UNIVERSITY OF MARYLAND
Department of Physics
College Park, Maryland

Ph.D. PHYSICS QUALIFYING EXAMINATION - PART II

August 30th, 2013 **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

This problem studies interplay between scattering and bound states, and shows that bound states can be obtained as pole singularities in the scattering matrix $\hat{S}$.

Consider an arbitrary potential $V(x)$ in one dimension vanishing for $|x| > a$. The wave functions $\psi(x)$ of energy E are superpositions of plane waves outside of the potential:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x \le -a, \\ Ce^{ikx} + De^{-ikx}, & x \ge a, \end{cases} \qquad E = \frac{\hbar^2 k^2}{2m}. \tag{1}$$

(a) **[2 points]** Explain why the terms with A and D in Eq. (1) represent the incoming waves, whereas the terms with B and C represent the outgoing waves.

(b) **[5 points]** A linear relation between the incoming and outgoing waves is represented by the 2×2 scattering matrix $\hat{S}$:

$$\begin{pmatrix} C \\ B \end{pmatrix} = \hat{S} \begin{pmatrix} A \\ D \end{pmatrix}, \qquad \hat{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}. \tag{2}$$

Show that the matrix $\hat{S}$ is unitary, i.e. $\hat{S}^\dagger \hat{S} = \hat{1}$. *Hint:* Use probability flux conservation.

(c) **[5 points]** Suppose the potential $V(x) = V(-x)$ is symmetric. In this case, you may consider a symmetric wave function $\psi_s(-x) = \psi_s(x)$ with $A = D$ and $B = C$.

Using probability flux conservation, show that the outgoing waves in $\psi_s(x)$ differ from the incoming waves by a phase factor $e^{i\phi}$. Prove the following relation for the matrix elements: $S_{11} + S_{12} = S_{22} + S_{21} = e^{i\phi}$.

(d) **[6 points]** Now consider a specific example of the delta-function potential

$$V(x) = \beta\, \delta(x), \qquad \gamma = \beta \frac{m}{\hbar^2}, \tag{3}$$

where β and γ are coefficients representing the strength of the potential. Calculate the sum of the matrix elements $S_{11} + S_{12} = e^{i\phi}$ in terms of γ and k.

Hint: Integrating Schrödinger's equation around $x = 0$, find a condition on $\psi(0)$ and the derivatives $\psi'(\pm\epsilon)$ at $\epsilon \to 0$. Applying this condition to $\psi_s(x)$ in Eq. (1), find $e^{i\phi}$.

(e) **[5 points]** Now let us formally treat $k = k' + ik''$ as a complex variable with real and imaginary parts k' and k''. Show that $S_{11} + S_{12}$ as a function of the complex variable k has a pole singularity on the imaginary axis at $k'' > 0$ for $\gamma < 0$. Examining Eqs. (1) and (2), show that the wave function $\psi_s(x)$ in this case corresponds to a bound state and find its exponential decay rate vs. $|x|$. Substituting the imaginary k into Eq. (1) for E, find the energy of this bound state.

(f) **[2 points]** Discuss briefly how the consideration in Part (e) changes when the potential (3) is repulsive with $\gamma > 0$.

Problem II.2

At times $t < 0$, a system described by a Hamiltonian H is in the quantum state $|n\rangle$ with the energy E_n

$$H|n\rangle = E_n|n\rangle.$$

At time $t = 0$, the system is perturbed by an external potential V, so the system Hamiltonian suddenly changes from H to $H + V$ for $t > 0$. Assume H and V to be time-independent. Let us denote the new set of energy eigenstates by primes in order to distinguish it from the old set:

$$(H + V)|m'\rangle = E_{m'}|m'\rangle.$$

(a) **[5 points]**

  (a) What is the probability of finding the system in a new eigenstate $|m'\rangle$ for $t > 0$, given that it was in the state $|n\rangle$ at $t < 0$? Does this probability change in time?

  (b) What is the change in the energy expectation value of the system $\Delta E = E(t > 0) - E(t < 0)$, in terms of matrix elements of V?

(b) **[10 points]** Suppose H is the Hamiltonian of a one-dimensional infinite square-well potential of width L, and the system is in the ground state $|n = 1\rangle$ of this potential at $t < 0$. At $t > 0$, the width of the well suddenly doubles from L to $2L$.

  (a) Explicitly calculate the probability of finding the system in an energy eigenstate $|m'\rangle$ of the expanded well for $t > 0$.

  Does this probability vanish for certain values of m'? Explain qualitatively.

  (b) What is ΔE in this case?

(c) **[10 points]** Suppose H is the Hamiltonian of a one-dimensional infinite square-well potential located at $0 < x < L$, and the system is in the ground state $|n = 1\rangle$ of this potential at $t < 0$. At $t > 0$, the following perturbation is applied:

$$V(x) = \begin{cases} V_0 & \text{for} \quad 0 < x < L/3, \\ 0 & \text{for} \quad L/3 < x < L. \end{cases}$$

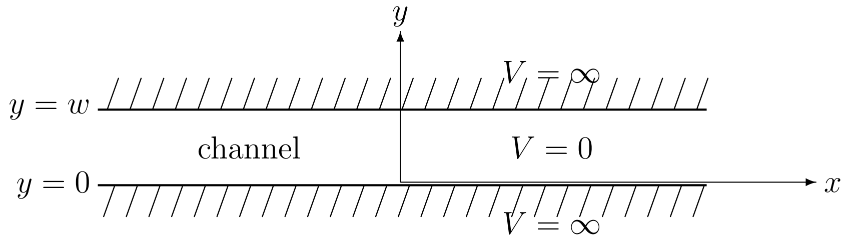
Explicitly calculate ΔE in this case. Do not assume that V_0 is small.

Useful formula:

$$\sin\alpha \, \sin\beta = \frac{\cos(\alpha - \beta) - \cos(\alpha + \beta)}{2}$$

Problem II.3

Assuming a two-dimensional geometry with rectangular coordinates x and y, consider a particle of mass m in an infinitely long channel of width w, with potential $V = 0$ in $0 < y < w$ and $V = +\infty$ in $y < 0$ and $y > w$, as shown in the Figure.



(a) **[2 points]** Write down the Schrödinger equation for a wavefunction $\psi(x, y)$ of energy E in the channel. What are the appropriate boundary conditions on ψ at $y = 0$ and at $y = w$?

(b) **[5 points]** Show that there are solutions for $\psi(x, y)$ that are of the form

$$\psi_n(x, y) = \begin{cases} u_n(y)e^{\pm ik_n x}, \; k_n = \sqrt{k_0^2 - (n\pi/w)^2} & \text{for} \quad n \leq n_*, \\ u_n(y)e^{\pm \alpha_n x}, \; \alpha_n = \sqrt{(n\pi/w)^2 - k_0^2} & \text{for} \quad n \geq n_* + 1, \end{cases} \tag{1}$$

Here $n = 1, 2 \ldots$ is an integer that enumerates the functions u_n by increasing eigenvalue, and n_* is the largest value of n for which $(n\pi/w)^2 < k_0^2 \equiv 2mE/\hbar^2$. The functions $u_n(y)$ are orthonormal, $\int_0^w u_n(y)u_m(y)dy = \delta_{nm}$ and complete, $\sum_{n=1}^{\infty} u_n(y)u_n(y') = \delta(y - y')$. What are the functions $u_n(y)$?

For what range of energies are there no propagating modes (i.e. $n_* = 0$)?

The Green's function for the domain $0 < y < w$ of the Figure is defined to be the solution of the equation

$$\left\{ \frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + E \right\} G(x, x', y, y') = \delta(x - x')\, \delta(y - y'). \tag{2}$$

For $0 < y < w$, $0 < y' < w$, appropriate boundary conditions on G, and outgoing waves at $x \to +\infty$ and $x \to -\infty$, it can be written as

$$G(x, x', y, y') = \frac{m}{\hbar^2} \sum_{n=1}^{\infty} \frac{e^{-\gamma_n |x-x'|}}{\gamma_n} u_n(y')u_n(y), \tag{3}$$

where $\gamma_n = \alpha_n$ for $n \geq n_* + 1$ and $\gamma_n = -ik_n$ for $n \leq n_*$.

(c) **[7 points]** Verify that Eq. (3) for G satisfies Eq. (2).

II.3 (Continued)

(d) [**5 points**] Now assume that there is a weak, localized scattering potential $V_s(x,y)$ placed in the channel, where $|V_s(x,y)| \ll E$ everywhere (i.e., the potential is weak), and $V_s(x,y) = 0$ for $|x| > \Delta$ (i.e., the potential is localized in x). Let $\overline{V}_s = \max_{x,y} |V_s(x,y)|$ characterize the strength of the potential, with $\varepsilon = \overline{V}_s/E$ a small parameter.

Consider a solution of the Schrödinger equation for this problem of the form $\psi = \psi_0 + \psi_1$, where ψ_0 is a solution for $V_s = 0$, and ψ_1 is a small correction, due to V_s, of size ε compared to ψ_0. Write a formula for ψ_1 in terms of ψ_0 and the Green's function G of Eq. (2), to first order in ϵ.

(e) [**6 points**] Finally, consider the situation in which $k_0\Delta \ll 1$, $n_* = 1$, and ψ_0 is a wave incident from the left:

$$\psi^{(0)} \to Au_1(y)e^{ik_1x} \text{ for } x \to -\infty.$$

This wave scatters off the scattering potential, producing a reflected wave,

$$\psi^{(1)} = SAu_1(y)e^{ik_0|x|} = SAu_1(y)e^{-ik_1x} \text{ for } x \to -\infty$$

and a transmitted wave,

$$\psi^{(0)} + \psi^{(1)} = TAu_1(y)e^{ik_1x} \text{ for } x \to +\infty$$

For $\varepsilon \ll 1$, to lowest order in ε, the scattering coefficient S is proportional to ε, while the transmission coefficient T is equal to one plus a correction term proportional to ε. Find S and T up to order ε in terms of integrals over V_s and u_1.

Problem II.4

Let H_0 be the Hamiltonian of a spinless nonrelativistic particle in a central potential $V_0(r)$. Energy eigenstates are the eigenstates of angular momentum and can be labeled as $|n, l, m\rangle$. Apart from the $(2l+1)$-fold degeneracy arising from spherical symmetry, there are no other degeneracies in the spectrum of H_0. This problem concerns how the spectrum changes when a perturbation V of a particular form is added to H_0, so that $H = H_0 + V$ with

$$V(r, \theta, \phi) = \lambda\, e^{-r^2/R^2}\, r^K\, Y_K^0(\theta, \phi).$$

Here the perturbing potential is written in spherical coordinates, the parameter λ represents the strength of the potential, R is a constant with units of length, K is a positive integer, and Y_l^m is a spherical harmonic.

At various stages of this problem, you may find helpful to think about parity, time reversal, and spherical tensors. You should assume that quantities never vanish accidentally, i.e. they only vanish for reasons of symmetry. If Clebsch-Gordan coefficients arise, simply state your result in terms of them. You do not need to evaluate them explicitly.

In Parts (a) and (b), work to all orders in the strength λ of the perturbation.

(a) [**5 points**] When the perturbation is included, does the quantum number m remain a good quantum number for the system? If so, explain briefly why or why not.

(b) [**5 points**] The perturbation breaks the $(2l+1)$-fold degeneracy. Is there any surviving degeneracy in the spectrum? If not, explain briefly why not. If so, identify the degeneracy and explain briefly its origin.

In Parts (c)-(e), you may assume that the strength parameter λ is small. Let us denote by $\Delta E_{n,l,m}$ the energy shift of the state $|n, l, m\rangle$ (as labeled in the unperturbed eigenbasis) due to the perturbation. For small λ, one might generically expect that the energy shift is given by the first-order perturbation theory, so that $\Delta E_{n,l,m} \propto \lambda$. However, under certain circumstances, the first-order perturbation vanishes, and this linear dependence on λ is absent. In these cases, the dominant behavior is quadratic in λ: $\Delta E_{n,l,m} \propto \lambda^2$.

(c) [**5 points**] Recall that the perturbation depends on the integer K, which specifies the spherical harmonic. Consider the case $K = 3$, where $V = \lambda\, e^{-r^2/R^2}\, r\, Y_3^0(\theta, \phi)$. Determine which energy levels, if any, have a quadratic dependence on λ as the leading behavior. (*Hint:* This amounts to asking for which states the first-order perturbation vanish. Consideration of parity may be helpful.)

(d) [**5 points**] Consider the case $K = 6$, where $V = \lambda\, e^{-r^2/R^2}\, r^6\, Y_6^0(\theta, \phi)$. Using the Wigner-Eckart theorem, determine which energy levels, if any, have a quadratic dependence on λ as the leading behavior.

(e) [**5 points**] Consider the case $K = 2$, where $V = \lambda\, e^{-r^2/R^2}\, r^2\, Y_2^0(\theta, \phi)$. In this case, $\Delta E_{n,l=1,m} \propto \lambda$ for the states with $l = 1$. You may assume this linear dependence to be correct without proving it. Using the Wigner-Eckart theorem, express the ratio of the energy shifts $\Delta E_{n,l=1,m}/\Delta E_{n,l=1,m'}$ in terms of Clebsch-Gordan coefficients.

Problem II.5

This problem is inspired by Einstein's model of a solid, where vibrations of atoms in a crystal lattice are modeled using a set of independent harmonic oscillators.

Consider a system of N one-dimensional non-interacting harmonic oscillators of frequency ω in thermal equilibrium at temperature T.

(a) [**5 points**] First suppose the oscillators are *classical*. Find the partition function, $Z_N^{(\mathrm{c})}(T)$, of the system of N classical oscillators.

(b) [**4 points**] Calculate the energy, $U^{(\mathrm{c})}$, and heat capacity, $C^{(\mathrm{c})}$, of the classical oscillator system. Here and in Part (e) below, you may find the following equation for the energy useful:

$$U = -\frac{\partial}{\partial \beta} \ln Z,$$

where $\beta = 1/k_B T$, and k_{B} is the Boltzmann constant.

(c) [**2 points**] Explain how to derive your result for $C^{(\mathrm{c})}$ using the equipartition theorem.

(d) [**5 points**] Now suppose the oscillators are *quantum*. Find the partition function, $Z_N^{(\mathrm{q})}(T)$, of the system of N quantum oscillators.

(e) [**4 points**] Calculate the energy, $U^{(\mathrm{q})}$, and heat capacity, $C^{(\mathrm{q})}$, of the quantum oscillator system.

(f) [**3 points**] At what temperatures do the quantum oscillators behave as classical ones? Take the classical limit in your result for $C^{(\mathrm{q})}$ and reproduce the corresponding classical result, $C^{(\mathrm{c})}$.

(g) [**2 points**] How does $C^{(\mathrm{q})}$ behave in the limit $T \to 0$? Sketch $C^{(\mathrm{q})}$ vs. T from $T = 0$ to high temperatures.