#### STONY BROOK UNIVERSITY

## DEPARTMENT OF PHYSICS AND ASTRONOMY

Graduate Placement Exam Part 2, Aug. 22, 2012 (18:00 - 22:30)

General Instructions: This exam is for incoming graduate students who wish to demonstrate mastery in one or more areas of the graduate core curriculum, in order to skip one or more of the first-year courses. Do two of the three problems in either or both areas. Each problem is worth 20 points, and unless stated otherwise, all parts of each question have equal weight.

Each solution should typically take less than 45 minutes.

Use one exam book for each problem, and label it carefully with the problem topic and number and your name. Make sure to do every part of the problems you choose.

You may use a one page help sheet, a calculator, and with the proctor's approval, a foreign language dictionary. No other materials may be used.

# Quantum Mechanics 1

A particle of mass m moves in a three-dimensional spherically-symmetric potential

$$V(r) = -u\delta(r-a), \quad u > 0.$$

- (a) Reduce the radial part of the Schrödinger equation to the effective one-dimensional problem and write down the appropriate boundary conditions the wavefunction of a bound state should satisfy in this problem.
- (b) Find the condition on u for the potential to have at least one bound state.
- (c) Compare this result to a one-dimensional quantum particle in attractive  $\delta$ -function potential.

## **SOLUTION:**

(a) For a spherically symmetric potential, solution of the Schrödinger equation can be obtained by the separation of variables in the spherical coordinate system. The equation for the radial part R(r) of the wavefunction is

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[V(r) + \frac{\hbar^2l(l+1)}{2mr^2}\right]R(r) = ER(r),$$

and by substitution  $R(r) = \psi(r)/r$  is reduced to the one-dimensional form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]\psi(r) = E\psi(r), \quad r \ge 0,$$

where l is the magnitude of the angular momentum. Since angular momentum increases the total potential in the effective one-dimensional problem, the minimum value of the potential strength u for the existence of the bound state will arise naturally for l=0. In this case, the radial equation for the bound states (E<0) reduces for the potential  $V(r)=-u\delta(r-a)$  in the problem and  $r\neq a$  to

$$\psi''(r) - k^2 \psi(r) = 0,$$

where the wavevector k gives the state energy  $E = -\hbar^2 k^2/(2m)$ .

The wavefunction that solves this equation and satisfies the appropriate boundary condition

$$\psi(r) \to 0 \quad \text{for } r \to 0, \ r \to \infty,$$

should have the following form:

$$\psi(r) = \begin{cases} A \sinh(kr), & 0 \le r < a, \\ Be^{-kr}, & r > a, \end{cases}$$

where A, B are some constants.

(b) For the  $\delta$ -function potential,  $\psi(r)$  should satisfy the following conditions at r=a:

$$\psi(a+0) = \psi(a-0); \quad \psi'(a+0) - \psi'(-0) = -(2mu/\hbar^2)\psi(a).$$

Applied to the wavefunction above, these conditions give the following equation for the wavevector k:

$$x \coth x = \lambda - x$$
,  $x \equiv ka > 0$ ,  $\lambda \equiv 2mua/\hbar^2$ .

Analyzing this equation qualitatively, we see that it has a solution only if  $\lambda > 1$ , i.e.

$$u > \hbar^2/(2ma) .$$

For smaller values of u, there are no bound states.

(c) We see that, in agreement with general properties of the Schrödinger equation, the 3-dimensional  $\delta$ -function potential should be sufficiently strong to create a bound state. In contrast to this, arbitrary weak attractive 1-dimensional potential has a bound state.

# Quantum Mechanics 2

Consider the scattering of two non-relativistic particles of mass m and charge e with relative momentum p interacting through the screened Coulomb interaction

$$V(r) = \frac{e^2}{4\pi\epsilon r}e^{-\lambda r}.$$

- (a) Calculate the differential cross section  $\frac{d\sigma}{d\Omega}(\theta)$  for scattering through an angle  $\theta$  in the Born approximation treating the particles as distinguishable.
- (b) Now take the two particles to be electrons and find  $\frac{d\sigma}{d\Omega}(\theta)$  in the state with total spin S=0 and S=1.

## **SOLUTION:**

(a) The relative motion of the two particles is described by the Schrödinger equation with the reduced mass m/2:

$$\left[-\frac{\hbar^2}{m}\nabla^2 + V(r)\right]\psi(\bar{r}) = E\psi(\bar{r}), \qquad (1)$$

and energy  $E = p^2/m$ . In the Born approximation, the scattering amplitude  $f(\theta)$  that determines the differential cross section,  $\frac{d\sigma}{d\Omega}(\theta) = |f(\theta)|^2$  is given by the standard expression:

$$f(\theta) = -\frac{m}{4\pi\hbar^2}V(\bar{q}),$$

where  $\bar{q} = \bar{k} - \bar{k}'$  is the change of the relative wavevector  $\bar{k} = \bar{p}/\hbar$  in the scattering process, related to the scattering angle as  $q = 2k\sin(\theta/2)$ , and  $V(\bar{q})$  is the Fourier component of the potential V(r):

$$V(\bar{q}) = \int d^{(3)}r \, V(r)e^{i\bar{q}\bar{r}}.$$

For the screened Coulomb interaction in the problem, the integral can be taken directly:

$$V(\bar{q}) = \frac{e^2}{\epsilon} \frac{1}{q^2 + \lambda^2} \,,$$

giving the scattering amplitude:

$$f(\theta) = -\frac{1}{a(q^2 + \lambda^2)}, \quad a = \frac{4\pi\epsilon\hbar^2}{me^2}.$$

Expressing the factor  $q^2$  through the angle  $\theta$  we obtain finally the differential cross section:

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{a^2} \frac{1}{[2k^2(1-\cos\theta) + \lambda^2]^2}.$$

(b) When the two particles are identical, the total wavefunction should have certain symmetry with respect to the interchange of particle coordinates. In the scattering process described by the Schrödinger equation (1), this interchange corresponds to changing sign of  $\bar{r}$ , i.e., to changing sign of the relative momentum  $\bar{p}$ . Thus, the wavefunction in this case is the combination of two components, with momentum  $\bar{p}$  and  $-\bar{p}$ . Accordingly, the amplitude of scattering in the certain direction is the sum of the "single-particle" scattering amplitudes at angle  $\theta$  and  $\pi - \theta$ . If the two electrons have total spin S=0, their orbital wavefunction should be symmetric. Therefore, the two amplitudes should be added together:

$$f^{(S=0)}(\theta) = f(\theta) + f(\pi - \theta),$$

and

$$\frac{d\sigma^{(S=0)}}{d\Omega}(\theta) = \frac{1}{a^2} \left[ \frac{1}{2k^2(1-\cos\theta) + \lambda^2} + \frac{1}{2k^2(1+\cos\theta) + \lambda^2} \right]^2.$$

If the two electrons have total spin S=1, their orbital wavefunction should be antisymmetric, and the two amplitudes should be subtracted:

$$f^{(S=1)}(\theta) = f(\theta) - f(\pi - \theta),$$

so that

$$\frac{d\sigma^{(S=1)}}{d\Omega}(\theta) = \frac{1}{a^2} \left[ \frac{1}{2k^2(1-\cos\theta) + \lambda^2} - \frac{1}{2k^2(1+\cos\theta) + \lambda^2} \right]^2.$$

# Quantum Mechanics 3

Find the vector  $\bar{\Omega}$  in the following relation for an angular momentum operator  $\bar{J}$  normalized to  $\hbar$ :

$$e^{-i\frac{\pi}{2}J_x}e^{-i\frac{\pi}{2}J_y}e^{-i\frac{\pi}{2}J_z} = e^{-i\bar{\Omega}\cdot\bar{J}},$$

- (a) first, in the specific case of the angular momentum j = 1/2;
- (b) for arbitrary j, using the geometric interpretation of the operators in this relation.

## **SOLUTION:**

(a) For j = 1/2, angular momentum operator  $\bar{J}$  normalized to  $\hbar$  is  $\bar{J} = (1/2)\{\sigma_x, \sigma_y, \sigma_z\} \equiv \bar{\sigma}/2$ , where  $\sigma$ 's are the Pauli matrices. One can simplify the equation given in the problem using the standard relations for matrices  $\sigma$ , e.g.,

$$e^{-i\bar{\phi}\cdot\bar{\sigma}} = \cos\phi - i\bar{n}\cdot\bar{\sigma}\sin\phi,$$

where  $\bar{\phi}$  is an arbitrary vector of length  $\phi = |\bar{\phi}|$  in the direction  $\hat{n} = \bar{\phi}/\phi$ . Comparing the two sides of the simplified equation:

$$\frac{-i}{\sqrt{2}}(\sigma_x + \sigma_z) = \cos(\Omega/2) - i\hat{n} \cdot \bar{\sigma}\sin(\Omega/2),$$

we see that

$$\cos(\Omega/2) = 0$$
,  $n_x = n_z = 1/\sqrt{2}$ ,  $n_y = 0$ ,

i.e.,  $\Omega = \pi$ , giving finally

$$\bar{\Omega} = \frac{\pi}{\sqrt{2}} \{1, 0, 1\}.$$

(b) For arbitrary magnitude of the angular momentum, the vector  $\bar{\Omega}$  can be found by recognizing that the operators of the angular momentum are generators of rotation. Three operators on the l.h.s. of the equation in the problem represent a sequence of three rotations by the angle  $\pi/2$  around axes z, y, and x. A convenient way of finding one rotation equivalent to this sequence is to see how the unit vectors  $\hat{x}, \hat{y}, \hat{z}$  along the corresponding axes are transformed by this sequence of rotations. Considering the sequence of three active (i.e., rotating a vector, not the coordinate system) counterclock-wise rotations, one finds the transformation of the unit vectors:

$$\hat{x} \rightarrow \hat{z}$$
,  $\hat{y} \rightarrow -\hat{y}$ ,  $\hat{z} \rightarrow \hat{x}$ .

Now, one can check directly that this transformation is induced by the rotation represented by the same vector  $\bar{\Omega}$  found above: rotation through angle  $\pi$  around the axis set by the unit vector  $\hat{n} = (1/\sqrt{2})\{1,0,1\}$ . Therefore, this vector  $\bar{\Omega}$  makes the equation in the problem valid for the angular momentum operators of arbitrary magnitude.

## Statistical Mechanics 1

An ideal classical gas, confined in a container with the linear size scale L, had been in thermal equilibrium at temperature T. Then a small hole of size a << L was opened in the wall of the container for a short time interval t such that  $a << v_0 t << L$ , where  $v_0$  is the r.m.s. velocity of the molecules in equilibrium. Find the r.m.s. velocity of the escaped molecules and compare it with  $v_0$ . On the basis of the comparison, what would be the most immediate observable effect of the gas emission?

# **SOLUTION:**

Due to the condition  $v_0t \ll L$ , during the period of the hole being open, we can neglect collisions of molecules with walls. Hence only the molecules flying directly into the hole may escape. Moreover, velocity of such molecules should satisfy the condition  $v \geq r/\Delta t$ , where r is the initial distance of the molecule from the hole. (Due to the condition  $a \ll r$ , satisfied for most escaped molecules, it is not important which exactly part of the hole we are speaking about.) Hence, the number of escaped molecules with velocities within the range [v, v + dv] is proportional to  $r^3 = (v\Delta t)^3$ :

$$dN = \text{const} \times (v\Delta t)^3 w(v) dv$$

where the distribution of initial velocities is described by the Maxwell distribution,

$$w(v) \propto \exp^{-mv^2/2T}$$

(Since molecules from each point may reach the hole only if they fly in a certain direction, the distribution should be for one velocity component only.) As a result,

$$dN = c(vt)^3 \exp^{-mv^2/2T} dV$$

where c is some constant. Now the average  $v^2$  of the escaped molecules may be calculated as

$$< v^2> = \frac{\int v^2 dN}{\int dN} = \frac{c \int_0^\infty v^2 (v\Delta t)^3 \exp^{-mv^2/2T} dV}{c \int_0^\infty (v\Delta t)^3 \exp^{-mv^2/2T} dV} = \frac{2T}{m} \frac{\int_0^\infty \zeta^5 \exp^{-\zeta^2 d\zeta}}{\int_0^\infty \zeta^3 \exp^{-\zeta^2 d\zeta}} = \frac{2T}{m} \frac{\Gamma(3)/2}{\Gamma(2)/2} = \frac{4T}{m}$$

Comparing the result with the r.m.s. velocity  $v_0 = \delta v$  of the gas as a whole, for their ratio we get

$$\frac{\langle v^2 \rangle^{1/2}}{v_0} = \left(\frac{4}{3}\right)^{1/2} \approx 1.154.$$

The immediately observable result of the escape of (on the average) hotter molecule is cooling of the remaining gas.

## Statistical Mechanics 2

Consider a classical 2D particle free to move within area A.

- a) (2 pts) Define pressure in 2D
- b) (8 pts) Calculate the average energy, entropy, free energy, and the equation of state starting from the microcanonical distribution,
- c) (8 pts) Calculate the average energy, entropy, free energy, and the equation of state **starting from the canonical distribution**, and

(2 pts) Now consider a system of many quantum particles. Indicate the modifications needed (i) if the particles are fermions and (ii) if the particles are bosons.

Hint: The volume of an n dimensional hypersphere is

$$V_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2} + 1)}$$

# **SOLUTION:**

- (a) In 2D, P = dF/dl = dp/dt/dl in which l is a coordinate measuring the boundary of the area A.
- (b) The number of quantum states of the ensemble with an energy below  $E_n$  is

$$\Sigma_n = \frac{g^N}{(2\pi\hbar)^{2N}} \int_{p_i^2/2m < E, 0 < j < 2N} d^{2N}q d^{2N}p = \frac{(gA)^{2N}}{(2\pi\hbar)^{2N}} p_E^{2N} V_{2N} = \frac{(gA)^{2N}}{(2\pi\hbar)^{2N}} (2mE_N)^N \frac{\pi^N}{\Gamma(N+1)}$$

with

$$g(E_N) = \frac{d\Sigma_N}{dE_N} = \frac{NA^N}{\Gamma(N+1)} \left(\frac{m}{2\pi\hbar^2}\right)^N E_N^{N-1},$$

 $S_N = \log g(EN) + \operatorname{const} = N \log A + (N-1) \log E_N + N \log \left(\frac{m}{2\pi\hbar^2}\right) + \log N - \log[\Gamma(N+1)] + \operatorname{const},$ 

and

$$S_N \to_{N\to\infty} N \log \left[ A \left( \frac{m}{2\pi\hbar^2} \right) \left( \frac{E_N}{N} \right) \right] + N + \text{const},$$

and

$$\frac{1}{T} \equiv \left(\frac{\partial S_N}{\partial E_N}\right)_A = \frac{N}{E_N}$$

so that the average energy  $E \equiv E_N/N$  per particle equals T (in accordance with the equipartition theorem), and

$$S \equiv \frac{S_N}{N} = \log \left[ A \left( \frac{m}{2\pi\hbar^2} \right) T \right] + N + \text{const.}$$

From here,

$$F \equiv E - TS = -T\left\{1 + \log\left[A\left(\frac{m}{2\pi\hbar^2}\right)T\right]\right\} = -T\log A + f(T), \quad (*)$$

where

$$f(T) \equiv -T \left[ \log \left( \frac{mT}{2\pi\hbar^2} \right) + 1 \right].$$

In our 2D system, the usual conjugate pair of variables P, V has to be replaced with pair  $\sigma$ , A, where  $\sigma$  is the surface "anti-tension", i.e. the pressure force exerted per unit length of the border contour. As a result

$$\sigma = -\left(\frac{\partial F}{\partial A}\right)_T,$$

and together with Eq. (\*) this gives essentially the same equation of state as in 3D case:

$$\sigma = \frac{T}{A}.$$

(c) Applying the canonical distribution to a single classical particle, we have

$$Z \equiv \Sigma_n e^{-E_n/T} \to \frac{gA}{(2\pi\hbar)^2} \int e^{-p^2/2mT} d^2p = \frac{gA}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} e^{-p_x^2/2mT} dp_x \int_{-\infty}^{\infty} e^{-p_y^2/2mT} dp_y = \frac{gA}{(2\pi\hbar)^2} 2\pi mT,$$

so that

$$F = -T \log Z = -T \log \left( gA \frac{mT}{2\pi\hbar^2} \right),$$

the same formula as from the first method (besides the insubstantial addition of 1 to the logarithm), thus launching the thermodynamics autopilot to calculate the balance of the same results.

## Statistical Mechanics 3

A quantum particle is free to move over a spherical surface of radius r. Calculate its heat capacity, in the limit of low and high temperatures. (Quantify the conditions.)

#### **SOLUTION:**

The eigenfunctions of this motion are the spherical harmonics indexed by two integer quantum numbers, l=0,1,... and m with  $-l \le m \le +l$ . The corresponding eigenenergies depend on l only,

$$E_l = \frac{\hbar^2}{2mr^2}l(l+1),$$

so that every energy level (besides the ground-state one) is (2l+1)-degenerate. This means that the statistical sum of the Gibbs distribution is

$$Z = \Sigma_l = 0^{\infty} (2l+1)e^{-\left(\frac{\hbar^2}{2mr^2T}l(l+1)\right)}.(**)$$

In the high temperature limit,  $T >> \hbar^2/2mr^2$ , the sum (\*\*) converges at l >> 1, and may be replaced with an integral:

$$Z \to \int_{l=0}^{\infty} 2le^{-\left(\frac{\hbar^2}{2mr^2T}l^2\right)} = \frac{2mr^2T}{\hbar^2} \int_{0}^{\infty} e^{-\zeta}d\zeta = \frac{2mr^2T}{\hbar^2}$$

so that average energy

$$E \to \frac{1}{Z} \int_{l=0}^{\infty} E_i 2l e^{-\left(\frac{\hbar^2}{2mr^2T}l^2\right)} dl = T$$

giving heat capacity  $c \to 1$ . This result is natural, because in an inertial system which whose origin (in the given instant) coincides with the particle position, the energy of the 3D rotator may be expressed as

$$E_n = \frac{p^2}{2m} = \frac{p_1^2 + p_2^2}{2m},$$

with momentum vector  $\vec{p}$  having 2 mutually perpendicular Cartesian components (in two arbitrary directions perpendicular to sphere's radius). According to the equipartition theorem, the average energy of each of these "half-degrees of freedom" is T/2.

In the low-temperature limit  $T \ll \hbar^2/2mr^2$ , the terms of statistical sum drop fast (exponentially) with l, one may keep only two first terms - with l=0 and l=1:

$$Z \approx 1 + 3e^{-\frac{\hbar^2}{mr^2T}}$$
 and  $\log Z \approx 3e^{-\frac{\hbar^2}{mr^2T}}$ .

From here the average energy is

$$E = -\frac{\partial}{\partial (1/T)} \log Z = 3 \frac{\hbar^2}{mr^2} e^{-\frac{\hbar^2}{mr^2T}},$$

and the heat capacity is

$$c = \frac{\partial E}{\partial T} = 3\left(\frac{\hbar^2}{mr^2T}\right)^2 e^{-\frac{\hbar^2}{mr^2T}}.$$

Hence at  $T \to 0$  the heat capacity is exponentially is exponentially small - the property common for all systems with a finite gap between the zero-point energy and the excited states. Note also that the degeneracy of the excited states of the system does affect all its thermodynamic properties, in particular being responsible for factor 3 in the final result.