Ph.D. Comprehensive Exam

Department of Physics
Georgetown University

Part I: Monday, July 15, 2013, 1:00pm - 5:00pm

Instructions:

- This is a closed-book, closed-notes exam. The only electronic devices allowed are calculators provided by the department.
- Each problem is worth 50 points.
- You should submit work for all of the problems. In many cases, even if you get stuck on one part of a problem, you may be able to make progress on subsequent parts.
- Please work different problems on separate sheets of paper.
- Show all your work.

NAME:

---

1. A stationary spin-$\frac{1}{2}$ particle is in a uniform and constant external magnetic field $\vec{B} = B_0\hat{z}$. The Hamiltonian operator of the system is given by

$$H = -\mu B_0 \sigma_z,$$

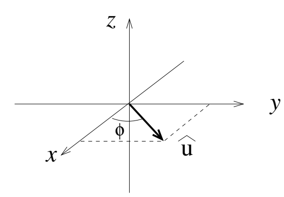
where $\mu > 0$. The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(a) Determine the energy eigenvalues and normalized eigenvectors of the Hamiltonian (in the basis of σ_z eigenvectors).

(b) Determine the eigenvalues and normalized eigenvectors of σ_x (in the basis of σ_z eigenvectors).

(c) Let $\hat{u}$ be a unit vector that lies in the xy plane and points at an angle ϕ from the $+x$ axis. The component of $\vec{\sigma}$ along $\hat{u}$ is denoted σ_u. Determine the eigenvalues and normalized eigenvectors of σ_u (in the basis of σ_z eigenvectors).



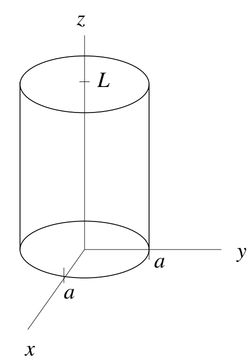
(d) At time $t = 0$, a measurement of σ_x yields the lowest eigenvalue of σ_x. Determine the probability that, at time $t > 0$, a measurement of σ_x will find the highest eigenvalue of σ_x. Plot your result for the probability as a function of time.

NAME:

---

2. A particle of mass μ is inside a cylindrical box of height L and radius a. The Hamiltonian is given by

$$H = \frac{P^2}{2\mu} + V(r, z, \phi),$$



where

$$V(r, z, \phi) = \begin{cases} 0 & \text{if } r < a \text{ and } 0 < z < L \\ \infty & \text{otherwise,} \end{cases}$$

and

$$P^2 = P_r^2 + P_z^2 + L_z^2/r^2.$$

Note that the wave function can be written in separable form:

$$\Psi(r, z, \phi) = R(r)Z(z)\Phi(\phi),$$

where (r, z, ϕ) represent cylindrical coordinates.

(a) Write down the Schrodinger equation for the confined particle in coordinate representation.

(b) What differential equation and boundary condition must $\Phi(\phi)$ satisfy? Determine the function $\Phi(\phi)$ (up to an overall normalization constant) for the particle confined in the box.

(c) What differential equation and boundary conditions must $Z(z)$ satisfy? Determine the function $Z(z)$ (up to an overall normalization constant) for the particle confined in the box.

(d) Determine the differential equation that the radial function $R(r)$ must satisfy.

(e) Explain what would have to be done to determine the energy eigenvalues. (You do not need to find them.)

In coordinate representation:

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$P_z = -i\hbar \frac{\partial}{\partial z}$$

$$P_r^2 = -\hbar^2 \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right)$$

NAME:

---

3. A charge, q, is located at position $\vec{r'} = (0, 0, d)$, where $d > 0$. An infinite, grounded conducting block lies in the region $z < 0$ such that its surface is at $z = 0$. Using the image charge method in Cartesian coordinates,

   a) find an expression for the potential at **any** point $\vec{r} = (x, y, z)$ in the region

      i) $z > 0$

      ii) $z < 0$

   b) find expressions for all 3 electric field components and show that the electric field is normal to the surface of the conductor, i.e. at $z = 0$.

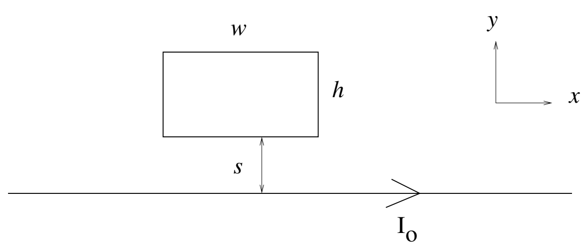
   c) find an expression for $\sigma(x, y, 0)$, the induced charge at the surface of the conductor.

   d) find the work required to bring the charge, q, from ∞ to the position $\vec{r'}$.

NAME:

---

4. A $h \times w$ rectangular loop is made of wire with cross sectional area A and resistivity ρ. The loop lies on a table a distance s from a very long straight wire, as shown below. The long straight wire carries a current I_0.



(a) Find the flux of $\vec{B}$ through the loop.

(b) If someone pulls the loop directly away from the wire (in the $+y$ direction), with constant speed v, determine

- ∗ the emf around the loop;
- ∗ the magnitude of the current in the loop;
- ∗ the direction of current flow in the loop.

(c) If the wire loop were replaced by a wooden loop of the same dimensions, which, if any, of your answers in part (b) would change? Explain.

(d) If the original wire loop were pulled with constant speed v in the $+x$ direction, which, if any, of your answers in part (b) would change? Explain.

Ph.D. Comprehensive Exam

Department of Physics
Georgetown University

Part II: Tuesday, July 16, 2013, 1:00pm - 5:00pm

Instructions:

- This is a closed-book, closed-notes exam. The only electronic devices allowed are calculators provided by the department.
- Each problem is worth 50 points.
- You should submit work for all of the problems. In many cases, even if you get stuck on one part of a problem, you may be able to make progress on subsequent parts.
- Please work different problems on separate sheets of paper.
- Show all your work.

NAME:

---

1. Consider a one-dimensional lattice with electrons in s-wave bands that are allowed to hop between nearest neighbors with a hopping integral given by $-t$. This is called a tight-binding representation for the bandstructure of the material. The single-particle Hamiltonian for this system can be written as a tridiagonal matrix with $-t$ on each of the subdiagonals and 0 on the diagonals ($H_{ij} = -t$ for $j = i \pm 1$ and 0 otherwise). Assume the lattice spacing is a.

   (a) Approximate the infinite lattice by a finite chain of length N with periodic boundary conditions given by site 1 being identified as the same as site $N+1$. Show that the eigenvalue equation
   $$\sum_{j=1}^{N} H_{ij}\psi_j(k) = \epsilon(k)\psi_i(k) \tag{1}$$
   is solved by the (unnormalized) eigenfunctions $\psi_j(k) = \exp(ikaj)$ with $k = 0, 2\pi/aN$, $\ldots$, $2\pi(N-1)/aN$ and eigenvalues $\epsilon(k) = -2t\cos(ka)$. Determine the first Brillouin zone. Plot the bandstructure in the first Brillouin zone. Determine the bandwidth of the band (total range in energy for the allowed eigenvalues).

   (b) Derive the (single-spin) density of states in energy per unit length for the band. The (single-spin) density of states, $D(E)$ satisfies
   $$\begin{aligned} D(E) &= \frac{1}{2\pi}\int_0^{2\pi/a} dk\delta[E - \epsilon(k)] \\ &= \frac{1}{2\pi}2\left|\frac{dk}{d\epsilon}\right|_{\epsilon\to E} \end{aligned} \tag{2}$$
   where the factor of two comes from the two k points where $E = \epsilon(k)$.

   (c) The electron density satisfies
   $$n = 2\int_{-\infty}^{\infty} dEf(E-\mu)D(E) \tag{3}$$
   where the 2 comes from the spin degeneracy and $f(E-\mu) = 1/[1+\exp((E-\mu)/k_BT)]$ is the Fermi-Dirac distribution function. Prove that the electron density satisfies $n = 1/a$ if $\mu = 0$ for all temperatures. *Hint*: $f(E-\mu) = [\tanh((E-\mu)/2k_BT)+1]/2$. One part of this breakup is even and one part is odd.

   (d) In the case where $n = 1/a$ ($\mu = 0$), explain why the energy density $U(T)$ as a function of T, is given by
   $$U(T) = 2\int_{-\infty}^{\infty} dEEf(E)D(E) \tag{4}$$
   Determine explicit values of the integrals in the limits $T \to 0$ and $T \to \infty$ by replacing the Fermi-Dirac distribution by its limiting values in those cases.

NAME:

---

2. Consider a 2D square lattice with N_{TOT} atoms, lattice spacing a, and one atom of mass m per lattice point. The phonon dispersion relation is given by

$$\omega(k) = (4C/m)^{1/2} \sin(ka/2),$$

where C is the force constant between nearest neighbors and $k = |\vec{k}|$ is the magnitude of the wave vector $\vec{k}$.

   (a) In the long wavelength limit, show that the dispersion can be written as $\omega(k) = vk$. Obtain the density of modes (number of modes per unit frequency range) and show that it is proportional to ω.

   (b) Explain what the Debye frequency is. Use the linear frequency dependence of the density of modes to express the Debye frequency as a function of v and N_{TOT}.

   (c) Use the Debye model to show that the heat capacity is proportional to T^2 at low temperature.

   (d) Explain what the Debye temperature is and how it is related to the Debye frequency.

NAME:

---

3. Consider an isolated system of N identical diatomic molecules at low densities, so that they can be considered an *ideal gas*.

   (a) Show that, according to classical statistics, the heat capacity at constant volume is given by $C_v = \frac{7}{2}Nk_B$. You can do this using the equipartition theorem, but if you do, you must first *derive* the equipartition theorem.

   (b) Experimentally, the heat capacity of diatomic gasses only approaches $3.5Nk_B$ at high temperatures, close to the temperatures where the molecules disassociate. Explain in a few sentences why the heat capacity at low temperature is instead given by $C_v = \frac{3}{2}Nk_B$.

   (c) For the specific case of the vibrational degrees of freedom, show that their contribution to the head capacity is given by

$$C_v = Nk_B \left(\frac{\theta}{T}\right)^2 \frac{\exp\left(\frac{\theta}{T}\right)}{\left[\exp\left(\frac{\theta}{T}\right) - 1\right]^2}$$

   where the vibrational motion can be described as a harmonic oscillator with frequency ω and $\theta = \hbar\omega/k_B$. You may find it useful to recall the relationship for $|p| < 1$

$$1 + p + p^2 + ... = 1/(1-p).$$

   (d) Show that the contribution of the vibrational modes to the specific heat vanishes at low temperatures, and approaches the classical result at high temperatures. Be explicit about the appropriate condition for "low" and "high" temperatures.

Some potentially useful integrals:

$$\int_0^\infty e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty xe^{-ax^2} dx = \frac{1}{2a}$$

$$\int_0^\infty x^2e^{-ax^2} dx = \frac{1}{4}\sqrt{\frac{\pi}{a^2}}$$

NAME:

---

4. Consider a system of N molecules, each of which consists of three identical spin $\frac{1}{2}$ particles located on the corners of a microscopic equilateral triangle. The Hamiltonian of one such molecule is given by

$$H = J(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1) = \frac{J}{2}(S^2 - S_1^2 - S_2^2 - S_3^2),$$

where J is a positive constant, $\vec{S}_1$, $\vec{S}_2$, and $\vec{S}_3$ are the spin operators for the three spin $\frac{1}{2}$ particles, and $\vec{S} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$.

a. Show that the eigenvalues of H are $\pm\frac{3}{4}\hbar^2 J$ and each energy level is fourfold degenerate.

b. Calculate the canonical partition function for a system of N such molecules.

c. Calculate the internal energy for a system of N such molecules.

d. What is the internal energy for $T \to 0$ and for $T \to \infty$? Briefly interpret your results.

e. Calculate the heat capacity for a system of N such molecules.

f. What is the heat capacity for $T \to 0$ and for $T \to \infty$? Briefly interpret your results.

g. Calculate the entropy for a system of N such molecules.

h. What is the entropy for $T \to 0$ and for $T \to \infty$? Briefly interpret your results.