PHYS 522: Statistical Mechanics

Homework #1

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1. Evaluate the density matrix ϱ of an electron in a magnetic field in the representation that makes $\hat{\sigma}$ diagonal. Next, show that the value of $\langle\sigma\rangle$, resulting from this representation, is precisely the same as the one obtained in class.

Solution:

The pauli spin operator σ_x is diagonal in the representation where the basis states are eivenstates of S_x operator. In S_z representation the S_x states are given by

$$|S_x;\pm\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle \pm |-\rangle\right)$$

The transformation operator that takes from S_z representation to S_x representation is given by operator

$$U = |S_x;+\rangle\langle+| + |S_x;-\rangle\langle-|$$

So the matrix representation of this operator is

$$U = \begin{bmatrix} \langle S_x;+|+\rangle & \langle S_x;+|-\rangle \\ \langle S_x;-|+\rangle & \langle S_x;-|-\rangle \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

The operator in the new basis can be obtained from the old basis with the transformation.

$$\sigma_z' = U^\dagger \sigma_z U = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

The Hamiltonian of the system in new basis is

$$\mathcal{H}' = \mu \boldsymbol{B}\cdot\boldsymbol{\sigma}' = -\mu B_z \sigma_z'$$

The density operator in cannonical ensemble is given by

$$\hat{\varrho}' = \frac{e^{-\beta\mathcal{H}}}{\operatorname{Tr}\left(e^{-\beta\mathcal{H}}\right)} \tag{1}$$

Carrying out the taylor expansion of the numerator in the density operator

$$\begin{aligned} e^{-\beta\mathcal{H}'} = e^{\beta\mu B_z\sigma_z'} &= 1 + \frac{\beta\mu B_z\sigma_z'}{1!} + \frac{(\beta\mu B_z\sigma_z')^2}{2!} + \frac{(\beta\mu B_z\sigma_z')^3}{3!} + \frac{(\beta\mu B_z\sigma_z')^4}{4!} + \dots \\ &= \left[1 + \frac{(\beta\mu B_z)^2}{2!} + \frac{(\beta\mu B_z)^4}{4!} + \dots\right] + \sigma_z'\left[\frac{\beta\mu B_z}{1!} + \frac{(\beta\mu B_z)^3}{3!} + \dots\right] \\ &= \cosh(\beta\mu B_z) + \sigma_z \sinh(\beta\mu B_z) \end{aligned} \tag{2}$$

where we have used the fact that $\sigma_z'^{2n} = 1; \quad \sigma_z'^{2n+1} = \sigma_z'$ for all n in $\{0, 1, \dots\}$ Also we have

$$\operatorname{Tr}(1) = 2 \qquad \operatorname{Tr}(\sigma_z') = 0$$

So taking trace of Eq. (**??**) we get

$$\mathrm{Tr}(e^{-\beta\mathcal{H}'}) = \mathrm{Tr}(\cosh(\beta\mu B_z) + \sigma_z \sinh(\beta\mu B_z)) = \cosh(\beta\mu B_z)\mathrm{Tr}(1) + \sinh(\beta\mu B_z)\mathrm{Tr}(\sigma_z') = 2\cosh(\beta\mu B_z)$$

So the density operator (1) becomes

$$\hat{\varrho}' = \frac{\cosh(\beta\mu B_z) + \sigma_z \sinh(\beta\mu B_z)}{2\cosh(\beta\mu B_z)} = \frac{1}{2} + \frac{1}{2}\sigma_z' \tanh(\beta\mu B_z)$$

Now the expectation value of operator σ_z for the

$$\langle\sigma_z'\rangle = \mathrm{Tr}(\hat{\varrho}\sigma_z') = \mathrm{Tr}\left(\frac{1}{2}\sigma_z + \frac{1}{2}\sigma_z^2 \tanh(\beta\mu B_z)\right) = \mathrm{Tr}\left(\frac{1}{2}\sigma_z + \frac{1}{2}\tanh(\beta\mu B_z)\right) = \tanh(\beta\mu B_z)$$

This gives the expectation value of the operator. This expression is the same as the one we obtained using the basis states where σ_z was diagonal instead of σ_x that we have here. □

2. Derive the uncertainties, $\Delta x, \Delta p$ and ΔE, of a free particle in 3D box using the density matrix expression in the coordinate representation. Then calculate the uncertainty product $\Delta x \cdot \Delta p$.

Solution:

For a particle in a box the the density matrix is given by

$$\langle r|\hat{\varrho}|r'\rangle = \frac{1}{V}\exp\left[-\frac{m}{2\beta\hbar^2}|\boldsymbol{r} - \boldsymbol{r'}|^2\right]$$

The average position of the particle is given by

$$\langle\boldsymbol{r}\rangle = \mathrm{Tr}(\boldsymbol{r}\hat{\varrho}) = \frac{1}{V}\int \left|\exp\left[-\frac{m}{2\beta\hbar^2}|\boldsymbol{r} - \boldsymbol{r'}|^2\right] r\right|_{\boldsymbol{r}=\boldsymbol{r'}} d^3r = \frac{3}{4}R$$

The average squared position is given by

$$\left\langle\boldsymbol{r}^2\right\rangle = \mathrm{Tr}(\boldsymbol{r}^2\hat{\varrho}) = \frac{1}{V}\int \left|\exp\left[-\frac{m}{2\beta\hbar^2}|\boldsymbol{r} - \boldsymbol{r'}|^2\right] r^2\right|_{\boldsymbol{r}=\boldsymbol{r'}} d^3r = \frac{3}{5}R^2$$

So the uncertainity in the position of particle is given by

$$\Delta r = \sqrt{\langle\boldsymbol{r}^2\rangle - \langle\boldsymbol{r}\rangle^2} = \frac{1}{4}\sqrt{\frac{3}{5}}R$$

Now the average value of momentum is given by

$$\langle\boldsymbol{p}\rangle = \mathrm{Tr}(\boldsymbol{p}\hat{\varrho}) = \frac{-i\hbar}{V}\int \left|\frac{\partial}{\partial r}\exp\left[-\frac{m}{2\beta\hbar^2}|\boldsymbol{r} - \boldsymbol{r'}|^2\right]\right|_{\boldsymbol{r}=\boldsymbol{r'}} d^3r = -i\frac{\hbar}{V}\int 0 d^3r = 0$$

The average momentum squared is

$$\left\langle\boldsymbol{p}^2\right\rangle = \mathrm{Tr}(\boldsymbol{p}^2\hat{\varrho}) = -\frac{\hbar^2}{V}\int \left|\frac{\partial^2}{\partial r^2}\exp\left[-\frac{m}{2\beta\hbar^2}|\boldsymbol{r} - \boldsymbol{r'}|^2\right]\right|_{\boldsymbol{r}=\boldsymbol{r'}} d^3r = 3mkT$$

Again the uncertainity in momentum is given by

$$\Delta p = \sqrt{\langle\boldsymbol{p}^2\rangle - \langle\boldsymbol{p}\rangle^2} = \sqrt{3mkT}$$

So the uncertainity product is

$$\Delta r \cdot \Delta p = \frac{3}{4}\sqrt{\frac{mkT}{5}}R$$

This gives the uncertainity product in position and momentum. □

3. Prove that

$$\langle q|e^{-\beta\mathcal{H}}|q'\rangle = \exp\left[-\beta\mathcal{H}\left(-i\hbar\frac{\partial}{\partial q}, q\right)\right]\delta(q-q'),$$

where

$$\mathcal{H}\left(-i\hbar\frac{\partial}{\partial q}, q\right)$$

is the Hamiltonian of the system in the q-representation, which formally operates upon the Dirac delta function, $\delta(q-q')$. Write δ-function is a suitable form; apply this result to a free particle.

Solution:

let $\psi_n(q) = \langle n|q\rangle$ be energy eigenfunction with eigenvalue E_n in configuration space q. Then by schrodingers equation we have

$$\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q)\psi_n(q') = E_n\psi_n(q')$$

Since we know that for operators $A\psi(x) = \lambda\phi(x) \implies f(A)\phi(x) = f(\lambda)\phi(x)$

$$e^{-\beta\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q)}\psi_n(q') = e^{-\beta E_n}\psi_n(q')$$

This can be used to write

$$\begin{aligned}\langle q|e^{-\beta\mathcal{H}}|q'\rangle &= \sum_n \langle q|n\rangle\ \langle n|e^{-\beta\mathcal{H}}|q'\rangle \qquad \left(\text{Inserting } \sum_n |n\rangle\langle n|\right)\\ &= \sum_n \psi_n(q)e^{-\beta E_n}\psi_n^*(q')\\ &= e^{\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q)}\sum_n \psi_n(q)\psi_n^*(q')\end{aligned}$$

But since the the eigenfunctions of the Hamiltonian are orthogonal to each other we get $\sum_n \psi^*(q')\psi(q) = \delta(q-q')$ we get

$$\langle q|e^{-\beta\mathcal{H}}|q'\rangle = e^{\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q)}\delta(q-q') \tag{3}$$

This is the required expression for the matrix element of the dnesity operator $e^{-\beta\mathcal{H}}$.

We can also write the δ–function using the fourier transform representaation of δ–function as

$$\delta(q-q') = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{ik(q-q')}dk \tag{4}$$

For a free particle the Hamiltonian can be written as

$$\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q) = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q'^2} \tag{5}$$

Now using (5) and (4) this in (3) we get

$$\begin{aligned}\langle q|e^{-\beta\mathcal{H}}|q'\rangle &= \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{\mathcal{H}(-i\hbar\frac{\partial}{\partial q}, q)}e^{ik(q-q')}dk\\ &= \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{-\frac{\beta\hbar^2}{2m}+ik(q-q')}dk\end{aligned}$$

This can be solved by completing the square in the exponential and using the gamma function the final result is

$$\langle q|e^{-\beta\mathcal{H}}|q'\rangle = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}} e^{-\frac{m}{2\beta\hbar^2}(q-q')^2}$$

This is the matrix element of the density operator for the free particle in a box. □

4. Derive the density matrix ρ for a free particle in the momentum representation and study its main properties, such as the average energy, momentum.
Solution:
The Hamiltonian of the free particle in moementum representation is

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

Let $|\psi_k\rangle$ be the momentum wavefunction of the particle then the expression for the momentum wavefunction is

$$_k(r) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

Since the momentum eigenfunctions make complete set of states they are orthonormal

$$\langle\psi_k|\psi_k'\rangle = \delta_{k,k'}$$

Now the cannonical partition function of the system is

$$\begin{aligned} Q(V,T) &= \text{Tr}e^{-\beta\mathcal{H}} \\ &= \sum_k \langle\psi_k|e^{-\beta\mathcal{H}}|\psi_k\rangle \\ &= \sum_k e^{-\frac{\beta\hbar^2}{2m}k^2} \end{aligned}$$

Since the states are very close in momentum sapce we can replace the sum by integral

$$\begin{aligned} Q(V,T) &= \frac{V}{(2\pi)^3}\int dK e^{-\frac{\beta\hbar^2}{2m}k^2} \\ &= \frac{V}{(2\pi)^3}\left(\frac{2m\pi}{\beta\hbar^2}\right)^{\frac{3}{2}} \\ &= \frac{V}{\lambda^3} \end{aligned}$$

The matrix element of this operator now become

$$\langle\psi_k|\hat{\varrho}|\psi_k'\rangle = \frac{\lambda^3}{V} e^{-\frac{\beta\hbar^2}{2m}k^2}\delta_{k,k'}$$

Ths is the requried density matrix representation in momentum sapce. □

5. We showed in class that linearly polarized light corresponds to apure state and non-polarized light is in a mixed state. What is the circularly polarized, a mixed state or a pure state? Verify your statement
Solution:
Polarized light must be pure state because, at any given time it only has components The two plane polarized components x be represented by A $\begin{bmatrix}1\\0\end{bmatrix}$ a and y plane polarized be represented by $\begin{bmatrix}0\\1\end{bmatrix}$. The

most general polarization of the light can be written as the linear combination of these two plane polarized conponents as

$$P_{\text{gen}} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} e^{i\theta_1} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{i\theta_2}$$

where a and b in general are complex numbers. For a circularly polarize. If the two plane polarized components have a total phase difference of $n\pi$ then the light is plane polarized. But for the phase difference $\delta = \theta_2 - \theta_1 = (2n+1)\frac{\pi}{2}$ the light is circularly polarized. Let the phase $\theta_1 = 0$ and $_2 = \pi/2$ such the phase difference is $\pi/2$ we get

$$P_{\text{circular}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{i}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Now for this representation, the density matrix can be obtained easily as

$$\hat{\varrho} = \begin{bmatrix} aa^* & ab^* \\ ba^* & bb^* \end{bmatrix} = \begin{bmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{bmatrix}$$

This prepresents a pure state as

$$\hat{\varrho}^2 = \begin{bmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{bmatrix} \times \begin{bmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{bmatrix} = \hat{\varrho}$$

This verifies that the circularly polarized light is pure state. □