

PHY5524 Problem Set 7: Solution

Problem 1

The unitary transformation which diagonalizes σ_x , which in the usual basis ($\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \uparrow$, $\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \downarrow$) is given by $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (1)$$

as can be seen explicitly, as follows,

$$U\sigma_xU^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2)$$

Now, for the Hamiltonian

$$H = -\mu_B B \sigma_z \quad (3)$$

the density matrix in the usual basis is

$$\hat{\rho} = \frac{1}{2 \cosh \beta \mu_B B} \begin{pmatrix} e^{\beta \mu_B B} & 0 \\ 0 & e^{-\beta \mu_B B} \end{pmatrix} \quad (4)$$

In the new basis the density matrix is then,

$$U\hat{\rho}U^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{2 \cosh \beta \mu_B B} \begin{pmatrix} e^{\beta \mu_B B} & 0 \\ 0 & e^{-\beta \mu_B B} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (5)$$

$$= \frac{1}{2} \frac{1}{2 \cosh \beta \mu_B B} \begin{pmatrix} e^{\beta \mu_B B} + e^{-\beta \mu_B B} & e^{\beta \mu_B B} - e^{-\beta \mu_B B} \\ e^{\beta \mu_B B} - e^{-\beta \mu_B B} & e^{\beta \mu_B B} + e^{-\beta \mu_B B} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \tanh \beta \mu_B B \\ \tanh \beta \mu_B B & 1 \end{pmatrix} \quad (6)$$

Finally, to calculate $\langle \sigma_z \rangle$, note that $U\sigma_zU^\dagger = \sigma_x$, i.e.,

$$U\sigma_zU^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (7)$$

Thus, applying the formula,

$$\langle \hat{A} \rangle = \text{Tr} [\hat{A} \hat{\rho}] \quad (8)$$

in the new basis we find

$$\langle \sigma_z \rangle = \text{Tr} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & \tanh \beta \mu_B B \\ \tanh \beta \mu_B B & 1 \end{pmatrix} \right] = \frac{1}{2} \text{Tr} \left[\begin{pmatrix} \tanh \beta \mu_B B & 1 \\ 1 & \tanh \beta \mu_B B \end{pmatrix} \right] = \tanh \beta \mu_B B \quad (9)$$

which is, reassuringly, the same answer we obtained in the original basis in which σ_z is diagonal.

Problem 2

The unsymmetrized energy eigenstates for N free particles in a box are of the form

$$\psi_{\vec{k}_1, \vec{k}_2, \dots, \vec{k}_N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \psi_{\vec{k}_1}(\vec{r}_1) \psi_{\vec{k}_2}(\vec{r}_2) \cdots \psi_{\vec{k}_N}(\vec{r}_N) = \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \vec{k}_1, \vec{k}_2, \dots, \vec{k}_N \rangle \quad (10)$$

where

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}} \quad (11)$$

is a one-particle momentum eigenstate with wave vector \vec{k} .

To find the density matrix in the position basis we need to compute the matrix elements of $e^{-\beta H}$ in the position basis,

$$\begin{aligned} \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | e^{-\beta \hat{H}} | \vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N \rangle &= \sum_{\vec{k}_1, \vec{k}_2, \dots, \vec{k}_N} \sum_{\vec{k}'_1, \vec{k}'_2, \dots, \vec{k}'_N} \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \vec{k}_1, \vec{k}_2, \dots, \vec{k}_N \rangle \langle \vec{k}_1, \vec{k}_2, \dots, \vec{k}_N | e^{-\beta H} | \vec{k}'_1, \vec{k}'_2, \dots, \vec{k}'_N \rangle \\ &\quad \times \langle \vec{k}'_1, \vec{k}'_2, \dots, \vec{k}'_N | \vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N \rangle \end{aligned} \quad (12)$$

where on the RHS we have inserted complete sets of eigenstates on both sides of the $e^{-\beta H}$ operator.

For free particles we have

$$\langle \vec{k}_1, \vec{k}_2, \dots, \vec{k}_N | e^{-\beta H} | \vec{k}'_1, \vec{k}'_2, \dots, \vec{k}'_N \rangle = \delta_{\vec{k}_1, \vec{k}'_1} \delta_{\vec{k}_2, \vec{k}'_2} \dots \delta_{\vec{k}_N, \vec{k}'_N} e^{-\beta \frac{\hbar^2}{2m} (k_1^2 + k_2^2 + \dots + k_N^2)} \quad (13)$$

Therefore

$$\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | e^{-\beta \hat{H}} | \vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N \rangle = \sum_{\vec{k}_1, \dots, \vec{k}_N} \langle \vec{r}_1, \dots, \vec{r}_N | \vec{k}_1, \dots, \vec{k}_N \rangle \langle \vec{k}_1, \dots, \vec{k}_N | \vec{r}'_1, \dots, \vec{r}'_N \rangle e^{-\beta \frac{\hbar^2}{2m} (k_1^2 + \dots + k_N^2)} \quad (14)$$

$$\begin{aligned} &= V^N \int \frac{d^3 k_1}{(2\pi)^3} \dots \int \frac{d^3 k_N}{(2\pi)^3} \psi_{\vec{k}_1, \dots, \vec{k}_N}(\vec{r}_1, \dots, \vec{r}_N) \psi_{\vec{k}_1, \dots, \vec{k}_N}^*(\vec{r}'_1, \dots, \vec{r}'_N) e^{-\beta \frac{\hbar^2}{2m} (k_1^2 + \dots + k_N^2)} \\ &= \left(V \int \frac{d^3 k_1}{(2\pi)^3} \psi_{\vec{k}_1}(\vec{r}_1) \psi_{\vec{k}_1}^*(\vec{r}'_1) e^{-\beta \frac{\hbar^2 k_1^2}{2m}} \right) \dots \left(V \int \frac{d^3 k_N}{(2\pi)^3} \psi_{\vec{k}_N}(\vec{r}_N) \psi_{\vec{k}_N}^*(\vec{r}'_N) e^{-\beta \frac{\hbar^2 k_N^2}{2m}} \right) \end{aligned} \quad (15)$$

$$= \left(\int \frac{d^3 k}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}'_1)} e^{-\beta \hbar^2 k^2 / 2m} \right) \dots \left(\int \frac{d^3 k}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{r}_N - \vec{r}'_N)} e^{-\beta \hbar^2 k^2 / 2m} \right) \quad (16)$$

$$= \left(\frac{2\pi m k_B T}{h^2} \right)^{3N/2} e^{-\frac{m}{2\beta \hbar^2} |\vec{r}_1 - \vec{r}'_1|^2} \dots e^{-\frac{m}{2\beta \hbar^2} |\vec{r}_N - \vec{r}'_N|^2} \quad (17)$$

where, in the last equality, we have used the result for the one particle matrix element,

$$\langle \vec{r} | e^{-\beta H} | \vec{r}' \rangle = \int \frac{d^3 k}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{r} - \vec{r}')} e^{-\beta \hbar^2 k^2 / 2m} = \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} e^{-\frac{m}{2\beta \hbar^2} |\vec{r} - \vec{r}'|^2} \quad (18)$$

derived in class by completing the square.

The partition function for the N particle system is then

$$Q_N = \text{Tr}[e^{-\beta H}] = \int d^3 r_1 \dots d^3 r_N \langle \vec{r}_1, \dots, \vec{r}_N | e^{-\beta H} | \vec{r}_1, \dots, \vec{r}_N \rangle \quad (19)$$

$$= V^N \left(\frac{2\pi m k_B T}{h^2} \right)^{3N/2} \quad (20)$$

Note that, because we have used the *unsymmetrized* wave function, there is no Gibbs factor of $\frac{1}{N!}$.

Finally, it follows that the diagonal matrix elements of the density matrix in the position basis are

$$\langle \vec{r}_1, \dots, \vec{r}_N | \rho | \vec{r}_1, \dots, \vec{r}_N \rangle = \frac{1}{Q_N} \langle \vec{r}_1, \dots, \vec{r}_N | e^{-\beta H} | \vec{r}_1, \dots, \vec{r}_N \rangle = \frac{1}{V^N} \quad (21)$$

As shown in class, this expectation value is the joint probability density to find particles at the points $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N$. The fact that this is simply a constant, independent of the particle coordinates, indicates that there are no spatial correlations between the particles. Again, this is a consequence of using *unsymmetrized* wave functions to describe the gas.