22.51 - Interaction of Radiation with Matter

Home Work Set No. 6

1. Thermodynamics of a photon gas.

In class it was shown that the Helmholtz free energy F (T, N, V) of a thermodynamic system is related to its partition function Z (T, N, V) by

$$F = -k_B T \ell n Z(T, N, V). \quad (1)$$

If we use a thermodynamic relation

$$dF = -pdV - SdT, \quad (2)$$

then we can compute the pressure by a formula

$$p = -\left(\frac{\partial F}{\partial V}\right)_{N,T} = k_B T\left(\frac{\partial \ell n Z}{\partial V}\right)_{N,T}. \quad (3)$$

For a single mode of radiation field in thermal equilibrium at temperature T, we learned in class how to calculate the partition function Z. So we can write down the free energy as

$$F = k_B T \ell n(1 - e^{-\beta h\nu}). \quad (4)$$

But for a multimode field, we have to compute the sum over modes to get the total free energy, namely,

$$F = k_B T \int_0^\infty d\nu g(\nu) \ell n(1 - e^{-\beta h\nu}). \quad (5)$$

(a) Show that, for a radiation field contained in a box of volume V,

$$g(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2 d\nu. \quad (6)$$

(b) Show that the pressure of a photon gas is, according to eq 3,

$$p = \frac{8\pi^5}{45c^3h^3}(k_B T)^4 . \tag{7}$$

(c) Likewise, show that the total energy is

$$E = \frac{8\pi^5 V}{15c^3h^3}(k_B T)^4 . \tag{8}$$

and hence by comparing eqs 7 and 8, one get an interesting relation

$$p = E/3V. \tag{9}$$

Discuss the physical meaning of the last equation in terms of classical radiation pressure.

2. Let a particle of spin 1/2 and of magnetic moment $\vec{\mu}$ traveling in y-direction passes through a homogeneous magnetic field $\vec{B}_0$ parallel to the z-direction. The particle spin in this field will be oriented in either the +z or -z direction. Let us assume that it points in the +z direction. When passing the point y=0 at t=0, the particle enters an additional field $\vec{B}_1$ parallel to the x-direction. It leaves this auxiliary field at $y = \ell$ at $t = t_0$. We would like to find out the probability of a spin flip during this time interval. You are asked to proceed to the solution in the following way.

(a) Schrödinger equation of a particle of a magnetic moment $\vec{\mu} = \mu\vec{\sigma}$ in a magnetic field $\vec{B}$ is

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi - \mu\vec{\sigma}\cdot\vec{B}\,\psi \tag{10}$$

For $t<0$, only the field $\hat{z}B_0$ acts. Let the wave function be:

$$\psi(y,t) = e^{i(ky-\omega t)}\begin{bmatrix}1\\0\end{bmatrix} \tag{11}$$

Show that the energy of the particle is

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} - \mu B_0 \tag{12}$$

(b) At t=0, the field $\hat{x}B_1$ is switched on and spin state of the particle may change, so that write for t>0,

$$\psi(\mathrm{y},\mathrm{t}) = \mathrm{e}^{\mathrm{i}(\mathrm{ky}-\omega_0 \mathrm{t})}\left\{\mathrm{a}(\mathrm{t})\begin{bmatrix}1\\0\end{bmatrix} + \mathrm{b}(\mathrm{t})\begin{bmatrix}0\\1\end{bmatrix}\right\}; \qquad \hbar\omega_0 = \frac{\hbar^2 \mathrm{k}^2}{2\mathrm{m}} \tag{13}$$

For a weak field, the Lorentz force acting perpendicular to the y-direction may be neglected so the momentum $\hbar k$ in y-direction is unchanged.

(c) In the combined field, the magnetic interaction is

$$\vec{\mu}\cdot\vec{B} = \mu(B_0\sigma_z + B_1\sigma_x) \tag{14}$$

where $\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices. Show that

$$(\vec{\mu}\cdot\vec{B})\begin{bmatrix}a\\b\end{bmatrix} = \mu\begin{bmatrix}B_0 + B_1 b\\ B_1 a - B_0 b\end{bmatrix} \tag{15}$$

(d) By substituting eq. 15 into eq. 10, show that the Schrödinger equation can be reduced to a pair of first order differential equations:

$$i\hbar\dot{a} = -\mu(B_0 a + B_1 b) \tag{16}$$

$$i\hbar\dot{b} = -\mu(B_1 a - B_0 b) \tag{17}$$

(e) Show that the solution of eq.16 andeq.17 is

$$a(t) = \cos\omega' t + \frac{iB_0}{\sqrt{B_0^2 + B_1^2}}\sin\omega' t \tag{18}$$

$$b(t) = \frac{iB_1}{\sqrt{B_0^2 + B_1^2}} \sin \omega' t \tag{19}$$

which satisfies a normalization condition

$$|a(t)|^2 + |b(t)|^2 = 1 \tag{20}$$

where $\hbar\omega' = \mu\sqrt{B_0^2 + B_1^2}$.

(f) Find the probability for the spin flip by computing $|b(t_0)|^2$ for $t_0 = \ell / v = m\ell / \hbar k$.

(g) Show that the probability of non-spin flip has a minimum value

$$|a(t_0)|^2{}_{\min} = \frac{B_0^2}{B_0^2 + B_1^2} \tag{21}$$

If $$\frac{\mu}{\hbar}\sqrt{B_0^2 + B_1^2}\,\frac{\ell}{v} = \frac{\pi}{2} \tag{22}$$

3. You are asked to work out the distribution function of coordinate in a harmonic oscillator. Remember the coordinate and its conjugate momentum operators are given by:

$$\hat{Q} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right), \qquad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^+ - \hat{a}\right). \tag{23}$$

The distribution function of Q, f(Q) is given by

$$f(Q) = \langle Q|\hat{\rho}|Q\rangle = \sum_{n=0}^{\infty}\langle Q|n\rangle\rho_{nn}\langle n|Q\rangle = \sum_{n=0}^{\infty}|\psi_n(Q)|^2\rho_{nn} \tag{24}$$

where $\rho_{nn} = \langle n|\hat{\rho}|n\rangle$ is the diagonal element of the density operator, and $\psi_n(Q) = \langle Q|n\rangle$ is the wave function of the harmonic oscillator in the nth excited state, which is real.

(a) Show that

$$f(Q) = \frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)}\psi_n^2(Q)\,. \tag{25}$$

(b) Show that

$$\psi_n(Q)\frac{d}{dQ}\psi_n(Q) = \langle n|Q\rangle\langle Q|\frac{i}{\hbar}\hat{P}|n\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left[\sqrt{n}\psi_n\psi_{n-1} - \sqrt{n+1}\psi_n\psi_{n+1}\right] \tag{26}$$

(c) Show that

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\left[\sqrt{n}\psi_n\psi_{n-1} - \sqrt{n+1}\psi_n\psi_{n+1}\right] = \left(e^{-\beta\hbar\omega} - 1\right)\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\left[\sqrt{n+1}\psi_n\psi_{n+1}\right] \tag{27}$$

(d) From Eq. (26) and (27), deduce that

$$\frac{df(Q)}{dQ} = \frac{2}{Z}\sqrt{\frac{m\omega}{2\hbar}}e^{-\beta\hbar\omega/2}\left(e^{-\beta\hbar\omega} - 1\right)\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\left[\sqrt{n+1}\psi_n\psi_{n+1}\right] \tag{28}$$

(e) Use the same operator technique to further show that

$$2Qf(Q) = \frac{2}{Z}\sqrt{\frac{\hbar}{2m\omega}}e^{-\beta\hbar\omega/2}\left(e^{-\beta\hbar\omega} + 1\right)\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\left[\sqrt{n+1}\psi_n\psi_{n+1}\right] \tag{29}$$

(e) From Eq. (28) and (29), derive a differential equation

$$\frac{df(Q)}{dQ} = -2\sigma^2 Qf(Q) \tag{30}$$

where

$$\sigma^2 = \frac{m\omega}{\hbar}\frac{1-e^{-\beta\hbar\omega}}{1+e^{-\beta\hbar\omega}} \tag{31}$$

(f) Establish finally the distribution function

$$f(Q) = \frac{1}{\sqrt{2\pi\langle Q^2\rangle}}e^{-\frac{Q^2}{2\langle Q^2\rangle}} \tag{32}$$

where $\langle Q^2 \rangle = 1/2\sigma^2$ is the second moment of the distribution.

(g) Use the distribution Eq. (32) to prove the Bloch theorem

$$\langle \exp(Q) \rangle = \exp\left[\frac{1}{2}\langle Q^2 \rangle\right] \tag{33}$$

(e) Show that the Bloch theorem also holds for $\hat{Q}$ which is a linear function of the coordinate operator.

4. A spin 1/2 nucleus is subject to a strong dc magnetic field B_0 in the z-direction and a weak rf field of magnitude B_x, at the Larmore frequency ω_0, in the x-direction. The Hamiltonian can be written as:

$$H = -\gamma B_0 \hat{I}_z - \gamma B_x \hat{I}_x \cos\omega_0 t = -\hbar\omega_0 \hat{I}_z - \hbar\Omega \hat{I}_x \cos\omega_0 t = H_0 + \hat{W}(t) \tag{34}$$

where $\hbar\hat{I}$ is the spin operator.
Denoting the eigen values and eigen vectors of H_0 by ,

$$\begin{aligned} H_0\left|\frac{1}{2}\right\rangle &= -\frac{\hbar\omega_0}{2}\left|\frac{1}{2}\right\rangle \\ H_0\left|-\frac{1}{2}\right\rangle &= \frac{\hbar\omega_0}{2}\left|-\frac{1}{2}\right\rangle \end{aligned} \tag{35}$$

(a) show that the state vector

$$|\psi(0)\rangle_x = \frac{1}{\sqrt{2}}\left|\frac{1}{2}\right\rangle + \frac{1}{\sqrt{2}}\left|-\frac{1}{2}\right\rangle \tag{36}$$

represents the spin vector pointing in the x-direction.

(b) Write down the state vectors for the cases of the spin vectors pointing in the y-direction, i.e. $|\psi(0)\rangle_y$, and the -y-direction, $|\psi(0)\rangle_{-y}$.

(c) You are next asked to solve the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \left(H_0 + W(t)\right)|\psi(t)\rangle \tag{37}$$

by using the expansion, in the Schrödinger picture,

$$|\psi_s(t)\rangle = c_1(t)e^{\frac{i}{2}\omega_0 t}\left|\frac{1}{2}\right\rangle + c_2(t)e^{-\frac{i}{2}\omega_0 t}\left|-\frac{1}{2}\right\rangle \tag{38}$$

or equivalently, in the interaction picture,

$$|\psi_I(t)\rangle = c_1(t)\left|\frac{1}{2}\right\rangle + c_2(t)\left|-\frac{1}{2}\right\rangle \tag{39}$$

under an initial condition that the spin vector lies along the y-direction at t = 0.
By substituting Eq. 11 into Eq. 10, obtain two first order differential equations for the amplitudes $c_1(t)$ and $c_2(t)$. It is valid to make the so called rotating wave approximation by neglecting the terms oscillating with high frequencies. This amounts to take

$$e^{\pm i\omega_0 t}\cos\omega_0 t \approx \frac{1}{2}. \tag{40}$$

Solve for the amplitudes $c_1(t)$ and $c_2(t)$ and discuss their physical meanings.

(d) From the resultant state vector in the interaction picture, $|\psi_I(t)\rangle$, describe the directions of the spin vectors at times $\frac{\Omega t}{2} = 0,\ \pi/2,\ \pi,\ 3\pi/2,$ and 2π.

5. The so-called Mössbauer effect is the phenomenon of resonance absorption of a gamma ray by a nucleus imbedded in a condensed medium, a gas, a liquid or a crystalline solid. A gamma ray is a photon emitted in a process of de-excitation of a nuclear excited state to a lower energy level. Let us denote this transition energy by E_0. Then if one send in an external monochromatic photon of an energy E, closed to E_0, the resonance absorption cross-section by the nucleus imbedded in the condensed medium can be written as:

$$\sigma_a(E) = \frac{\sigma_0\Gamma^2}{4}\sum_{n,n_0} g_{n0}\frac{\left|\langle n|e^{i\vec{p}\cdot\vec{R}/\hbar}|n_0\rangle\right|^2}{\left(E_0 - E + \varepsilon_n - \varepsilon_{n_0}\right)^2 + \Gamma^2/4}, \tag{41}$$

where Γ is the natural width of the excited state of the nucleus, $\vec{p}$ the momentum of the incident gamma ray photon, $\vec{R}$ the position vector of the center of mass of the absorbing nucleus, $|n_0\rangle$ and $|n\rangle$ the initial and the final states of the condensed medium, ε_{n_0} and ε_n, their respective energy eigenvalues. g_{n0} is the statistical weight factor of the initial state.

(A) Show that the cross-section formula can be transformed into the form

$$\sigma_a(E) = \frac{\sigma_0 \Gamma}{4\hbar} \int_{-\infty}^{\infty} dt \exp\left[-i\omega t - \left(\frac{\Gamma}{2\hbar} \right) |t| \right] F_s(p,t) \tag{42}$$

where $$F_S(p,t) = \left\langle \exp\left(-i\vec{p}\cdot\vec{R}(0)/\hbar\right) \exp\left(i\vec{p}\cdot\vec{R}(t)/\hbar\right) \right\rangle_T, \tag{43}$$

and $$\hbar\omega = E - E_0 . \tag{44}$$

Thus the resonance absorption cross-section of gamma rays can be put into nearly the same form as for the neutron inelastic scattering cross-section. In particular, it is obvious that one can use the Mössbauer effect to study the dynamics of liquids by measuring the time Fourier transform of the self-intermediate scattering function $F_s(p,t)$.

(B) In order to accomplish the above transformation, you need to first write

$$\frac{1}{\left(E_0 - E + \varepsilon_n - \varepsilon_{n_0}\right)^2 + \Gamma^2/4} = \int_{-\infty}^{\infty} \frac{\delta\left[\rho - \left(\varepsilon_n - \varepsilon_{n_0}\right)/\hbar\right]}{\left(E - E_0 - \hbar\rho\right)^2 + \Gamma^2/4} \tag{45}$$

and then use a Fourier transform formula

$$\int_{-\infty}^{\infty} \frac{\exp(-it\rho)d\rho}{\left(E - E_0 - \hbar\rho\right)^2 + \Gamma^2/4} = \frac{1}{\hbar}\frac{2\pi}{\Gamma} \exp\left[-it(E - E_0)/\hbar - (\Gamma/2\hbar)|t|\right]. \tag{46}$$

(C) Let $\vec{p} = \hbar\vec{K}$, then for a diffusing nucleus in a liquid, it is shown in class that

$$F_s^{cl}(K,t) = \exp\left(-K^2 D|t|\right) \tag{47}$$

thus by substituting Eq.47 into Eq. (42), show that one gets

$$\sigma_a(E) = \frac{\sigma_0 \Gamma}{4} \exp\left(\frac{\hbar\omega}{2k_B T}\right) \exp\left(-\frac{\hbar^2 K^2}{8Mk_B T}\right) \frac{\Gamma + 2\hbar K^2 D}{(E - E_0)^2 + (\Gamma + 2\hbar K^2 D)^2/4} \tag{48}$$

where the first two exponential factors are the quantum correctionterms for the detail balance factor and the recoil factor we discussed in the class respectively. The last resonance factor in Eq.48 shows that there is a diffusion broadening of the resonance absorption line by an amount:

$$\Delta E = 2\hbar K^2 D = \frac{2E_\gamma^2 D}{\hbar c^2}\,. \tag{49}$$

For example, radioactive isotope Fe^{57} emits Mössbauer gamma rays with energy of 14.4 KeV. Iron in a liquid state has typical diffusion constants of $D \approx 10^{-5}$ $\mathrm{cm}^2/\mathrm{sec}$. Thus the broadening is $\Delta E \approx 6x10^{-3}$ eV. This is to be compared with the natural width of the resonance line $\Gamma \approx 10^{-8}$ eV.

(D) You can read the details of this theory in a paper by K.S. Singwi and A, Sjölander, Phys. Rev. **120**, 1093 (1960).