy, if a ground state energy exists. (2 points)

(b) Determine the constant c so that $\phi(x; a)$ is normalized. (1 point)

(c) Determine the optimal value of a that makes $\phi(x; a)$ the best approximation to the ground state. (4 points)

(d) Determine the value of the energy for this best approximation. (1 point)

(e) Given that we know the analytical solution of the full 1D harmonic oscillator, we can readily determine the ground state solution of the half-oscillator since the first excited state of the full harmonic oscillator will have a node at $x = 0$. Compare the energy of the exact solution and your best approximation above. (2 points)

6. **Harmonic Oscillator**

(a) A particle of mass m is subject to a potential $V(x) = \frac{1}{2}kx^2$. One of the energy eigenstates (unnormalized) is sketched below. Is this the ground state, first excited state, second excited state, or the third? Explain your answer. (1 point)

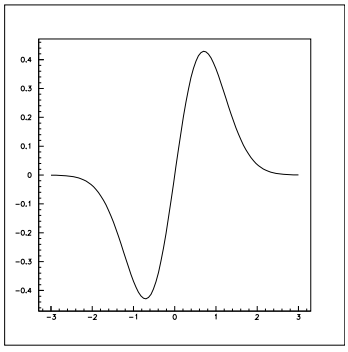

Figure 2: Energy Eigenstate

(b) A simple harmonic oscillator is in the ground state. An instantaneous force imparts momentum p_o to the system such that the new state vector is given by $|\Psi\rangle = e^{-ip_0\hat{x}/\hbar}|0\rangle$, where $|0\rangle$ is the ground state of the original oscillator. What is the probability that the system will stay in its ground state? (3 points)

(c) A particle of mass m in a one dimensional harmonic oscillator potential is in a state for which a measurement of the energy yields the values $\hbar\omega/2$ or $3\hbar\omega/2$, each with a probability of 1/2. The average value of the momentum at time t=0 is $\sqrt{m\omega\hbar/2}$. This information specifies the state of the particle completely. What is this state at time t? (3 points)

(d) A 1-dimensional harmonic oscillator is, at time t=0, in the state

$$|\Psi(t=0)\rangle = \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle)$$

where $|n\rangle$ is the n_{th} energy eigenstate. Find the expectation value of the position and energy at time t. (3 points)