

STONY BROOK UNIVERSITY

DEPARTMENT OF PHYSICS AND ASTRONOMY

Graduate Placement Exam Part 2, Aug. 24, 2011 (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 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 is moving in a one-dimensional potential

$$U(x) = \begin{cases} -u\delta(x), & \text{for } -a < x < a, \\ +\infty, & \text{for } |x| \geq a, \end{cases}$$

with $u > 0$.

- (10 pts) Find the eigenenergies E_n and the eigenfunctions $\psi_n(x)$ of the even-numbered states (in the convention that the states are numbered successively starting with the ground state $n = 1$).
- (10 pts) Derive the transcendental equations that determine the energy E_1 of the ground state. Find this energy and the wavefunction $\psi_1(x)$ for a special value of the strength of the δ -function, $u = \hbar^2/ma$.

SOLUTION:

a. Since the potential is symmetric $U(-x) = U(x)$, the wavefunctions have definite parity, with the even-numbered states being odd, $\psi_n(-x) = -\psi_n(x)$. Therefore, for these states, $\psi_n(0) = 0$, and the δ -function in $U(x)$ does not have any effect on these states. This means that they coincide with the states in the same potential but without the δ -function part:

$$E_n = \frac{1}{2m}(\hbar\pi n/2a)^2, \quad \psi_n(x) = \sqrt{\frac{2}{a}} \sin(\pi n x/2a), \quad n = 2, 4, 6, \dots$$

b. Because of the negative δ -function part of the potential, the energy E_1 of the ground state can be, in principle, both positive and negative. Assuming first that $E_1 > 0$, the wavefunction that satisfies the boundary condition $\psi_1(\pm a) = 0$, and is even, $\psi_1(-x) = \psi_1(x)$, can be written as

$$\psi_1(x) = A \sin k(a - |x|), \quad E_1 = \frac{\hbar^2 k^2}{2m} > 0.$$

The boundary condition at $x = 0$ takes then the form:

$$Ak \cos ka = \frac{mu}{\hbar^2} A \sin ka,$$

a gives the equation for $\xi \equiv ka$, and therefore the energy E_1 :

$$\xi = \lambda \tan \xi, \quad \lambda \equiv \frac{mua}{\hbar^2}.$$

This equation shows qualitatively that such a solution for E_1 , i.e., this energy is positive, only if $\lambda < 1$, that is, for $u < \hbar^2/ma$. This means that if $u > \hbar^2/ma$, the energy E_1 is negative, and one should take the wavefunction $\psi_1(x)$ in the following form:

$$\psi_1(x) = A \sinh k(a - |x|), \quad E_1 = -\frac{\hbar^2 k^2}{2m} < 0.$$

Then, as above, the boundary condition at $x = 0$ gives the following equation for $\xi \equiv ka$:

$$\xi = \lambda \tanh \xi.$$

One can see qualitatively from this equation that it determines the energy $E_1 < 0$ in the regime when $\lambda > 1$, i.e. for $u > \hbar^2/ma$.

Comparison of the two equations for the ground state energy E_1 obtained above shows that for $u = \hbar^2/ma$, this energy vanishes, $E_1 = 0$. The wavefunction of the ground state in this case can be written as:

$$\psi_1(x) = A(a - |x|),$$

since then $(\psi_1)'' = 0$ for $x \neq 0$. For this special value of u , the wavefunction $\psi_1(x)$ of this form also satisfies both the boundary conditions at $x = \pm a$ and at $x = 0$:

$$\psi_1(\pm a) = 0; \quad (\psi_1)'(+0) - (\psi_1)'(-0) = (2mu/\hbar^2)\psi_1(0) = 2\psi_1(0)/a.$$

Integrating $|\psi_1(x)|^2$, we find the normalization constant:

$$A = (3/2a^3)^{1/2}.$$

Quantum Mechanics 2

Consider an isotropic three dimensional oscillator:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{m\omega^2 \mathbf{r}^2}{2}, \tag{1}$$

where $\mathbf{r} = (x, y, z)$ and $\mathbf{p} = (p_x, p_y, p_z)$.

- a. (10 pts) Find the eigenenergies E_n and their degeneracies d_n .
- b. (10 pts) Since the Hamiltonian is spherically symmetric, the energy eigenstates can be classified according to the angular momentum. What is the angular momentum l of the ground state? Using the basic properties of the wavefunction of the 1D oscillators and spherical harmonics, find l for the first excited energy level and construct the standard angular momentum states $|l, m\rangle$ out of the degenerate states of this energy.

SOLUTION:

(a.) By separation of variables in the cartesian coordinates, one sees that the problem is equivalent to three one-dimensional oscillators, along x , y , z axis. Therefore, the total energy is

$$E_n = \hbar\omega(n + 3/2),$$

where $n = 0, 1, 2, 3, \dots$ is the total number of excitations of the three 1D oscillators. In contrast to the unique ground state, all excited states are degenerate. The degeneracy d_n is equal to the number of ways one can distribute n excitations among 3 oscillators. To find d_n , one considers first the number l of the excitations of one of the oscillators, $l = 0, 1, \dots, n$, and count the number of ways the remaining $n - l$ excitations can be split between the two other oscillators. This number is seen directly to be $n - l + 1$, so that

$$d_n = \sum_{l=0}^n (n - l + 1) = \sum_{k=1}^{n+1} k = (n + 1)(n + 2)/2.$$

(b.) The first two normalized eigenfunctions of a 1D oscillator are

$$\psi_0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}, \quad \psi_1(x) = \frac{\sqrt{2}}{\pi^{1/4}} x e^{-x^2/2},$$

where the distances are measured in units of a characteristic oscillator length $\lambda = \sqrt{\hbar/(m\omega)}$. In this notations, the ground state of the 3D oscillator is

$$\psi_0(\mathbf{r}) = \frac{1}{\pi^{3/4}} e^{-(x^2+y^2+z^2)/2} = \frac{1}{\pi^{3/4}} e^{-r^2/2}.$$

Since this wavefunction in spherical coordinate system is independent of angles θ and ϕ of this system, it corresponds to the angular momentum $l = 0$.

The three degenerate states of the first excited energy level of the 3D oscillator are obtained by taking one of the 1D oscillators to be in the first excited state:

$$\psi_x(\mathbf{r}) = \frac{\sqrt{2}}{\pi^{3/4}} x e^{-r^2/2}, \quad \psi_y(\mathbf{r}) = \frac{\sqrt{2}}{\pi^{3/4}} y e^{-r^2/2}, \quad \psi_z(\mathbf{r}) = \frac{\sqrt{2}}{\pi^{3/4}} z e^{-r^2/2}.$$

Since $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$, comparing the angular dependence of these wavefunctions to spherical harmonics, we see that they all correspond to the angular momentum $l = 1$, and

$$|1, 0\rangle = |\psi_z\rangle, \quad |1, \pm 1\rangle = \frac{1}{\sqrt{2}}(|\psi_x\rangle \pm i|\psi_y\rangle).$$

Quantum Mechanics 3

Two spin-1/2 particles are in the singlet state $|s = 0\rangle \equiv |\psi\rangle$. Let $S^{\bar{n}_j}$, $j = 1, 2$, be the component of the spin of particle j in the direction defined by a unit vector \bar{n}_j .

- (12 pts) Calculate the correlator $\langle\psi|S^{\bar{n}_1}S^{\bar{n}_2}|\psi\rangle$ expressing the result in terms of the angle θ between the vectors \bar{n}_1 and \bar{n}_2 .
- (8 pts) What are the outcomes of individual measurements of the operator $S^{\bar{n}_1}S^{\bar{n}_2}$? Determine the probabilities of all individual outcomes in the singlet state.

SOLUTION:

(a.) Choosing the coordinate system such that the direction \bar{n}_1 coincides with the z axis, while the direction \bar{n}_2 lies in the $x - z$ plane, one can write the product of the two spin operators as follows:

$$S^{\bar{n}_1}S^{\bar{n}_2} = (\hbar/2)^2 \sigma_z^{(1)} \otimes [\cos \theta \sigma_z^{(2)} + \sin \theta \sigma_x^{(2)}],$$

where the superscripts indicate the spin the operators are acting on. Since the part of the operator acting on the first spin is diagonal ($\sigma_z^{(1)}$), the off-diagonal elements in the average of this operator over the singlet $|s = 0\rangle \equiv |\psi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ vanish, so that the average is:

$$\begin{aligned} \langle\psi|S^{\bar{n}_1}S^{\bar{n}_2}|\psi\rangle &= \frac{1}{2}(\hbar/2)^2 \left[\langle\uparrow|\sigma_z^{(1)}|\uparrow\rangle\langle\downarrow|[\cos \theta \sigma_z^{(2)} + \sin \theta \sigma_x^{(2)}]|\downarrow\rangle \right. \\ &\quad \left. + \langle\downarrow|\sigma_z^{(1)}|\downarrow\rangle\langle\uparrow|[\cos \theta \sigma_z^{(2)} + \sin \theta \sigma_x^{(2)}]|\uparrow\rangle \right] = -\frac{\hbar^2}{8}(\cos \theta + \cos \theta) = -\frac{\hbar^2}{4} \cos \theta. \end{aligned}$$

(b.) Diagonalizing the operator $S^{\bar{n}_1}S^{\bar{n}_2}$ given in part (a), we see that its eigenvalues, i.e., possible outcomes of measurement of this operator are $\pm\hbar^2/4$ independently of the angle θ . There are two eigenvectors that correspond to each of the eigenvalue. For $\hbar^2/4$:

$$|\psi_1^{(+)}\rangle = \cos(\theta/2)|\uparrow\uparrow\rangle + \sin(\theta/2)|\uparrow\downarrow\rangle, \quad \text{and} \quad |\psi_2^{(+)}\rangle = \sin(\theta/2)|\downarrow\uparrow\rangle - \cos(\theta/2)|\downarrow\downarrow\rangle.$$

For $-\hbar^2/4$:

$$|\psi_1^{(-)}\rangle = \sin(\theta/2)|\uparrow\uparrow\rangle - \cos(\theta/2)|\uparrow\downarrow\rangle, \quad \text{and} \quad |\psi_2^{(-)}\rangle = \cos(\theta/2)|\downarrow\uparrow\rangle + \sin(\theta/2)|\downarrow\downarrow\rangle.$$

Calculating the inner product between these eigenstates and the singlet $|s=0\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ one finds the probabilities of these outcomes of measurement:

$$p_+ = \sum_{j=1,2} |\langle\psi|\psi_j^{(+)}\rangle|^2 = \sin^2(\theta/2), \quad p_- = \sum_{j=1,2} |\langle\psi|\psi_j^{(-)}\rangle|^2 = \cos^2(\theta/2).$$

These probabilities give the average value in agreement with the one found in part (a).

Statistical Mechanics 1

A gas has the following properties:

- i. $C_V = aT^b$, and
- ii. work R_T necessary for its isothermal compression from volume V_2 to volume V_1 is $cT \ln(V_2/V_1)$, where a , b , and c are constants.

Calculate the equation of state, thermodynamic potentials, energy (E), enthalpy (H), free energy (F), Gibbs energy (G) and grand potential (Ω), and finally the entropy S of the gas. You may leave undetermined constants of integration in your answer.

SOLUTION:

For this case (given R_T), we know that

$$P(T, V_1) = -\left(\frac{\partial R_T}{\partial V_1}\right)_T = \frac{cT}{V_1}$$

which is the same as the equation of state of an ideal gas with $N = c$. Then we have

$$\frac{d^2 f}{dT^2} = -\frac{C_V}{NT} = -\frac{a}{c}T^{b-1}.$$

Integrating this twice gives

$$f = -\frac{a}{b(b+1)c}T^{b+1} + dT + g.$$

with d and g new constants of integration. After some algebraic rearranging this gives

$$f - T\frac{df}{dT} = \frac{a}{(b+1)c}T^{b+1} + g.$$

These are now used to derive the various thermodynamic potentials (in the most convenient order):

$$\begin{aligned}
S &= N \left(\ln \frac{V}{c} - \frac{df}{dT} \right) = c \ln \frac{V}{c} + \frac{a}{b} T^b - dc \\
F &= -cT \ln \frac{V}{c} + cf(T) = -cT \ln \frac{V}{c} - \frac{a}{b(b+1)c} T^{b+1} + c(dT + g) \\
E &= N \left(f - T \frac{df}{dT} \right) = \frac{a}{b+1} T^{b+1} + cg \\
H &= E + PV \\
G &= F + PV \\
\Omega &= -PV = -cT
\end{aligned}$$

Note that all but Ω involve undetermined constants from the original integration.

Statistical Mechanics 2

A round cylinder of radius R , containing an ideal classical gas is rotated about its symmetry axis with angular velocity ω . Assuming that the gas is in thermodynamic equilibrium with temperature T ,

- (12 pts) Calculate the gas pressure near the cylinder's side wall, if it is equal to P_a at the cylinder's axis, and
- (8 pts) formulate the condition of validity of your result in terms of strong inequalities between the following length scales: the de Broglie wavelength $r_Q \equiv h/(mT)^{1/2}$, effective particle size r_0 , average distance $r_A \equiv (V/N)^{1/3}$ between the particles, and cylinder radius R .

SOLUTION:

(a.) At equilibrium, the gas as the whole has to be at rest in the reference frame rotating with the cylinder. From classical mechanics we know that in this non-inertial reference frame we have to add, to all real forces, an inertial centrifugal "force"

$$\mathbf{F} = m\omega^2 \rho$$

where ρ is the vector perpendicular to the rotation axis and connecting this axis with the rotating particle. This force may be presented as $-\nabla U$, where U is the effective potential energy

$$U = -\frac{m\omega^2 \rho^2}{2} + U_0$$

with U_0 an arbitrary constant. The pressure of an ideal classical gas in the field of an external potential is given by:

$$P(\mathbf{r}) = P(0)e^{-(\frac{m\omega^2 R^2}{2T})}.$$

with $U(0) = 0$. Applying this equation to the points at the axis ($\rho = 0$) and at the wall ($\rho = R$) we get

$$P_W = P_a e^{(\frac{m\omega^2 R^2}{2T})}.$$

(b.) The condition that a gas behaves classically (negligible quantum effects) is $r_Q \ll r_A, R$, while that for an ideal gas (negligible particle interactions) is $r_0 \ll r_A, R$. A more tricky question is the relation between the particle's mean free path,

$$\ell \approx \frac{r_A^3}{r_0^3} \gg r \text{ and } R.$$

Let us assume $\ell \ll R$. Then at all distances between ℓ and R we may consider gas macroscopically, and apply to its small volume $\ell^3 \ll dA dr \ll R^3$ the following condition of mechanical equilibrium (relative to the cylinder):

$$dM\omega^2 r = dP dA$$

with $dM = mnd^3r = nm dr dA$. Using the equation of state $P = nT$ and assuming the same temperature everywhere, this yields

$$dP = m \frac{P}{T} \omega^2 r dr.$$

Integrating this immediately gives the same result as the Boltzmann formula.

Statistical Mechanics 3

A particle may occupy any of N similar sites, and jump from that site to any other one classically (i.e., without quantum-mechanical coherence between the jumps), with the same rate Γ . Find the correlation function and spectral density of fluctuations of the instantaneous occupancy $n(t)$ (equal to either 1 or 0) of any particular site.

SOLUTION:

The probability for the particle to occupy the (arbitrary) j -th site is

$$\frac{dW_j}{dt} = -(N-1)\Gamma W_j + \sum_{f=1}^N \Gamma W_f$$

Since the sum of all W_j should be equal to 1, the sum in the above equation equals to $\Gamma(1 - W_j)$, so that this is a linear differential equation for one variable:

$$\frac{dW_j}{dt} = -(N-1)\Gamma W_j + \Gamma(1 - W_j) = \Gamma(1 - NW_j)$$

and may be readily solved for arbitrary initial conditions:

$$W(t) = W(0)e^{-(N\Gamma t)} + W(\infty)(1 - e^{-(N\Gamma t)})$$

with $W_j(\infty) = 1/N$.

Now we can readily calculate all the averages of interest, starting from the (ensemble!) average of the occupancy:

$$\langle n(t) \rangle = \sum_{n=0,1} nW(n, t) = W(1, t)$$

But $W(1, t)$ is just the probability to have this particular site occupied at time t , i.e. the $W_j(t)$ given by $W(t)$ above, so

$$\langle n(t) \rangle = \langle n(0) \rangle e^{-(N\Gamma t)} + \frac{1}{N}(1 - e^{-(N\Gamma t)}).$$

The (auto-)correlation function of the instantaneous occupancy is

$$\langle n(t)n(t+\tau) \rangle = \sum_{n=0,1} nW(n, \infty) \sum_{n'=0,1} n'W(n', \tau|n, 0),$$

where the last W is the conditional probability of occupancy n' at time τ , conditioned by occupancy n at time 0. Since one of two possible occupancy numbers is zero, in this sum of generally four terms, only one term (with $n = n' = 1$) gives a nonvanishing contribution:

$$\langle n(t)n(t+\tau) \rangle = W(1, \infty)W(1, \tau|1, 0)$$

The first operand of this product equals $W(\infty) = 1/N$, while the second one is just $W(\tau)$ with the initial condition $W(0) = 1$, so that we get

$$\langle n(t)n(t+\tau) \rangle = \frac{1}{N} \left[\frac{1}{N} + \left(1 - \frac{1}{N}\right) e^{-N\Gamma\tau} \right]$$

The spectral density $S(\omega)$

$$S_n(\omega) \equiv \frac{1}{\pi} \text{Re} \int_0^\infty \frac{N-1}{N^2} e^{-N\Gamma t} e^{i\omega t} dt = \frac{N-1}{\pi N} \frac{\Gamma}{N^2(\Gamma^2 + \omega^2)}.$$

The result describes the Lorentzian line shape, with the low-frequency density scaling as $(N-1)/N^3$.