G25.2651: Advanced Statistical Mechanics

Problem set #4

Due: April 6, 2009

1. The energy of a quantum particle with magnetic moment $\boldsymbol{\mu}$ interacting with a magnetic field $\mathbf{B}$ is $E = -\boldsymbol{\mu} \cdot \mathbf{B}$. Consider an electron fixed in space interacting with a magnetic field in the z direction, so that $\mathbf{B} = (0, 0, B)$. The electron has a spin of 1/2, and its magnetic moment can be related to its spin $\hat{\mathbf{S}}$ by $\hat{\boldsymbol{\mu}} = \gamma \hat{\mathbf{S}}$ so that the Hamiltonian for the electron becomes

$$\hat{H} = -\gamma B \hat{S}_z$$

The spin operator $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ is given by

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

a. Suppose an ensemble of such systems is prepared such that the density matrix initially is

$$\rho(0) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

Calculate $\rho(t)$.

b. What are the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ at any time t?

c. Suppose now that the initial density matrix is

$$\rho(0) = \begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix}$$

For this case, calculate $\rho(t)$.

d. What are the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ at time t for this case?

e. What are the fluctuations in $\hat{S}_x$? Recall that

$$\Delta \hat{S}_x = \sqrt{\langle \hat{S}_x^2 \rangle - \langle \hat{S}_x \rangle^2}$$

f. Suppose finally that the density matrix is given initially by a canonical density matrix:

$$\rho(0) = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}(e^{-\beta \hat{H}})}$$

What is $\rho(t)$?

g. What are the expectation values of $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$?

2. The Hamiltonian for a free particle in one dimension is

$$\hat{H} = \frac{\hat{p}^2}{2m}.$$

a. Using the free-particle eigenfunctions, show that the density matrix is given by

$$\langle x | e^{-\beta \hat{H}} | x' \rangle = \left(\frac{m}{2\pi\beta\hbar^2} \right)^{1/2} \exp\left[-\frac{m}{2\beta\hbar^2} (x - x')^2 \right]$$

b. In class, we showed that an operator $\hat{A}$ in the Heisenberg picture evolves in time according to

$$\hat{A}(t) = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$$

If we transform to imaginary time $t = -i\tau\hbar$, then the evolution of an operator in imaginary time becomes

$$\hat{A}(\tau) = e^{\tau\hat{H}}\hat{A}e^{-\tau\hat{H}}$$

Using this evolution, derive an expression for the imaginary-time mean-square displacement of a free particle defined to be

$$R^2(\tau) = \langle[\hat{x}(0) - \hat{x}(\tau)]^2\rangle.$$

This function is generally used to quantify the delocalization of a particle.

3. Consider a particle with mass m moving in a one-dimensional harmonic oscillator potential $U(\hat{x}) = m\omega^2\hat{x}^2/2$. Show that the Euclidean action

$$S[x] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 + U(x(\tau))\right]$$

for the classical solution is given by

$$S_{\rm cl}(x, x'; \beta) = \frac{m\omega}{2\sinh(\beta\hbar\omega)}\left[(x^2 + x'^2)\cosh(\beta\hbar\omega) - 2xx'\right]$$

4. The following problem considers the path-integral theory for the tunneling of a particle through a barrier.

a. Show that the path integral expression for the density matrix can be written as:

$$\rho(x, x'; \beta) = \int_{x(-\beta\hbar/2)=x}^{x(\beta\hbar/2)=x'} \mathcal{D}[x] \exp\left[-\frac{1}{\hbar}\int_{-\beta\hbar/2}^{\beta\hbar/2} d\tau \left(\frac{1}{2}m\dot{x}^2 + U(x(\tau))\right)\right]$$

b. Consider a double well potential of the form

$$U(x) = \frac{\omega^2}{8a^2}(x^2 - a^2)^2$$

Show that, for a particle of unit mass, the dominant path for the density matrix $\rho(-a, a; \beta)$ is given by

$$x(\tau) = a\tanh[(\tau - \tau_0)\omega/2]$$

in the low temperature limit with negligible error in the endpoint conditions. This path is called an *instanton* or *kink* solution. Discuss the behavior of this trajectory in imaginary time τ.

c. Calculate the classical imaginary-time action for the kink solution.