5500 Problem Set 4

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Question I.

A density operator can always be written in the form $\rho = \sum_k |\psi_k\rangle\langle\psi_k|$, where the vectors $|\psi_k\rangle$ need neither be normalized, nor orthogonal. Suppose we have two representations of this kind with the vectors $|\psi_k\rangle$ and $|\phi_k\rangle$; if not, you can always pad the smaller set with zero vectors to achieve the same size. Show that the corresponding density operators ρ_ψ and ρ_ϕ are the same if there exists a unitary matrix u_{pq} such that $|\psi_p\rangle = \sum_q u_{pq} |\phi_q\rangle$. The decomposition of a density operator into a mixture of pure states is in general not unique.

The reverse also holds: ρ_ψ and ρ_ϕ are the same density operator only if a unitary matrix u_{pq} as per above exists. The proof, though, is substantially tougher.

$$\begin{aligned}
\rho_\psi &= \sum_k |\psi_k\rangle\langle\psi_k| \\
\sum_p |\psi_p\rangle &= \sum_q u_{pq} |\phi_q\rangle \\
\sum_i |\psi_i\rangle\langle\psi_i| &= \sum_{ijk} u_{ij} u)^*_{ik} |\phi_j\rangle\langle\phi_k| \\
&= \sum_{jk} \left(\sum_i u^\dagger_{ki} u_{ij} \right) |\phi_j\rangle\langle\phi_k| \\
&= \sum_{jk} \delta_{kj} |\phi_j\rangle\langle\phi_k| \\
&= \sum_j |\phi_j\rangle\langle\phi_j| \\
&= \rho_\phi
\end{aligned}$$

This shows the desired result that the corresponding density operators are the same given there exists such a unitary operator u_{pq} such that $|\psi_p\rangle = \sum_q u_{pq} |\phi_q\rangle$.

Question II.

(a) Calculate the integrals that come up all over the place in statistical mechanics:

$$\int_0^\infty \mathrm{d}x\, x^n e^{-\lambda x}$$
$$\int_0^\infty \mathrm{d}x\, x^n e^{-\lambda x^2}$$

Presently it is enough to find an algorithm for the values of the integrals for $n = 0, 1, ...$ assuming $\lambda > 0$.

For the first integral, we can integrate by parts n times to get

$$\int_0^\infty \mathrm{d}x\, x^n e^{-\lambda x} = \frac{n!}{\lambda^{n+1}}$$

The second integral depends on the parity of n, and we can attack it using a substitution as follows:

$$\begin{aligned}
I &= \int_0^\infty \mathrm{d}x\, x^n e^{-\lambda x^2} \\
x &\equiv \lambda^{-1/2} y \\
\mathrm{d}x &= \lambda^{-1/2}\,\mathrm{d}y \\
y^2 &= \lambda x^2 \\
I &= \lambda^{-1/2} \int_0^\infty e^{-y^2} (\lambda^{-1/2} y)^n\,\mathrm{d}y \\
&= \lambda^{-(n+1)/2} \int_0^\infty e^{-y^2} y^n\,\mathrm{d}y
\end{aligned}$$

We can implement the following identity:

$$\begin{aligned}
-\frac{\partial}{\partial\lambda} I_{n-2} &= -\frac{\partial}{\partial\lambda} \int_0^\infty e^{-\lambda x^2} x^{n-2}\,\mathrm{d}x \\
&= -\int_0^\infty -x^2 e^{-\lambda x^2} x^{n-2}\,\mathrm{d}x \\
&= \int_0^\infty -x^2 e^{-\lambda x^2} x^{n}\,\mathrm{d}x \\
&= I_n
\end{aligned}$$

For even $n = 2k$,

$$\begin{aligned}
I_n &= \left(-\frac{\partial}{\partial\lambda}\right) I_{n-2} \\
&= \left(-\frac{\partial}{\partial\lambda}\right)^2 I_{n-4} \\
&= \left(-\frac{\partial}{\partial\lambda}\right)^{n/2} I_0 \\
&= \frac{\sqrt{\pi}}{2} \frac{\partial^{n/2}}{\partial\lambda^{n/2}} \lambda^{-1/2}
\end{aligned}$$

So we are left with

$$\begin{aligned}
I &= \frac{(k-\frac{1}{2})!}{2\lambda^{k+1/2}} \\
&= \frac{(2k-1)!!}{2^{k+1}\lambda^k} \sqrt{\frac{\pi}{\lambda}}
\end{aligned}$$

Odd $n = 2k + 1$ follows similarly to give

$$\begin{aligned}
I &= \frac{\partial^{(n-2)/2}}{\partial \lambda^{(n-2)/2}} I_1 \\
I_1 &= \frac{1}{2\lambda} \\
I_{\text{odd}} &= \frac{k!}{2\lambda^{k+1}}
\end{aligned}$$

In terms of n we have

$$\begin{aligned}
I_{even} &= \frac{(n-1)!!}{2^{n/2+1}\lambda^{n/2}} \\
I_{odd} &= \frac{[1/2(n-1)]!}{2\lambda^{(n+1)/2}}
\end{aligned}$$

(b) However, the results are good for a complex parameter λ as well, provided that $\Re(\lambda > 0)$. Demonstrate this for the integral $\int_{-\infty}^{\infty} \mathrm{d}x \, e^{-\lambda x^2}$.

We can begin this by doing the integral as if $\lambda \in \mathbb{R}$.

$$\begin{aligned}
I &= \int_{-\infty}^{\infty} e^{-\lambda x^2} \, \mathrm{d}x \\
I^2 &= \int_{-\infty}^{\infty} e^{-\lambda x^2} \, \mathrm{d}x \int_{-\infty}^{\infty} e^{-\lambda y^2} \, \mathrm{d}y \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\lambda(x^2+y^2)} \, \mathrm{d}x \, \mathrm{d}y \\
&= \int_{0}^{\infty} \int_{0}^{2\pi} e^{-\lambda\rho^2} \rho \, \mathrm{d}\rho \, \mathrm{d}\phi \\
&= \frac{\pi}{\lambda} \\
I &= \left(\frac{\pi}{\lambda}\right)^{\frac{1}{2}}
\end{aligned}$$

Which is good for a complex $\lambda = \mathrm{Re}\{\lambda\} + i \, \mathrm{Im}\{\lambda\}$

Question III.

Take it as an axiom that every hermitian operator represents an observable quantity. Show that the SM postulate of random phases is equivalent to the statement that there is no time evolution in the expectation value of any observable (that does not explicitly depend on time in the Schrodinger picture). Assume that the system is isolated, a good approximation over short enough time scales.

The postulate of random phases says that the density operator in an eigenbasis of the system Hamiltonian is diagonal. The time evolution of the density operator in the Liouville-von Neumann equation is a unitary transformation of the density operator

$$\rho(t) = U \rho(t_0) U^{\dagger}$$

The random phases postulate implies that $\rho(t)$ and $\rho(t_0)$ are diagonal, and The expectation value of an observable A is given by $\langle A\rangle = \mathrm{Tr}\{\rho A\}$, so we can say

$$\begin{aligned}\langle A(t)\rangle &= \mathrm{Tr}\{\rho(t)A\}\\ &= \mathrm{Tr}\Big\{U\rho(t_0)U^\dagger A\Big\}\\ &= \mathrm{Tr}\{\rho(t_0)A\}\\ &= \langle A(t_0)\rangle\end{aligned}$$

Given that the unitary operators are a symmetry transformation, we use the result $[U, A] = 0$ to go from the second to third line, which solves the problem immediately. Thus the expectation value of an observable is invariant with time under the SM postulate of random phases.

Another attack on this problem would be to show by Ehrenfest's theorem that $\mathrm{Tr}\{\rho[A, H]\} = 0$ which follows quickly from commutator algebra.

Question IV.

In the microcanonical (and soon-upcoming canonical) ensemble the occupation probability of an energy eigenstate depends only on the energy. This seemingly still leaves a problem with the random-phase postulate if the energy happens to be degenerate: there are infinitely many different ways of picking an orthonormal set of vectors that span a degenerate manifold. So, for which choice of the orthonormal vectors is the density operator diagonal? Show that this problem is a non-problem: If the density operator within a manifold of states is an equal mixture of states for one choice of the orthonormal set of states, it is an equal mixture for all choices.

If we assert that there must be a choice of the degenerate eigenstates which diagonalizes the Hamiltonian, then that choice diagonalizes the density operator as well, since a diagonal Hamiltonian implies a diagonal density operator in the chosen eigenbasis.

We can continue this to say that any choice of the degenerate eigenbasis which is a rotation of the basis posed above also diagonalizes the density operator given our results from the first problem of this homework.