UNIVERSITY OF MARYLAND
Department of Physics
College Park, Maryland

Ph.D. PHYSICS QUALIFYING EXAMINATION - PART II

August 26, 2011 **9 a.m. - 1 p.m.**

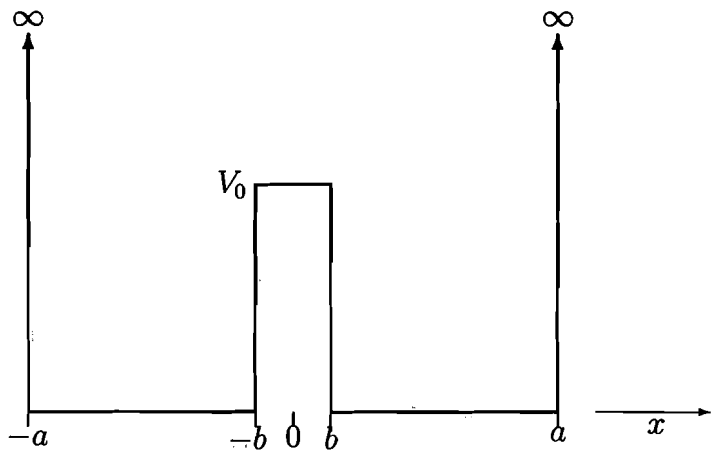
Do any four problems. Each problem is worth 25 points.

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.

Problem II.1

The goal of this problem is to find the wave functions for stationary eigenstates of a particle with mass m and energy $E < V_0$ in the one dimensional potential well shown below. It has infinite barriers at $x = +a$ and $-a$. In the middle of the well, there is a barrier of height V_0 and width $2b$ between $x = -b$ and $x = b$, centered at $x = 0$.



(a) **[5 points]** The wave functions $u(x)$ of the eigenstates may be assumed to be real and non-degenerate. Hence show that they will have definite parity, that is, $u(x)$ is an even or an odd function of x.

(b) **[5 points]** What are the boundary conditions that $u(x)$ must satisfy at the boundaries $x = \pm a$, and the continuity conditions at $x = \pm b$?

(c) **[5 points]** Answer the following questions separately for the even and the odd case:

Represent the wave function $u_e(x)$ (or $u_o(x)$) by different functions in the two outer regions ($|x| > b$) and the inner region ($|x| < b$). Write the wave function in the outer region, $x > b$, that satisfies the boundary condition at $x = a$ in terms of the wave vector k, which is related to the energy E by $E = \hbar^2 k^2/(2m)$, and a normalization constant A. (Parity then determines $u(x)$ for $x < -b$.)

Similarly for the inner region write the wave function in terms of $\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)$ and a normalization constant B.

(d) **[5 points]** Use the continuity conditions at $x = b$ to eliminate A and B, and obtain a relation between k and κ that could be solved for the energy E (but do not attempt to solve this transcendental equation).

(e) **[5 points]** Consider the limit $b \to 0$, $V_0 \to \infty$ in a manner such that $2bV_0 \to \Omega$, where Ω is finite, and the energy E remains finite. There are still solutions of even parity and odd parity, but the limit becomes complicated for even parity solutions. Therefore find only the solutions for odd parity explicitly. Find the quantization condition for k, and the corresponding energy eigenvalues.

Problem II.2

A simple model for electron states in an ordered solid crystal uses the Schrödinger equation with a one-dimensional periodic potential $V(x+a) = V(x)$. The energy eigenfunctions in such a periodic potential can be written in the form

$$\psi_k(x) = u_k(x)\, e^{ikx}, \qquad u(x+a) = u(x), \tag{1}$$

where k is a quantum number called the quasi-momentum, and $u(x)$ is a periodic function with the same period a as the potential $V(x)$. (Eq. (1) is known as Bloch's theorem in physics and Floquet's theorem in mathematics.) Introducing the wavenumber $q = 2\pi/a$ and expanding $u(x)$ into a Fourier series, Eq. (1) can be rewritten as

$$\psi_k(x) = e^{ikx} \sum_{n=-\infty}^{+\infty} c_n e^{inqx}, \qquad q = 2\pi/a, \tag{2}$$

where c_n are Fourier coefficients with the integer index n.

In this problem, we apply this general theory to the special case where the periodic potential is $V(x) = 2W\cos(qx)$, so that the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_k(x)}{\partial x^2} + 2W\cos(qx)\,\psi_k(x) = E_k\,\psi_k(x). \tag{3}$$

and m is the mass of the electron.

(a) **[4 points]** By substituting Eq. (2) into Eq. (3) and equating the coefficients in front of the exponential terms $e^{ikx+inqx}$ for each n, obtain a recursive relation between the coefficients c_n with different n.

The wavefunction (2) is completely characterized by the set of c_n, so $\psi_k(x)$ can be represented as a vector $|\psi\rangle_k = (\ldots, c_{-2}, c_{-1}, c_0, c_1, c_2, \ldots)$. (To save space and simplify notation, we will write such vectors both as rows and columns.) Show that the recursive relation between the coefficients c_n can be written in matrix form as

$$\begin{pmatrix} \ddots & W & 0 & 0 & 0 \\ W & \frac{\hbar^2(k-q)^2}{2m} & W & 0 & 0 \\ 0 & W & \frac{\hbar^2k^2}{2m} & W & 0 \\ 0 & 0 & W & \frac{\hbar^2(k+q)^2}{2m} & W \\ 0 & 0 & 0 & W & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ c_{-1} \\ c_0 \\ c_1 \\ \vdots \end{pmatrix} = E_k \begin{pmatrix} \vdots \\ c_{-1} \\ c_0 \\ c_1 \\ \vdots \end{pmatrix}. \tag{4}$$

(b) **[4 points]** Now let us assume that W is small and can be treated using perturbation theory. First, let us use non-degenerate perturbation theory. The energy eigenvector $|\psi\rangle_k = |\psi\rangle_k^{(0)} + |\psi\rangle_k^{(1)}$ can be written as a sum of the unperturbed term $|\psi\rangle_k^{(0)}$ and the first-order correction $|\psi\rangle_k^{(1)}$. The unperturbed term $|\psi\rangle_k^{(0)}$ has $c_0 = 1$ and $c_{n\neq 0} = 0$, i.e. $\psi_k^{(0)}(x) = e^{ikx}$. Using first-order non-degenerate perturbation theory in W, find the coefficients c_n in $|\psi\rangle_k^{(1)}$. Using these coefficients, write down the wavefunction $\psi_k(x) = \psi_k^{(0)}(x) + \psi_k^{(1)}(x)$ to the first order in W.

II.2 (Continued)

(c) **[4 points]** Now study the eigenenergy corrections $E_k = E_k^{(0)} + E_k^{(1)} + E_k^{(2)}$ using non-degenerate perturbation theory in W. Here the unperturbed term is $E_k^{(0)} = \hbar^2 k^2/2m$. Calculate the first- and the second-order correction terms $E_k^{(1)}$ and $E_k^{(2)}$.

(d) **[4 points]** Observe that non-degenerate perturbation theory produces formally divergent results when $k \to \pm q/2$. What is the origin of this divergence? Plot the diagonal elements of the matrix (1) as a series of displaced parabolas vs. k. What is the significance of the intersection points between these parabolas?

(e) **[5 points]** When $k \to \pm q/2$, some diagonal elements in the matrix (1) become equal, so we must to use a degenerate perturbation theory instead of the non-degenerate one. Let us focus specifically on $k \to q/2$. In this case, we can truncate the infinite matrix (1) to a 2×2 matrix involving only the coefficients c_0 and c_{-1}, because the other terms are non-degenerate:

$$\begin{pmatrix} \frac{\hbar^2(k-q)^2}{2m} & W \\ W & \frac{\hbar^2 k^2}{2m} \end{pmatrix} \begin{pmatrix} c_{-1} \\ c_0 \end{pmatrix} = E_k \begin{pmatrix} c_{-1} \\ c_0 \end{pmatrix} \qquad \text{for} \quad k \approx q/2. \tag{5}$$

To simplify the equations, introduce the deviation $\delta k = k - q/2$ and expand the diagonal terms of the matrix (5) to the first order in δk. Then, diagonalize the matrix (5) and obtain two energy eigenvalues $E_k^{\pm}$. Sketch the two energies as functions of δk. Does the difference $E_k^+ - E_k^-$ ("the energy gap") go to zero at some value of k, or does it remain non-zero?

(f) **[4 points]** Now, qualitatively generalize your consideration to the other degenerate points of the matrix (1), i.e. the points where the displaced parabolas, representing the diagonal matrix elements, intersect. Qualitatively sketch the energy eigenvalues E_k vs. k by modifying your original sketch due to the effect of non-zero W.

Briefly discuss the implications of your results for the electronic properties of solids. What is the difference in the electronic energy spectrum between metals and insulators?

Problem II.3

Consider a monoenergetic beam of neutrons of mass m and energy E moving in the x direction and normally incident on a block of ferromagnetic material. The material fills the entire $x > 0$ region and has a uniform internal magnetic field $\boldsymbol{B}$ of strength B_0 in the positive z direction. The spin of the neutrons is $s = 1/2$, and their magnetic moment is $\gamma \boldsymbol{S}$. The spin-independent part of the potential energy of the neutrons is represented by $V(x) = 0$ for $x \leq 0$ in vacuum and by $V(x) = V_0 > 0$ for $x > 0$ inside the material.

(a) **[2 points]** Write the Hamiltonian for the neutrons inside the magnetized material and sketch the potential energy of the neutrons with spins up and down as a function of the coordinate x from $-\infty$ to $+\infty$.

(b) **[5 points]** Show that the wave functions $\psi_+(x)$ for the spin-up neutrons and $\psi_-(x)$ for the spin-down neutrons satisfy the following equation for $x > 0$:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0 \mp \frac{\hbar\omega_0}{2}\right)\psi_\pm(x) = E\,\psi_\pm(x),$$

where $\omega_0 = \gamma B_0$.

(c) **[5 points]** Write down the general solutions for the wave functions $\psi_\pm(x)$ for both regions $x < 0$ and $x > 0$ for the special case where $V_0 - \hbar\omega_0/2 < E < V_0 + \hbar\omega_0/2$. Indicate this position of E on your sketch made in Part (a).

Hint: The problem is closely analogous to the case of a one-dimensional reflection from a potential step.

(d) **[10 points]** Using the continuity conditions at $x = 0$, solve for the ratio of constants needed in the general wave functions you wrote down in Part (c). Calculate the reflection coefficients $R_\pm$ for neutrons with spins up and down in terms of m, E, V_0, and ω_0:

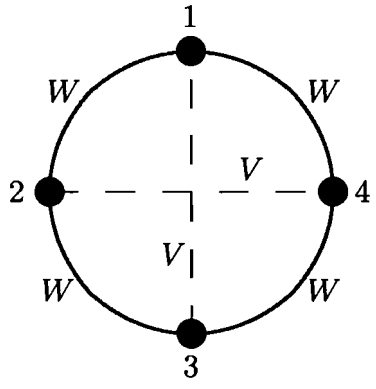
$$R_\pm = \left|\frac{B_\pm}{A_\pm}\right|^2,$$

where $A_\pm$ and $B_\pm$ represent the amplitudes of the incident and reflected plane waves in the neutron wave function.

(e) **[3 points]** Suggest how the result from Part (d) could be utilized in a neutron scattering experiment.

Problem II.4

Consider a molecule consisting of four identical atoms arranged in a ring (see Figure). We study the energy spectrum and the energy eigenfunctions of an electron in this molecule and the symmetry of these wavefunctions, ignoring the electron spin.



Let us label the four atoms by the index $j = 1, 2, 3, 4$, as shown in the Figure. Then ψ_j is the wavefunction of the electron on the atom j, and the electron state is described by the 4-component vector $|\psi\rangle = (\psi_1, \psi_2, \psi_3, \psi_4)$. (To save space and simplify notation, we will write such vectors both as rows and columns.) In the basis of the four atomic states, the Hamiltonian $\hat{H}$ of the system can be written as a 4×4 matrix. Taking into account only the (real) matrix elements W of $\hat{H}$ between the nearest neighboring atoms, as shown in the Figure, we obtain the following time-independent Schrödinger equation

$$\hat{H}|\psi\rangle = \begin{pmatrix} 0 & W & 0 & W \\ W & 0 & W & 0 \\ 0 & W & 0 & W \\ W & 0 & W & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \tag{1}$$

(a) **[9 points]** Show that the eigenfunctions of Eq. (1) can be taken as $\psi_j = e^{ijk}$, i.e. $|\psi\rangle_k = (e^{ik}, e^{i2k}, e^{i3k}, e^{i4k})$, where k is a parameter, and $i = \sqrt{-1}$. Substitute $|\psi\rangle_k$ into Eq. (1) and show that the equation is satisfied when k is properly selected. Show that there are four permitted values of k and find their values k_n and the corresponding eigenenergies E_n, where $n = 1, 2, 3, 4$.

Show that $|\psi\rangle_k$ does not change when we change $k \to k + 2\pi$, so, without loss of generality, we can restrict k_n to the interval $(0, 2\pi)$ and label the values of k_n in increasing order.

Are there degeneracies among the eigenvalues E_n?

(b) **[8 points]** Now let us also take into account the weaker matrix elements V of $\hat{H}$ between the next-nearest neighboring atoms, as shown by the dashed lines in the Figure. Write down $\hat{H}$ in that case and show that the Schrödinger equation becomes

$$\hat{H}|\psi\rangle = \begin{pmatrix} 0 & W & V & W \\ W & 0 & W & V \\ V & W & 0 & W \\ W & V & W & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \tag{2}$$

II.4 (Continued)

Show that the eigenvectors of Eq. (2) are the same vectors $|\psi\rangle_k$ with the same values k_n and find the new eigenenergies E_n.

Are there still degeneracies among the eigenvalues E_n?

(c) **[8 points]** Now let us discuss the symmetries of the eigenfunctions. First, let us consider a cyclic permutation of the atoms, i.e. a translational shift along the ring: $1 \to 2$, $2 \to 3$, $3 \to 4$, $4 \to 1$. In terms of the wavefunctions, the shift operator $\hat{S}$ is defined as $\hat{S}\psi_j = \psi_{j+1}$ with the periodic boundary condition.

Is the Hamiltonian $\hat{H}$ in Eqs. (1) and (2) invariant under the shift operation? Is it possible for a wavefunction $|\psi\rangle_k$ to be an eigenstate of both $\hat{S}$ and $\hat{H}$ operators simultaneously?

Verify explicitly that the energy eigenstates $|\psi\rangle_k$ are also the eigenstates of the shift operator, i.e. $\hat{S}|\psi\rangle_k = (e^{i2k}, e^{i3k}, e^{i4k}, e^{ik}) = \lambda_S|\psi\rangle_k$ for the permitted values k_n, and find the eigenvalues λ_S.

(d) **[8 points]** Now let us discuss invariance upon the time-reversal operation. Consider the time-dependent Schrödinger equation with a real Hamiltonian $\hat{H} = \hat{H}^*$

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi. \tag{3}$$

Suppose we reverse the time direction by changing $t \to -t$ in Eq. (3). Show that Eq. (3) can be restored to the original form if we simultaneously apply the complex conjugation operation and replace $\psi \to \psi^*$.

Relatedly, show that if ψ is an eigenfunction of $\hat{H}\psi = E\psi$ for a real $\hat{H}$, then ψ^* is also an eigenfunction of $\hat{H}$ with the same eigenvalue E.

Write the four eigenfunctions $|\psi\rangle_k = (e^{ik}, e^{i2k}, e^{i3k}, e^{i4k})$ explicitly for the permitted values k_n and examine how these functions transform upon the complex conjugation operation $|\psi\rangle_k^*$. If $|\psi\rangle_k \neq |\psi\rangle_k^*$, then we conclude that there are two different eigenvectors for the same energy eigenvalue, i.e. the eigenenergy is degenerate. How many such cases are present in our problem?

Show that by making linear combinations of the degenerate eigenstates, $|\psi\rangle_k + |\psi\rangle_k^*$ and $i|\psi\rangle_k - i|\psi\rangle_k^*$, it is possible to make all eigefunctions real. However, these energy eigefunctions will not be eigenstates of the shift operator. Construct such real eigenfunctions for our problem.

Problem II.5

Half of the Nobel Prize in Physics in 2005 was awarded to Roy J. Glauber for his contributions to the quantum theory of optical coherence and for his role in the discovery of coherent states of the electromagnetic radiation field.

Quantized electromagnetic radiation can be described using the harmonic oscillator Hamiltonian $\hat{H} = \hbar\omega(\hat{a}^+\hat{a}+\frac{1}{2})$, which is defined in terms of the energy quantum $\hbar\omega$ and the creation and annihilation operators $\hat{a}^+$ and $\hat{a}$. The energy eigenstates are the eigenstates $|n\rangle$ of the number operator $\hat{n} = \hat{a}^+\hat{a}$, which are interpreted as the states with n photons.

(a) **[6 points]** Glauber studied the coherent states, which are the eigenstates $|v\rangle$ of the annihilation operator $\hat{a}$ with complex eigenvalues v:

$$\hat{a}|v\rangle = v|v\rangle. \tag{1}$$

The coherent states (1) can be expanded in terms of the complete orthonormal set of the number states as

$$|v\rangle = \sum_{n=0}^{\infty} c_n|n\rangle. \tag{2}$$

Substituting Eq. (2) into Eq. (1) and using the formula $\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$, derive a recursion relation between the coefficients c_n. Solve this recursion relation and find c_n up to an overall normalization constant.

(b) **[5 points]** From the appropriate normalization condition for $|v\rangle$, show that overall normalization can be achieved by setting $c_0 = \exp(-|v|^2/2)$.

Hint: Recall the Taylor expansion for e^x.

(c) **[6 points]** Calculate the probability $P(n) = |\langle n|v\rangle|^2$ of finding n photons in the coherent state $|v\rangle$ and show that it is given by a Poisson distribution.

(d) **[3 points]** Determine the mean number of photons $\langle n\rangle$ in the coherent state $|v\rangle$.

(e) **[3 points]** Determine the variance $\Delta n^2 = \langle n^2\rangle - \langle n\rangle^2$ (or equivalently the photon number uncertainty $\Delta n = \sqrt{\Delta n^2}$) of the coherent state $|v\rangle$.

(f) **[2 points]** Are coherent states with different v and v' orthogonal? To answer this question examine the scalar product $\langle v|v'\rangle$.