PHYS852 Quantum Mechanics II, Spring 2010
HOMEWORK ASSIGNMENT 2: SOLUTIONS

Topics covered: Entropy, thermal states

1. [20] **Thermalized Free Particle**: In a gas of N particles, the state of particle 1 can be described by a reduced density matrix, defined in coordinate representation by

$$\rho_1(\mathbf{r}_1, \mathbf{r}_1') = \int d^3r_2 \ldots d^3r_N \langle \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N|\rho|\mathbf{r}_1', \mathbf{r}_2, \ldots, \mathbf{r}_N'\rangle, \tag{1}$$

where ρ is the full N-particle density operator. The full Hamiltonian separates as

$$H = H_1 + H_2 + \ldots + H_N + V_{1,2} + V_{1,3} + \ldots + V_{N-1,N} \tag{2}$$

where $H_n = \frac{P_n^2}{2M_n}$ and $V_{n,n'} = V(\mathbf{r}_n - \mathbf{r}_n')$ are the kinetic and short-range interaction terms, respectively. We can assume that the interactions with the $N-1$ other particles will thermalize the state of particle 1, so that

$$\rho_1(\mathbf{r}_1, \mathbf{r}_1') = \frac{1}{Z}\langle \mathbf{r}_1|e^{-\beta H_1}|\mathbf{r}_1'\rangle, \tag{3}$$

(a) [10] In a given basis, the diagonal elements of ρ give the probabilities for the system to be in the corresponding basis states. Show that the thermalized particle is equally likely to be at any position.

(b) [10] The off-diagonal elements of ρ measure the 'coherence' between the corresponding basis states. Show that there is a characteristic coherence length scale, λ_c, such that the coherence between position states becomes negligible only for $|\mathbf{r}-\mathbf{r}'| \gg \lambda_c$. Give the dependence of λ_c on the temperature T.

The probability to find the thermalized particle at position r is:

$$\begin{aligned} P_1(\mathbf{r}) &\propto \rho_1(\mathbf{r},\mathbf{r}) \\ &\propto \langle \mathbf{r}|e^{-\frac{P^2}{2Mn_bT}}|\mathbf{r}\rangle \\ &\propto \int d^3p \langle \mathbf{r}|e^{-\frac{P^2}{2Mk_bT}}|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{r}\rangle \\ &\propto \int dp_x dp_y dp_z e^{-\frac{p_x^2+p_y^2+p_z^2}{2Mk_bT}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \\ &\propto \int dp_x dp_y dp_z e^{-\frac{p_x^2+p_y^2+p_z^2}{2Mk_bT}} \end{aligned} \tag{4}$$

at which point we see that it is independent of $\mathbf{r}$, which indicates that the particle is equally likely to be found anywhere. The question becomes, how much of this 'uncertainty' is coherent superposition and how much is just ignorance? To answer this, we look at the off-diagonal element, $\rho_1(\mathbf{r},\mathbf{r}')$,

$$\rho_1(\mathbf{r},\mathbf{r}') \propto \int dp_x dp_y dp_z e^{-\frac{p_x^2+p_y^2+p_z^2}{2Mk_bT}} e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')/\hbar} \propto e^{-\frac{Mk_bT(\mathbf{r}-\mathbf{r}')^2}{2}} \tag{5}$$

putting this in the form $\exp\left[-\frac{(\mathbf{r}-\mathbf{r}')^2}{\lambda_c^2}\right]$ shows that the coherence decays drops off rapidly for $|\mathbf{r}-\mathbf{r}'| > \lambda_c = \sqrt{\frac{2}{Mk_bT}}$. This shows that the coherence length increases as the temperature decreases, which makes sense because a pure coherent superposition has zero entropy, and should therefore be obtained in the $T \to 0$ limit.

2. [30] **Thermalized Spin-1/2 System**: Consider a rigid lattice of spin-1/2 particles, of mass m and charge q, placed in a uniform magnetic field of magnitude B_0. The spins interact with each-other via magnetic dipole-dipole interactions, so that the reduced density operator of a single spin will be thermalized. Because the particle has no motional degrees of freedom, its density operator has a 2×2 matrix representation.

   (a) [10] Compute the single-particle thermal density operator for a given temperature T.

   (b) [10] Compute the partition function, and use it to compute the mean energy of the particle as a function of T.

   (c) [5] What is the critical temperature T_c, below which the particle is effectively frozen in the lowest energy level?

   (d) [5] Show that as $T \to \infty$, the thermal state goes to the maximum entropy state $\rho = \frac{I}{d}$, where I is the identity operator, and d is the Hilbert space dimension.

Choosing the z-axis along the field directions gives

$$H = -\vec{\mu} \cdot \vec{B} = -\frac{\hbar g q B_0}{4M} \sigma_z \tag{6}$$

The thermal density operator is

$$\rho_T = \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \exp\left[\frac{\beta \hbar g q B_0}{4M} \sigma_z\right] \to \frac{1}{Z} \begin{pmatrix} e^{\beta/\beta_0} & 0 \\ 0 & e^{-\beta/\beta_0} \end{pmatrix} \tag{7}$$

where

$$\beta_0 = \frac{4M}{\hbar g q B_0} \tag{8}$$

The partition function is

$$Z = \mathrm{Tr}\{e^{-\beta H}\} = 2\cosh(\beta/\beta_0) \tag{9}$$

The mean energy is then

$$E_T = -\frac{d}{d\beta} \ln Z = -\frac{1}{Z} \frac{d}{d\beta} Z = -\frac{\tanh(\beta/\beta_0)}{\beta_0} = -\tanh(T_c/T) k_b T_c \tag{10}$$

where

$$T_c = \frac{\hbar g q B_0}{4M k_b} \tag{11}$$

is the temperature below which the system becomes frozen in the ground state. In the limit $T \to \infty$, we have $\beta \to 0$, so that

$$\rho_\infty = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{I}{d} \tag{12}$$

3. [30] **Thermalized Spherical Oscillator**: For the spherically symmetric 3D harmonic oscillator, governed by

$$H = \frac{P^2}{2M} + \frac{1}{2}M\omega^2 R^2, \tag{13}$$

compute the thermal energy distribution function, the partition function, and the thermal mean energy, $E(T) = \langle H \rangle$. What is the leading order term in $E(T)$ as $T \to \infty$?

We can quantize using the principle quantum number, so that

$$H = \sum_{n=0}^{\infty}\sum_{m=1}^{d_n} \hbar\omega(n+1)|n,m\rangle\langle n,m| \tag{14}$$

where from 851/lecture 29, we recall that

$$d_n = \frac{1}{2}(n^2 + 3n + 2). \tag{15}$$

The partition function is then

$$\begin{aligned} Z = \mathrm{Tr}\{e^{-\beta H}\} &= \sum_{n=0}^{\infty}\sum_{m=1}^{d_n} e^{-\beta\hbar\omega(n+1)} \\ &= e^{-\beta\hbar\omega}\sum_{n=0}^{\infty} d_n e^{-\beta\hbar\omega n} \\ &= \frac{1}{2}e^{-\beta\hbar\omega}\sum_{n=0}^{\infty}(n^2+3n+2)\left(e^{-\beta\hbar\omega}\right)^n \end{aligned} \tag{16}$$

now

$$\sum_n e^{-\beta\hbar\omega n} = \frac{1}{1-e^{-\beta\hbar\omega}} \tag{17}$$

and

$$\begin{aligned} \sum_n n e^{-\beta\hbar\omega n} &= -\frac{1}{\hbar\omega}\frac{d}{d\beta}\sum_n e^{-\beta\hbar\omega n} \\ &= -\frac{1}{\hbar\omega}\frac{d}{d\beta}\frac{1}{1-e^{-\beta\hbar\omega}} \\ &= \frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2} \\ &= \frac{1}{2(\cosh(\beta\hbar\omega)-1)} \end{aligned} \tag{18}$$

likewise

$$\begin{aligned} \sum_n n^2 e^{-\beta\hbar\omega} &= \frac{1}{(\hbar\omega)^2}\frac{d^2}{d\beta^2}\frac{1}{1-e^{-\beta\hbar\omega}} \\ &= \frac{1}{4}\coth(\beta\hbar\omega/2)\mathrm{csch}(\beta\hbar\omega/2) \end{aligned} \tag{19}$$

Thus we find

$$Z = \frac{1-2e^{\beta\hbar\omega}-e^{2\beta\hbar\omega}}{2(1-e^{\beta\hbar\omega})^3} \tag{20}$$

The thermal Energy distribution is then

$$P_T(E) = \frac{1}{Z}\sum_{n=0}^{\infty}\delta(E-\hbar\omega(n+1))\left(1+\frac{3n}{2}+\frac{n^2}{2}\right)e^{-\beta\hbar\omega(n+1)} \tag{21}$$

The thermal mean energy is

$$\begin{aligned} E_T &= -\frac{1}{Z}\frac{d}{d\beta}Z \\ &= \hbar\omega\frac{2e^{\frac{2\hbar\omega}{k_bT}}\left(3+\sinh(\frac{\hbar\omega}{k_bT}\right)}{1-3e^{\frac{\hbar\omega}{k_bT}}+e^{\frac{2\hbar\omega}{k_bT}}+e^{\frac{3\hbar\omega}{k_bT}}} \end{aligned} \tag{22}$$

The leading term in the series expansion around $\beta = 0$ gives

$$\lim_{T\to\infty} E_T = 3k_bT \tag{23}$$

which is the standard classical result for a 3d oscillator.