PHYS852 Quantum Mechanics II, Spring 2010
HOMEWORK ASSIGNMENT 2

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

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

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

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

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.

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.

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

$$H = \frac{P^2}{2M} + \frac{1}{2} M\omega^2 R^2, \tag{4}$$

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 $T \to \infty$?