# UNIVERSITY OF MARYLAND Department of Physics College Park, Maryland

## Ph.D. PHYSICS QUALIFYING EXAMINATION - PART II

January 20, 2012 9 a.m. - 1 p.m.

Do any four problems. Each problem is worth 25 points.

Put all answers on your answer sheets.

Be sure your Qualifier ID Number is at the top right corner of each sheet and turn in solutions to four problems only. If five solutions are turned in we will grade #1 - #4.

Consider a particle of mass m moving in one dimension along the positive z-axis and experiencing a constant gravitational force F from the earth. The surface of the earth at z=0 is impenetrable and represented by an infinite potential barrier. The classical Hamiltonian is

$$H = \frac{p_z^2}{2m} + Fz, \qquad z > 0.$$

- (a) [2 points] Write down the corresponding time-independent Schrödinger equation for the wavefunction  $\psi(z)$  of the particle and sketch the confining potential V(z).
- (b) [2 points] State the boundary conditions on  $\psi(0)$  and  $\psi(\infty)$  that the wavefunction must obey at z=0 and  $z=\infty$ .

How many bound states are possible? Are there any unbound states?

- (c) [9 points] Using the variational method, find approximate expressions for the ground-state energy  $E_1$  and the ground-state wavefunction  $\psi_1(z)$ . Take the variational wavefunction of the form  $\psi(z) = Cz \exp(-z/l)$ , where C is a normalization constant, and l is a variational parameter. Determine the optimal value  $l_1$  of the variational parameter in terms of F, m, and the Planck constant  $\hbar$ . What is the dimensionality and the physical meaning of  $l_1$ ? Verify that your answers for  $l_1$ ,  $E_1$ , and  $\psi_1(z)$  have correct dimensionality.
- (d) [2 points] Now let us investigate excited energy states. First, consider classical motion of the particle with an energy E > 0. Determine the turning point  $z_t$ , which is a maximum value of z beyond which the particle cannot go for the given energy E. Then, qualitatively describe behavior of the wavefunction  $\psi_E(z)$  in the classically-permitted and classically-forbidden regions  $z < z_t$  and  $z > z_t$ . Sketch  $\psi(z)$  for the ground state and the first two excited states, paying attention to the different behavior for  $z < z_t$  and  $z > z_t$ .
- (e) [8 points] Determine the highly excited energy levels  $E_n$  using the quasiclassical WKB approximation. Use the Bohr-Sommerfeld quantization condition in the form

$$\int_0^{z_t} p_z(z) \, dz = \pi \hbar \left( n - \frac{1}{4} \right), \qquad n = 1, 2, 3, \dots$$

Explain briefly and qualitatively why the right-hand side of this equation for our problem contains (n-1/4), rather than the more common expression (n-1/2).

(f) [2 points] Verify that your answer for  $E_n$  has correct dimensionality.

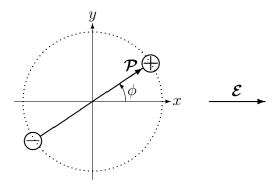
Verify that your answers for  $E_1$  from the variational method and from the WKB approximation agree by the order of magnitude (i.e. up to numerical coefficients).

State briefly and qualitatively for which energy levels  $E_n$  the WKB approximation is applicable.

Useful integral:  $\int_0^\infty x^n e^{-x/a} dx = n! a^{n+1}$ .

A diatomic molecule with moment of inertia I is constrained to rotate freely in the xy plane with angular momentum  $L_z$ . The molecule has a permanent electric dipole moment  $\mathcal{P}$  along the molecule axis, whose magnitude  $\mathcal{P}_0$  is independent of the rotational motion or external conditions. The Hamiltonian for the quantum system is

$$\hat{H} = \frac{(\hat{L}_z)^2}{2I}.\tag{1}$$



- (a) [4 points] The orientation of the dipole moment  $\mathcal{P}$  relative to the x axis is specified by the angle  $\phi$  as shown in the figure. Write down Hamiltonian (1) in the  $\phi$  representation and obtain the energy eigenvalues  $E_n$  and eigenfunctions  $\psi_n(\phi)$ . What is the degeneracy of each eigenstate?
- (b) [2 points] Now a weak uniform electric field  $\mathcal{E} = \mathcal{E}_0 \hat{e}_x$  is applied to the system along the x axis. Write down the new Hamiltonian for the system in terms of  $\phi$ , taking into account that the electric field  $\mathcal{E}$  couples to the dipole moment  $\mathcal{P}$ .
- (c) [5 points] Use perturbation theory to calculate the shifts of the energy eigenvalues to first order in  $\mathcal{E}_0$ . Does the perturbation lift the degeneracy to first order in  $\mathcal{E}_0$ ?
- (d) [6 points] Use perturbation theory to calculate the corresponding perturbed wave functions to first order in  $\mathcal{E}_0$ .
- (e) [5 points] Evaluate the expectation value  $\langle \mathcal{P}_x \rangle$  of the x component of the dipole moment operator  $\mathcal{P}$  in each energy eigenstate, and thereby deduce the electric polarizability

$$\alpha = \langle \mathcal{P}_x \rangle / \mathcal{E}_0 \tag{2}$$

of each state.

(f) [3 points] Provide a physical explanation for the difference in the signs of  $\alpha$  for the lowest energy eigenstate and the other states. (Hint: Classically, would the dipole spend more time aligned or anti-aligned with the applied field?)

A beam of electrons of mass m and energy  $E = \hbar^2 k^2/2m$  scatters off a homonuclear diatomic molecule, i.e., a molecule consisting of two identical atoms, separated by the distance a. Ignore recoil, vibration, and rotation of the molecule, and assume that it has a fixed position in space with a fixed vector a connecting the two atoms. Also assume that the state of the molecule does not change upon scattering, i.e., the scattering is elastic. Ignore the electron spin as well.

Suppose one atom produces a spherically-symmetrical potential  $U_0(r)$ , where r is the distance from the center of the atom. Then, the potential produced by the two atoms in the molecule is

$$U(\mathbf{r}) = U_0(r) + U_0(|\mathbf{r} - \mathbf{a}|). \tag{1}$$

This problem asks you to express scattering properties of the two-atom potential in terms of scattering properties of the single-atom potential using the Born approximation.

- (a) [4 points] Write down a formula for the scattering amplitude  $f_0(q)$  on the single-atom potential  $U_0(r)$  in the Born approximation. Here  $\mathbf{q} = \mathbf{k}' \mathbf{k}$  is the change of the electron wavevector from  $\mathbf{k}$  to  $\mathbf{k}'$  upon scattering. Express q in terms of k and the scattering angle  $\theta$ .
- (b) [4 points] Now obtain a formula for the scattering amplitude f(q) on the two-atom potential (1) in the Born approximation in terms of  $f_0(q)$  and  $\boldsymbol{a}$ .
- (c) [4 points] Express the differential cross-section of scattering on the molecule,  $d\sigma/d\Omega$ , in terms of the corresponding cross-section  $d\sigma_0/d\Omega$  for a single atom in the Born approximation.
- (d) [4 points] The orientation of the molecular axis is determined by the unit vector  $\mathbf{n} = \mathbf{a}/a$ . So far, we assumed that the vector  $\mathbf{n}$  has a fixed orientation. Now assume that the molecular axis orientations are random, and different orientations appear with equal probability. Average the differential cross-section of scattering over random orientations of  $\mathbf{n}$  and obtain the averaged cross-section  $\overline{d\sigma/d\Omega}$ .
- (e) [3 points] In the Born approximation, write down a general formula for the total cross-section of scattering on the single-atom potential,  $\sigma_0$ .
- (f) [3 points] Now assume that electrons have low energy, so that  $ka \ll 1$ , but the Born approximation is still applicable. Express the total cross-section of scattering on the molecule,  $\sigma$ , in terms of  $\sigma_0$ . Does it matter in this limit whether the orientation of the molecule is fixed or random?
- (g) [3 points] Now consider the high-energy limit where  $ka \gg 1$ , and also assume that the range  $r_0$  of the potential  $U_0(r)$  is much shorter than the interatomic distance a:  $r_0 \ll a$ . Express the total cross-section of scattering on the molecule,  $\sigma$ , in terms of  $\sigma_0$ . Does it matter in this limit whether the orientation of the molecule is fixed or random?

Consider a system consisting of two particles, A and B, each of spin 1. The two particles may form a bound state, which we treat as a composite particle C. The states of the particles are represented in the basis  $|j,m\rangle_{A,B,C}$ , where j and m are the quantum numbers of the angular momentum and its projection on the z axis, and the index A, B, or C indicates the particle. In this problem, assume conservation of angular momentum. Consider only the spin angular momentum of the particles and ignore the orbital angular momentum and the spatial part of the wave functions.

The particles A and B are bosons. Consider two cases: (i) the particles A and B are distinguishable (i.e. different), (ii) the particles A and B are indistinguishable (i.e. identical).

- (a) [5 points] Given that  $j_A = 1$  and  $j_B = 1$ , what are the possible values of the angular momentum  $j_C$  of the composite particle C? Answer the question in the two cases (i) and (ii). In the latter case, discuss the symmetry of the composite wave function with respect to interchange of the particles A and B.
- (b) [5 points] Suppose the Hamiltonian of the system is

$$\hat{H} = a \, (\hat{J}_{z,C})^2,$$

where  $\hat{J}_{z,C} = \hat{J}_{z,A} + \hat{J}_{z,B}$  is the z component of the angular momentum operator of the composite particle C, and a is a coefficient.

What are the eigenvalues of the Hamiltonian, and what are their degeneracies? Answer the question in the two cases (i) and (ii).

(c) [7 **points**] Suppose initially one of the particles A and B is in the state  $|1,1\rangle$  and another in the state  $|1,-1\rangle$ . Then, these particles combine to form the particle C. What are the possible states  $|j,m\rangle_C$  of the composite particle C in this case? What are the probabilities of finding the particle C in these states?

Answer the question in the two cases (i) and (ii). In the latter case, write down the properly symmetrized wavefunction of the initial state of the particles A and B.

(d) [8 points] Suppose the particle C is in the state  $|0,0\rangle_C$ . Suppose it is a metastable state, and the particle C decays to particles A and B. Write down the wavefunction of the two-particle system  $|\psi\rangle_{AB}$  in the basis of the states  $|1, m_1\rangle_A |1, m_2\rangle_B$ . What are the permitted combinations of the numbers  $m_1$  and  $m_2$  in this case? What are the probabilities of finding the particles A and B in these states?

Is it possible to write the wavefunction  $|\psi\rangle_{AB}$  of the two-particle system as a product  $|\psi\rangle_{A}|\psi\rangle_{B}$  in this case? If not, such a state is called an entangled state. Entangled states play important role in quantum information and quantum computing.

Suppose a measurement finds the particle A in the state  $|1,1\rangle_A$ . Then, what are the possible states  $|1,m\rangle_B$  of the particle B? Is there any uncertainty in the state of the particle B, once the state of the particle A has been measured?

See next page for useful equations

### II.4 (Continued)

Information about selected Clebsch-Gordan coefficients:

$$\begin{split} |1,1\rangle|1,-1\rangle &= \sqrt{\frac{1}{6}}\,|2,0\rangle + \sqrt{\frac{1}{2}}\,|1,0\rangle + \sqrt{\frac{1}{3}}\,|0,0\rangle \\ |1,-1\rangle|1,1\rangle &= \sqrt{\frac{1}{6}}\,|2,0\rangle - \sqrt{\frac{1}{2}}\,|1,0\rangle + \sqrt{\frac{1}{3}}\,|0,0\rangle \\ |0,0\rangle &= \sqrt{\frac{1}{3}}\,|1,1\rangle|1,-1\rangle - \sqrt{\frac{1}{3}}\,|1,0\rangle|1,0\rangle + \sqrt{\frac{1}{3}}\,|1,-1\rangle|1,1\rangle \end{split}$$

The 2011 Nobel Prize in physics was awarded for measurements of supernova radiation showing that the universe is expanding faster now than it was in the past. This acceleration is impossible in Newtonian gravity because gravity is always attractive. In General Relativity, however, the source of gravitational force is not just mass-energy (which is always positive) but also pressure, which can be negative. Thus negative pressure of an all-pervasive "dark energy" that fills the universe uniformly can produce the accelerated expansion.

This problem explores a semi-Newtonian model of this phenomenon. In this model, the gravitational force on a test mass m is given by  $m\mathbf{g}$ , and the gravitational acceleration vector  $\mathbf{g}$  satisfies the equation

$$\nabla \cdot \mathbf{g} = -4\pi G(\rho + 3P)/c^2,\tag{1}$$

where  $\rho$  is the source's energy density, P is its pressure, G is Newton's constant and c is the speed of light. The combination  $\rho + 3P$  comes from General Relativity and the three dimensions of space.

- (a) [5 points] Choose an arbitrary center of spherical symmetry, and find the spherically symmetric solution of equation (1) for g(r) assuming constant values  $\rho$  and P.
- (b) [5 points] Consider two test particles that start out at rest with respect to each other at t=0 in the field  $\mathbf{g}(\mathbf{r})$  you found in the previous part. Find the time dependence of their separation vector  $\mathbf{s}(t) = \mathbf{r}_2(t) \mathbf{r}_1(t)$  under the influence of the gravitational force, and show that the separation grows exponentially if  $\rho + 3P$  is negative. Use the non-relativistic Newton's equations of motion,  $\mathbf{F} = m\mathbf{a}$ .
- (c) [5 points] The equation of state of the dark energy is such that its energy density  $\rho$  and pressure P are constant everywhere and for all times. Use energy conservation to find a relation between  $\rho$  and P: As the universe expands uniformly in all directions, any volume V of space expands by an amount dV, creating more dark energy, so its vacuum energy increases by an amount  $\rho dV$ . Use the first law of thermodynamics to relate this to the work done on the growing volume, and so determine the pressure P in terms of the energy density  $\rho$ . (Gravity plays no role in this energy balance since V can be taken to be arbitrarily small.) You should find that if  $\rho$  is positive then  $\rho+3P$  is negative, so the dark energy produces accelerated expansion. Note: negative pressure means the force on an area is opposite to that produced by a conventional ideal gas filling a volume.
- (d) Constant dark energy density and pressure need not single out any preferred rest frame. Let's see how this can be, according to special relativity. (More direct ways than steps i.-iii. to arrive at iv. are also possible.)
  - i. [3 points] As a warm up, first consider the simpler case of a uniform electric charge density  $n_{\rm e}$  and current density  $j_{\rm e}^x$  in the x-direction. Find the charge density  $n_{\rm e}'$  in another reference frame moving with relative velocity v in the x-direction. Show that there is no choice of  $n_{\rm e}$  and  $j_{\rm e}^x$  such that, for all v,  $n_{\rm e}=n_{\rm e}'$ . Hint: Charge and current densities are components of a 4-vector.

- ii. [3 points] Suppose there is a dark energy density  $\rho$  in a given frame, and no momentum density, energy current, or pressure. What would be the energy density  $\rho'$  in another frame moving with relative velocity v in the x direction? Hint: Electric charge is a scalar, but energy is the time component of a 4-vector. Energy density changes because energy changes and because volume changes.
- iii. [3 points] Pressure in the x-direction can be thought of as the current density of x component of momentum in the x-direction. If we had nothing but isotropic pressure P in a given frame (with no energy density, momentum density, or energy current) what would be the energy density  $\rho'$  in another frame moving with relative velocity v in the x-direction?
- iv. [1 point] Now combine the previous two parts to see what is  $\rho'$  when there is both  $\rho$  and P. Show that the dark energy density is the same in all frames if and only if  $P = -\rho$ , which is the same condition inferred in part (c) using energy conservation!