UNIVERSITY OF MARYLAND
Department of Physics
College Park, Maryland

PHYSICS Ph.D. QUALIFYING EXAMINATION
PART II

January 25, 2019 9:00 a.m. – 1:00 p.m.

Do any four problems. Each problem is worth 25 points.
Start each problem on a new sheet of paper (because different faculty members will be grading each problem in parallel).

Be sure to write your Qualifier ID ("control number") at the top of each sheet — not your name! — and turn in solutions to four problems only. (If five solutions are turned in, we will only grade # 1 - # 4.)

At the end of the exam, when you are turning in your papers, please fill in a "no answer" placeholder form for the problem that you skipped, so that the grader for that problem will have something from every student.

You may keep this packet with the questions after the exam.

Problem II.1

The Schrödinger equation for the helium atom cannot be solved exactly. However, if we replace each of the Coulomb forces by a spring force, the system *can* be solved exactly. As an example, consider the Hamiltonian H in 3-dimensional space given by

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) + \frac{1}{2}m\omega^2\left(r_1^2 + r_2^2\right) - \frac{\lambda}{4}m\omega^2|\mathbf{r}_1 - \mathbf{r}_2|^2 \ , \tag{1}$$

with $0 \le \lambda < 1$. Here $\mathbf{r}_1$ and $\mathbf{r}_2$ represent the coordinates associated with the two electrons and m is the electron mass.

(a) [**5 points**] Neglecting the last term in H (i.e., setting $\lambda = 0$), determine the ground state energy of the two (uncoupled) 3D harmonic oscillators. Also write down the ground state wave function.

(b) [**8 points**] Use this uncoupled ground state wave function and first order perturbation theory to estimate the ground state energy of the full, coupled Hamiltonian H.

(c) [**6 points**] By a suitable change of variables, show how the full Hamiltonian H can be transformed into the sum of two independent simple harmonic oscillators in 3D,

$$H = \left[-\frac{\hbar^2}{2m}\nabla_u^2 + \frac{1}{2}m\omega^2 u^2\right] + \left[-\frac{\hbar^2}{2m}\nabla_v^2 + \frac{1}{2}\left(1-\lambda\right)m\omega^2 v^2\right] \ . \tag{2}$$

Explicitly give the $u = u(\mathbf{r}_1, \mathbf{r}_2)$ and $v = v(\mathbf{r}_1, \mathbf{r}_2)$ that satisfy this transformation.

(d) [**6 points**] Determine the exact ground state energy of the system.

How well does this answer agree with your estimate from part (b) above in the small-λ limit?

Possibly useful:

The normalized ground state wave function of a single harmonic oscillator in one dimension is given by

$$\psi(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \exp\left(-\alpha x^2/2\right) \ ,$$

where $\alpha = m\omega/\hbar$.

$$\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \qquad \int_0^{\infty} dx\, x e^{-\alpha x^2} = \frac{1}{2\alpha} \qquad \int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2} = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

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**]

(i) 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 $t < 0$?

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

(b) [**12 points**] Suppose H is the Hamiltonian of a one-dimensional infinite square-well potential of width L (from $x = 0$ to 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 to $2L$ (from $x = 0$ to $2L$) and keeps the new width for all $t > 0$.

(i) Explicitly calculate the probability of finding the system in an energy eigenstate $|m'\rangle$ of the expanded well for $t > 0$. Point out for which values of m' the probability vanishes.

(ii) What is ΔE in this case?

(c) [**8 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.

Possibly useful:

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

Problem II.3

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 spatial wave functions $\psi(x)$ of energy E are superpositions of plane waves outside of the potential:

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

(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) [**5 points**] Now consider a specific example: 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 $e^{i\phi}$ in terms of γ and k.

(e) [**6 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.4

Two particles interact via a spin-spin Hamiltonian term $A\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$, where A is a positive constant and $\boldsymbol{S}_{1,2}$ are the spin angular momenta of the two particles. Particle 1 has spin 1 and magnetic moment $\mu_\mathbf{1} = -\frac{\mu_\mathbf{B}}{\hbar}\mathbf{S_1}$, whereas particle 2 has spin $\frac{1}{2}$ and zero magnetic moment.

(a) **[6 points]** Without any magnetic field present, what are the energy levels of this system in terms of A and $\hbar$? And what is the degree of degeneracy of each level?

(b) **[8 points]** Write down all the energy eigenstates corresponding to the system energy levels in part (a), expressed as linear superpositions of products of single-particle spin states (i.e., terms of the form $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$).

Now consider what happens when the system is in a magnetic field of strength B.

(c) **[4 points]** What are the approximate energy eigenstates and eigenvalues if $B \gg \frac{A\hbar^2}{\mu_B}$?

(d) **[7 points]** Sketch the approximate energy eigenvalues as functions of magnetic field strength, from $0 \leq B \lesssim \frac{A\hbar^2}{\mu_B}$, and label the appropriate states. *Do not neglect the spin-spin interaction term from parts (a) and (b).*

Possibly useful:

$(\mathbf{V_1} + \mathbf{V_2})^2 = \mathbf{V_1}^2 + \mathbf{V_2}^2 + 2\,\mathbf{V_1} \cdot \mathbf{V_2}$ for vectors $\mathbf{V_1}$ and $\mathbf{V_2}$

$$J_\pm|j, m\rangle \;=\; \sqrt{j(j+1) - m(m \pm 1)}\;|j, m \pm 1\rangle$$

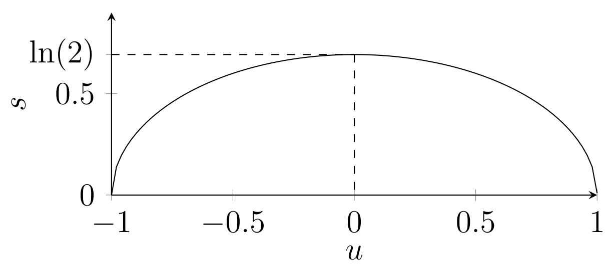
Problem II.5

The notion of negative absolute temperature is unusual but it can occur in, for example, quantum spin systems. To see this, consider a quantum system of N noninteracting magnetic dipoles each with spin $1/2$, having a magnetic moment μ_B, placed in a magnetic field $\mathbf{B}$. Assume a canonical ensemble description of this spin system with a temperature $T = 1/(k\beta)$, where k is Boltzmann's constant.

(a) [**5 points**] Write down the energy levels of this two-level system in terms of μ_B and B, the magnitude of the magnetic field. (You may wish to use a symbol such as ϵ to represent a relevant energy.)
Then determine the partition function Z_N in terms of β.

(b) [**9 points**] Calculate the free energy F, the entropy S, and the internal energy U of this system as a function of N and β.

A schematic plot of $s \equiv \frac{S}{Nk}$ versus $u \equiv \frac{U}{N\mu_B B}$ is provided in the figure below to aid you in answering the following questions:



(c) [**5 points**] What is the temperature T of the magnetic system in terms of the thermodynamic quantities in part (b)?
Copy the figure onto your answer sheet and indicate on the figure: (*i*) the places where $T = 0$, (*ii*) the region where negative temperature $T < 0$ appears, (*iii*) indicate with one arrow on each branch the direction of increasing T, and (*iv*) what is the temperature at the global maximum of the curve?

(d) [**2 points**] Explain what energy state the system is in at $T = 0$.

(e) [**4 points**] For each of the following, if you can't calculate the temperature exactly, describe it qualitatively.

(i) If a system of this nature at $T = 300K$ is brought into contact with an identical system at $T = -300K$, what is the final equilibrium temperature?

(ii) If a system of this nature at $T = 300K$ is brought into contact with an identical system at $T = -100K$, what is the final equilibrium temperature?