

**PH.D. QUALIFYING EXAM SOLUTIONS**  
**2000**

MATT THIESSE

MODERN

**Problem 1.** *Consider the Hamiltonian for one particle in two dimensions*

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 (x^2 + y^2).$$

*Is this system invariant under translations? Why or why not? Is it invariant under rotations around the z-axis? Why or why not? What are the corresponding conserved quantities, if any, in these two cases?*

If the Lagrangian is independent of a particular coordinate, it is invariant with respect to translations about that coordinate and that coordinate is called "cyclic". Looking at the Euler-Lagrange equation, if  $L$  doesn't depend on position, then

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} = 0$$

and the quantity  $\frac{\partial L}{\partial \dot{x}}$  would be an invariant of the system. However, since the given Lagrangian is dependent on position ( $x^2 + y^2 = r^2$ ) the system is not invariant under translations. Examining this Hamiltonian, it looks like we have some rotating object about the z axis. The total energy of the system is not the same at all points in space. The energy of a merry-go-round on the axis of rotation is zero but as you step outward the energy increases.

Writing the Lagrangian in polar coordinates, we get

$$L = \frac{1}{2}m \left( r^2 \dot{\theta}^2 + \dot{r}^2 \right) + \frac{1}{2}m\omega^2 r^2 = m\dot{\theta}^2 r^2 + \frac{1}{2}m\dot{r}^2$$

which is clearly independent of  $\theta$ . So, the Lagrangian is invariant under rotations. In other words, the total energy of the merry-go-round does not depend on the angular position. According to the E-L equations, we know that  $\frac{\partial L}{\partial \theta} = 0$  so

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = \frac{d}{dt} \left( 2m\dot{\theta} r^2 \right) = 0.$$

The angular momentum,  $m\omega r^2$ , is therefore a conserved quantity of the system.

For completeness, invariance under translations leads to linear momentum conservation. Invariance under rotations leads to angular momentum conservation. And time invariance

leads to energy conservation. The above Hamiltonian is invariant over time so the energy is conserved.

**Problem 2.** *In your own words, explain why one needs to symmetrize the state vectors of identical particles in quantum mechanics. What is the form of the symmetric and anti-symmetric states for a system of two identical particles (please, define your symbols)?*

When considering multi-particle systems, one must account for the state of each particle. Especially for identical particles, one must also *attempt* to keep track of each particle individually. For example, take positronium. Clearly the particles are not identical and we can write the state vector for the bound state as a linear combination of the possible orientations:

$$|\Psi\rangle = |\alpha\rangle|\beta\rangle + |\beta\rangle|\alpha\rangle.$$

But, if we now have two  $\alpha$  particles, the state vector for the bound state has two identical terms, indistinguishable by *any* possible observation. This wouldn't be a problem if the universe contained only Bosons, which are symmetric under permutations ( $|\alpha\rangle|\beta\rangle = |\beta\rangle|\alpha\rangle$ ). However, for Fermions, the exchange of a particle introduces a negative sign ( $|\alpha\rangle|\beta\rangle = -|\beta\rangle|\alpha\rangle$ ). So, using our previous example, the state vector for a bound state of two identical particles is

$$|\Psi\rangle = |\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle.$$

**Problem 3.** *Why is the Pauli exclusion principle automatically satisfied if the state vector of a system is properly symmetrized?*

Following directly from Problem 2, the electrons in an atom must all have different state vectors, according to the Pauli exclusion principle. Since electrons are fermions, the exchange of particles is antisymmetric. In particular, for a system of two electrons, the state vector is

$$|\Psi\rangle = |\alpha\rangle|\alpha\rangle - |\alpha\rangle|\alpha\rangle = 0.$$

Therefore, the composite state cannot exist for which two identical particles are in identical quantum states.

**Problem 4.** *An electron is scattered by a one-dimensional square well potential. The width of the square well is  $12\text{\AA}$  and the depth of the square well,  $V_0$ , is to be determined. A measurement of the transmission coefficient as a function of electron kinetic energy (in eV) is shown. Estimate  $V_0$ . Show your work, state any assumptions, and explain your strategy in solving the problem.*

*Helpful information:*  $\sqrt{\frac{2m_e}{\hbar^2}} = 0.512\text{\AA}^{-1}$

See Gilmore, Elementary Quantum Mechanics in One Dimension, 2004, chapter 7.

Since this is a scattered electron, we can assume  $E > 0$ .

To the left of the potential well, Schrödinger's equation reads

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} &= E\psi \\ \frac{d^2\psi}{dx^2} &= -\frac{2mE}{\hbar^2}\psi = -k^2\psi \end{aligned}$$

where  $k \equiv \frac{\sqrt{2mE}}{\hbar}$ . So  $\psi(x) = Ae^{ikx} + Be^{-ikx}$  in this region.

Inside the well,

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\psi &= E\psi \\ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} &= (E + V_0)\psi \\ \frac{d^2\psi}{dx^2} &= -\frac{2m(E + V_0)}{\hbar^2}\psi = -l^2\psi \end{aligned}$$

where  $l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}$ . So  $\psi(x) = C \sin(lx) + D \cos(lx)$  here.

To the right of the potential well,

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} &= E\psi \\ \frac{d^2\psi}{dx^2} &= -\frac{2mE}{\hbar^2}\psi = -k^2\psi \end{aligned}$$

So  $\psi(x) = Fe^{ikx} + Ge^{-ikx}$ . Assuming no incoming waves in this region,  $G = 0$  and so  $\psi(x) = Fe^{ikx}$ . The transmission coefficient is related to  $F$ :  $T = \frac{|F|^2}{|A|^2}$ .

Applying boundary conditions (continuity in  $\psi$  and  $\frac{d\psi}{dx}$  at the two sides of the well, which are labeled -a and a), we find four equations.

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= C \sin(-la) + D \cos(-la) \\ Ae^{-ika} + Be^{ika} &= -C \sin(la) + D \cos(la) \end{aligned} \quad (1)$$

$$\begin{aligned} ikAe^{-ika} - ikBe^{ika} &= lC \cos(-la) - lD \sin(-la) \\ &= lC \cos(la) + lD \sin(la) \\ ik(Ae^{-ika} - Be^{ika}) &= l(C \cos(la) + D \sin(la)) \end{aligned} \quad (2)$$

$$C \sin(la) + D \cos(la) = Fe^{ika} \quad (3)$$

$$\begin{aligned} lC \cos(la) - lD \sin(la) &= ikFe^{ika} \\ l(C \cos(la) - D \sin(la)) &= ikFe^{ika} \end{aligned} \quad (4)$$

Solving Eqn. 4 for  $C$ ,

$$\begin{aligned} C \cos(la) &= \frac{ik}{l} F e^{ika} + D \sin(la) \\ (5) \quad C &= i \frac{k}{l} F \frac{e^{ika}}{\cos(la)} + D \frac{\sin(la)}{\cos(la)} \end{aligned}$$

Substituting this expression for  $C$  into Eqn. 3,

$$\begin{aligned} i \frac{k}{l} F e^{ika} \frac{\sin(la)}{\cos(la)} + D \frac{\sin^2(la)}{\cos(la)} + D \cos(la) &= F e^{ika} \\ D \left( \frac{\sin^2(la) + \cos^2(la)}{\cos(la)} \right) &= F e^{ika} \left( 1 - i \frac{k}{l} \frac{\sin(la)}{\cos(la)} \right) \\ \frac{D}{\cos(la)} &= \\ (6) \quad D &= F e^{ika} \left( \cos(la) - i \frac{k}{l} \sin(la) \right) \end{aligned}$$

Substituting this back into the expression we found for  $C$  (Eqn. 5), we find that

$$\begin{aligned} C &= i \frac{k}{l} F e^{ika} \frac{1}{\cos(la)} + F e^{ika} \left( \cos(la) - i \frac{k}{l} \sin(la) \right) \frac{\sin(la)}{\cos(la)} \\ &= i \frac{k}{l} F e^{ika} \frac{1}{\cos(la)} + F e^{ika} \sin(la) - i \frac{k}{l} F e^{ika} \frac{\sin^2(la)}{\cos(la)} \\ &= i \frac{k}{l} F e^{ika} \frac{1 - \sin^2(la)}{\cos(la)} + F e^{ika} \sin(la) \\ &= i \frac{k}{l} F e^{ika} \cos(la) + F e^{ika} \sin(la) \\ (7) \quad C &= F e^{ika} \left( \sin(la) + i \frac{k}{l} \cos(la) \right) \end{aligned}$$

Replacing  $C$  and  $D$  with Eqn. 7 and 6, respectively, in Eqn. 1,

$$\begin{aligned} A e^{-ika} + B e^{ika} &= -F e^{ika} \left( \sin(la) + i \frac{k}{l} \cos(la) \right) \sin(la) + F e^{ika} \left( \cos(la) - i \frac{k}{l} \sin(la) \right) \cos(la) \\ &= F e^{ika} \left( -\sin^2(la) - 2i \frac{k}{l} \sin(la) \cos(la) + \cos^2(la) \right) \\ &= F e^{ika} \left( \cos^2(la) - \sin^2(la) - 2i \frac{k}{l} \sin(la) \cos(la) \right) \\ B e^{ika} &= F e^{ika} \left( \cos^2(la) - \sin^2(la) - 2i \frac{k}{l} \sin(la) \cos(la) \right) - A e^{-ika} \\ (8) \quad B &= F \left( \cos^2(la) - \sin^2(la) - 2i \frac{k}{l} \sin(la) \cos(la) \right) - A e^{-2ika} \end{aligned}$$

$$\begin{aligned}
ik \left( Ae^{-ika} - Be^{ika} \right) &= l \left( Fe^{ika} \left( \sin(la) + i\frac{k}{l} \cos(la) \right) \cos(la) + Fe^{ika} \left( \cos(la) - i\frac{k}{l} \sin(la) \right) \sin(la) \right) \\
i\frac{k}{l} \left( Ae^{-ika} - Be^{ika} \right) &= Fe^{ika} \left( 2 \sin(la) \cos(la) + i\frac{k}{l} \cos^2(la) - i\frac{k}{l} \sin^2(la) \right) \\
&= Fe^{ika} \left( i\frac{k}{l} (\cos^2(la) - \sin^2(la)) + 2 \sin(la) \cos(la) \right)
\end{aligned}$$

Replacing  $B$  with Eqn. 8,

$$\begin{aligned}
i\frac{k}{l} \left( 2Ae^{-ika} - Fe^{ika} \left( \cos^2(la) - \sin^2(la) - 2i\frac{k}{l} \sin(la) \cos(la) \right) \right) &= Fe^{ika} \left( i\frac{k}{l} (\cos^2(la) - \sin^2(la)) \right. \\
&\quad \left. + 2 \sin(la) \cos(la) \right) \\
2i\frac{k}{l} Ae^{-ika} - i\frac{k}{l} Fe^{ika} \left( \cos^2(la) - \sin^2(la) - 2i\frac{k}{l} \sin(la) \cos(la) \right) &=
\end{aligned}$$

$$\begin{aligned}
i\frac{k}{l} Ae^{-2ika} &= F \left[ i\frac{k}{l} (\cos^2(la) - \sin^2(la)) + \sin(la) \cos(la) + \frac{k^2}{l^2} \sin(la) \cos(la) \right] \\
&= F \left[ i\frac{k}{l} (\cos^2(la) - \sin^2(la)) + \left( 1 + \frac{k^2}{l^2} \right) \sin(la) \cos(la) \right] \\
F &= \frac{i\frac{k}{l} Ae^{-2ika}}{i\frac{k}{l} (\cos^2(la) - \sin^2(la)) + \left( 1 + \frac{k^2}{l^2} \right) \sin(la) \cos(la)} \\
&= \frac{Ae^{-2ika}}{\cos^2(la) - \sin^2(la) - i\frac{l}{k} \left( 1 + \frac{k^2}{l^2} \right) \sin(la) \cos(la)} \\
&= \frac{Ae^{-2ika}}{\cos^2(la) - \sin^2(la) - i \left( \frac{l}{k} + \frac{k}{l} \right) \sin(la) \cos(la)} \\
(9) \quad F &= \frac{Ae^{-2ika}}{\cos(2la) - i \left( \frac{k^2 + l^2}{2kl} \right) \sin(2la)}
\end{aligned}$$

Solving for the transmission coefficient,

$$\begin{aligned}
 T &= \frac{|F|^2}{|A|^2} \\
 &= \frac{1}{\left[ \cos(2la) + i \left( \frac{k^2 + l^2}{2kl} \right) \sin(2la) \right] \left[ \cos(2la) - i \left( \frac{k^2 + l^2}{2kl} \right) \sin(2la) \right]} \\
 T^{-1} &= \cos^2(2la) + \left( \frac{k^2 + l^2}{2kl} \right)^2 \sin^2(2la)
 \end{aligned}$$

$T$  will equal 1 when  $2la = n\pi$ .

$$\begin{aligned}
 \frac{2a}{\hbar} \sqrt{2m(E_n + V_0)} &= n\pi \\
 2m(E_n + V_0) &= \frac{n^2 \pi^2 \hbar^2}{(2a)^2} \\
 E_n + V_0 &= \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} \\
 V_0 &= \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} - E_n
 \end{aligned}$$

It is useful to note that these are the same energies as those allowed for the infinite square well.

When  $n = 1$  (the first time  $T = 1$  in the given graph, at approximately  $E \sim 1.25$  eV), we find

$$V_0 \sim \frac{\pi^2 \hbar^2}{2m(12\text{\AA})^2} - 1.25 \text{ eV}$$

$$\boxed{V_0 \sim 9.07 \text{ eV}}$$

**Problem 5.** *In the double helix DNA molecule, each base from one strand bonds to a base in the other strand. The correct matches A-T and G-C are more tightly bound than the incorrect matches (mismatches). At 300 K, the probability for a mismatch to occur is about  $10^{-9}$  per base pair. The DNA molecule can be assumed to be a thermodynamic system in equilibrium with a thermal reservoir. If the probability for a mismatch is determined entirely by the binding energy difference between the correct and incorrect base pairs, what is this energy difference? When the temperature is raised by 20 C, how will the mismatch probability affected?*

In a two-state system, the probability for either state to occur depends entirely on the energies of the two states. In particular, the probability for a state  $i$  is related to the partition function:

$$p_i = \frac{g_i e^{-\beta E_i}}{\sum_i g_i e^{-\beta E_i}}$$

where  $g_i$  is the degeneracy of each state, which in our case is 1. Since tightly bound states have energies lower than loosely bound states, we can arbitrarily set the energy of a mismatched state to be  $\varepsilon$  and the energy of a matched state to be 0. Therefore, the energy difference between the states will necessarily be  $\varepsilon$ . The probability for each state is

$$p_{\text{mismatch}} = \frac{e^{-\beta\varepsilon}}{e^{-\beta\varepsilon} + e^0} = 10^{-9}, \quad p_{\text{match}} = \frac{e^0}{e^{-\beta\varepsilon} + e^0} = 1 - 10^{-9}.$$

Taking  $p_{\text{mismatch}}$ , we can solve for  $\varepsilon$ .

$$e^{-\beta\varepsilon} = \frac{10^{-9}}{1 - 10^{-9}}$$

$$\varepsilon = -kT \ln \left( \frac{10^{-9}}{1 - 10^{-9}} \right)$$

At  $T = 300$  K,  $\varepsilon = 8.58 \times 10^{-20} \text{ N} \cdot \text{m} = 0.53574$  eV. So at  $T = 320$  K,  $\varepsilon = 9.156 \times 10^{-20} \text{ N} \cdot \text{m} = 0.57145$  eV. The mismatch probability at  $T = 320$  K is, therefore,

$$p_{\text{mismatch}} = \frac{e^{-k(320 \text{ K})(9.156 \times 10^{-20} \text{ N} \cdot \text{m})}}{e^{-k(320 \text{ K})(9.156 \times 10^{-20} \text{ N} \cdot \text{m})} + 1} = 0.999 \times 10^{-9}.$$

The probability for a mismatch decreases by a slight amount for a slightly higher temperature.

**Problem 6.** *A gas obeys the equation of state*

$$P = \frac{NkT}{V} + \frac{B(T)}{V^2}$$

where  $B$  is a function of temperature  $T$  only. Find the work done if the gas, initially at  $T$  and volume  $V$  is expanded isothermally and reversibly to volume  $2V$ .

The super awesome fundamental equation of thermodynamics is

$$U = TS - PV + \mu N$$

and in the differential form

$$dU = SdT + TdS - PdV - VdP + \mu dN + Nd\mu.$$

The first term goes away since the expansion is isothermal. The second term goes away since the expansion is reversible. The last two terms go away because the number of particles is not changing and the gas is not changing flavor. The fourth term goes away too and we are left with

$$dU = -PdV.$$

So, the work done is

$$\begin{aligned}
 W &= \int_V^{2V} \left( \frac{NkT}{V} + \frac{B(T)}{V^2} \right) dV \\
 &= NkT \ln V \Big|_V^{2V} - \frac{B(T)}{V} \Big|_V^{2V} \\
 &= NkT \ln 2 + \frac{B(T)}{2V}
 \end{aligned}$$

**Problem 7.** *By considering the number of micro states of a (small) system A in thermal contact with a larger reservoir A', derive the ratio of probabilities  $P(U_1)/P(U_2)$  of finding A with energy  $U_1$  or  $U_2$ , in terms of temperature T. State your assumptions.*

In the spirit of problem 5, the probability is related to the partition function of the system A:

$$P(U_{1,2}) = \frac{e^{-\beta U_{1,2}}}{\sum_i e^{-\beta U_i}}.$$

The ratio of probabilities cancels out the partition function so we get, simply,

$$\frac{P(U_1)}{P(U_2)} = \frac{e^{-U_1/kT}}{e^{-U_2/kT}} = e^{(U_2-U_1)/kT}.$$

Since the system A is in thermal contact with A', the temperature, T, is the same for all microstates. In addition, we assume that all microstates are equally likely.

**Problem A1: You call this exciting?** *Consider a one-dimensional simple harmonic oscillator of mass m and angular frequency  $\omega$  in its ground state at  $t = -\infty$ . It is acted upon by a spatially uniform time dependent **force** (not potential) given by*

$$F(t) = \frac{F_0 \tau}{\omega(\tau^2 + t^2)} \quad \text{for } -\infty < t < \infty.$$

(A). *Using time-dependent perturbation theory to first order calculate the probability that the oscillator is found in the first excited state at  $t = \infty$ .*

In time-dependent perturbation theory, we consider transitions between states. The amplitude for a certain transition to occur from state  $a$  to state  $a'$  under the influence of a perturbed Hamiltonian is (see Fermi Golden Rule):

$$c(t) = -\frac{i}{\hbar} \int_0^t dt' \langle a' | H_1(t') | a \rangle e^{ia'\omega t}.$$



The initial state  $|a\rangle$  is the ground state,  $|0\rangle$ . Let us calculate the amplitude for an arbitrary final state  $\langle a'|$ . To get the perturbed Hamiltonian,  $H_1$ , we integrate the perturbing force with respect to position:

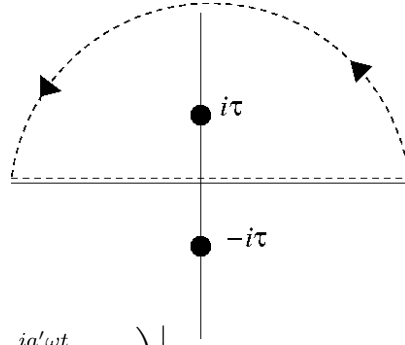
$$U = - \int F(t) dx = - \frac{F_0 \tau x}{\omega(\tau^2 + t^2)} = H_1(t, x).$$

Integrating over the entire temporal range of the perturbing Hamiltonian, the transition amplitude is therefore

$$\begin{aligned} c(t) &= -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt' \langle a' | \frac{-F_0 \tau x}{\omega(\tau^2 + t'^2)} | 0 \rangle e^{ia'\omega t'} \\ &= \frac{i}{\hbar} \frac{F_0 \tau}{\omega} \langle a' | x | 0 \rangle \int_{-\infty}^{\infty} \frac{e^{ia'\omega t}}{\tau^2 + t^2} \end{aligned}$$

Using the Hint from the end of the problem, we see that  $\langle a' | x | 0 \rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \delta_{a',1}$ . In addition, the integral is not possible using normal methods so a contour integral is required. The function  $\frac{e^{ia'\omega t}}{\tau^2 + t^2}$  has two simple poles, at  $\pm i\tau$ . Our contour (the upper semi-circle) encloses only one of the poles so the value of the integral becomes simply

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{e^{ia'\omega t}}{\tau^2 + t^2} &= 2\pi i \text{Res}(+i\tau) \\ &= 2\pi i \left( (t - i\tau) \frac{e^{ia'\omega t}}{(t + i\tau)(t - i\tau)} \right) \Big|_{t=i\tau} \\ &= \frac{\pi}{\tau} e^{-a'\omega\tau} \end{aligned}$$



And the amplitude becomes:

$$c(t) = \frac{i}{\hbar} \frac{F_0 \tau}{\omega} \langle a' | x | 0 \rangle \int_{-\infty}^{\infty} \frac{e^{ia'\omega t}}{\tau^2 + t^2} = \frac{i}{\hbar} \frac{F_0 \tau}{\omega} \left(\frac{\hbar}{2m\omega}\right)^{1/2} \delta_{a',1} \frac{\pi}{\tau} e^{-a'\omega\tau}.$$

To find the probability we take the modulus squared,

$$\begin{aligned} |c(t)|^2 &= \left( \frac{i}{\hbar} \frac{F_0}{\omega} \left(\frac{\hbar}{2m\omega}\right)^{1/2} \delta_{a',1} \pi e^{-a'\omega\tau} \right) \left( -\frac{i}{\hbar} \frac{F_0}{\omega} \left(\frac{\hbar}{2m\omega}\right)^{1/2} \delta_{a',1} \pi e^{-a'\omega\tau} \right) \\ &= \frac{F_0^2 \pi^2}{2m\hbar\omega^3} e^{-2a'\omega\tau} \delta_{a',1} \end{aligned}$$

So the probability to find the oscillator in the first excited state,  $a' = 1$ , is

$$|c(t)|^2 = \frac{F_0^2 \pi^2}{2m\hbar\omega^3} e^{-2\omega t}.$$

(B). Again, with time-dependent perturbation theory to first order calculate the probability that the oscillator is found in any other excited state at  $t = \infty$ .

In our general probability expression, we have a delta function,  $\delta_{a',1}$ . This ensures that any transition between the ground state and a state other than the first excited state is forbidden. So the oscillator has a probability of zero for such transitions. Even more generally, transitions are not possible between states which are more than one excitation level apart.

(C). Show that for  $\tau \gg 1/\omega$ , the probability for excitation is essentially negligible.

As  $\tau, \omega \rightarrow \infty$ , the probability,  $|c(t)|^2$ , decreases since  $\omega^3$  and  $e^{2\omega\tau}$  are in the denominator.

Hint: if  $x$  is the position operator,  $\langle n'|x|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1})$ .

**Problem A2:** Well, since you put it that way... Consider a particle in the state described by the wave function

$$\Psi = N(x + 2z) \exp[-\alpha(x^2 + y^2 + z^2)],$$

where  $N$  is a known normalization factor.

(A). With the help of the explicit expressions given below, write the wave function as a linear superposition of spherical harmonics.

The wave function can be written in terms of spherical coordinates by substituting  $x^2 + y^2 + z^2 = r^2$  and

$$x = \left(\frac{2\pi}{3}\right)^{1/2} r (Y_1^{-1} - Y_1^{+1})$$

and

$$z = \left(\frac{4\pi}{3}\right)^{1/2} r Y_1^0.$$

The wave function becomes

$$\Psi = N \left[ \left(\frac{2\pi}{3}\right)^{1/2} (Y_1^{-1} - Y_1^{+1}) + \left(\frac{16\pi}{3}\right)^{1/2} Y_1^0 \right] r e^{-\alpha r^2}.$$

(B). For the given wave function, what are the possible measurable pairs of values  $(\ell, m)$  and what are the respective probabilities?

The only possible for  $\ell$  is  $\ell = 1$ . The possible values for  $m$  are  $m = -1, 0, 1$ . The normalization factor  $N$  is found by setting the sum of the squares of the coefficients to 1.

$$N^2 \left( \frac{16\pi}{3} + \frac{2\pi}{3} + \frac{2\pi}{3} \right) = 1$$

$$N^2 = \frac{3}{20\pi}$$

So the probabilities for each set of quantum numbers are

$$p_{\ell=1, m=-1} = N^2 \frac{2\pi}{3} = \frac{1}{10}$$

$$p_{\ell=1, m=0} = N^2 \frac{16\pi}{3} = \frac{4}{5}$$

$$p_{\ell=1, m=1} = N^2 \frac{2\pi}{3} = \frac{1}{10}.$$

*Hint:*

$$Y_1^{\pm 1}(\theta, \phi) = \mp \left( \frac{3}{8\pi} \right)^{1/2} \sin \theta (\cos \phi \pm i \sin \phi) = \mp \left( \frac{3}{4\pi} \right)^{1/2} \frac{x \pm iy}{\sqrt{2}r}$$

$$Y_1^0(\theta, \phi) = \left( \frac{3}{4\pi} \right)^{1/2} \cos \theta = \left( \frac{3}{4\pi} \right)^{1/2} \frac{z}{r}$$

**Problem A3: A new angle.** Compute the angle between the bonds described by the wave function  $\Psi_1$  and  $\Psi_2$ :

$$\begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} +1 & +1 & +1 & +1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 \end{bmatrix} \begin{bmatrix} \phi_1 \\ x\phi_2 \\ y\phi_2 \\ z\phi_2 \end{bmatrix}$$

Here  $\phi_1(r)$  and  $\phi_2(r)$  are real, spherically symmetric functions normalized by

$$\int \phi_1^2 dV = 1 \quad \int (x\phi_2)^2 dV = 1$$

Using the rule for inner products,

$$\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_1 | \Psi_1 \rangle \langle \Psi_2 | \Psi_2 \rangle \cos \theta,$$

we get

$$\langle \Psi_1 | \Psi_2 \rangle = \frac{1}{4} \int (\phi_1^2 + (x\phi_2)^2 - (y\phi_2)^2 - (z\phi_2)^2) dV = 0$$

and

$$\langle \Psi_1 | \Psi_1 \rangle = \langle \Psi_2 | \Psi_2 \rangle = \frac{1}{4} \int (\phi_1^2 + (x\phi_2)^2 + (y\phi_2)^2 + (z\phi_2)^2) dV = 1$$

So, we get, quite simply  $0 = \cos \theta$  and the angle between the bonds described is

$$\theta = \frac{\pi}{2} + n\pi.$$

$\Psi_1$  and  $\Psi_2$  are orthogonal.

**Problem B1: Hot or Cold?** Consider a system of  $N(\gg 1)$  non interacting particles.  $U$ , the energy of the total system is fixed. Each particle has energy either 0 or  $\varepsilon(> 0)$ .  $n_0$  and  $n_1$  are the occupation numbers of the two states.

(A). What is the entropy of the system?

First, the total energy of the system is  $U = n_0(0) + n_1(\varepsilon) = n_1\varepsilon$ . So  $n_1 = \frac{U}{\varepsilon}$  and  $n_0 = N - \frac{U}{\varepsilon}$ . Now, the entropy of the system is

$$S = k \ln \Omega$$

where

$$\Omega = \binom{N}{n_0} = \frac{N!}{n_0!(N - n_0)!} = \frac{N!}{n_0!n_1!} = \frac{N!}{(N - \frac{U}{\varepsilon})! (\frac{U}{\varepsilon})!}.$$

So the entropy becomes

$$\begin{aligned} \frac{S}{k} &= \ln N! - \ln \left( N - \frac{U}{\varepsilon} \right)! - \ln \left( \frac{U}{\varepsilon} \right)! \\ &= N \ln N - N - \left( N - \frac{U}{\varepsilon} \right) \ln \left( N - \frac{U}{\varepsilon} \right) + N - \frac{U}{\varepsilon} - \frac{U}{\varepsilon} \ln \frac{U}{\varepsilon} + \frac{U}{\varepsilon} \\ &= N \ln N - N \ln \left( N - \frac{U}{\varepsilon} \right) + \frac{U}{\varepsilon} \ln \left( N - \frac{U}{\varepsilon} \right) - \frac{U}{\varepsilon} \ln \frac{U}{\varepsilon} \\ S &= kN \ln \left[ \frac{N}{N - \frac{U}{\varepsilon}} \right] + k \frac{U}{\varepsilon} \ln \left[ \frac{N - \frac{U}{\varepsilon}}{\frac{U}{\varepsilon}} \right] \end{aligned}$$

(B). Derive a relationship for the temperature as a function of  $U$ .

By definition,

$$\frac{\partial S}{\partial U} = \frac{1}{T}.$$

So,

$$\frac{\partial S}{\partial U} = \frac{k}{\varepsilon} \ln \left( \frac{N - \frac{U}{\varepsilon}}{\frac{U}{\varepsilon}} \right)$$

and, therefore,

$$\frac{1}{T} = \frac{k}{\varepsilon} \ln \left[ \frac{N - \frac{U}{\varepsilon}}{\frac{U}{\varepsilon}} \right].$$

(C). Under what range of values of  $n_0$  is the temperature  $T < 0$ ?

We can write the temperature in terms of  $n_0$  and  $n_1$ :

$$T = \frac{\varepsilon}{k} \ln \left[ \frac{n_1}{n_0} \right].$$

The temperature can only be negative if there are more particles in the low energy state than the high energy state ( $n_0 > n_1$ ). This negative temperature means the system is in a population inversion.

(D). Suppose such a system (call it I) with  $T < 0$  is brought into contact with another system (call it II) with  $T > 0$ . Explain the direction in which heat flows.

In a population inversion, the negative temperature system loses energy to raise the temperature. Heat flows from the colder system to the warm temperature.

**Problem B2: Do you hear what I hear?** At  $T=0$ , the velocity of sound  $u$  in a spin  $-1/2$  Fermi gas (i.e. an electron gas) is given by

$$u^2 = \left( \frac{\partial P}{\partial \rho} \right)_{T=0}$$

where  $\rho = mn$ , in which  $m$  is the mass of the gas particles and  $n$  is the number density.

(A). If  $\mu$  is the chemical potential, show that

$$\left( \frac{\partial P}{\partial \rho} \right)_T = \left( \frac{n}{m} \right) \left( \frac{\partial \mu}{\partial n} \right).$$

The differential form of the super special fundamental thermodynamic relationship is

$$dU = TdS + SdT - PdV - VdP + \mu dN + Nd\mu.$$

Since the system is held at constant temperature, the  $dT$  term goes away. Now, let us divide the entire equation by  $mVdn$  where  $n$  is the number density,  $N/V$ , and  $m$  is the mass. We get

$$\frac{dU}{mVdn} = \frac{TdS}{mVdn} - \frac{PdV}{mVdn} - \frac{VdP}{mVdn} + \frac{\mu dN}{mVdn} + \frac{Nd\mu}{mVdn}.$$

This simplifies to

$$\frac{dU}{mdN} = \frac{TdS}{mVdn} - \frac{PdV}{mVdn} + \frac{\mu}{m} + \frac{n}{m} \frac{d\mu}{dn} - \frac{dP}{d\rho}$$

where  $\rho = mn$ . Now, if we assume the entropy and the volume are constant, we can assume

$$\mu = \left( \frac{dU}{dN} \right)_{S,V}$$

and we can simplify our equation further:

$$\left(\frac{dP}{d\rho}\right)_T = \frac{n}{m} \frac{d\mu}{dn}.$$

(B). Find an expression for the total number of electrons in terms of fundamental constants and the momentum of the Fermi level,  $p_F$ .

$$N = \frac{4\pi gV}{3h^3} p_F^3$$

See Pathria pg 234.

(C). Find an expression for the total energy  $E$  of the gas.

See Pathria pg 235.

(D). Using the equation of state for a Fermi gas,  $PV = (2/3)E$ , calculate the sound velocity in the limit of zero temperature using the results of parts A-C, and expressing your results in terms of  $n$  and  $m$ .

Combine all the answers.