

Problem set 2

to be discussed end of May, 2011

see <http://tu-dresden.de/physik/tqo/lehre>

Entropy

We study properties of entropy $S(\rho) = -k_B \text{Tr}(\rho \ln \rho)$:

- a) Let ρ, ρ' be density operators: Show that

$$\text{Tr}[\rho(\ln \rho' - \ln \rho)] \leq 0$$

holds. [Hint: $\ln z \leq z - 1$]

- b) Show with a) that $S(\rho) \leq S(\rho_K)$ for all density operators ρ with $\text{Tr}\rho = 1$ and $\text{Tr}(\rho\hat{H}) = E$ (ρ_K the canonical ensemble).
- c) Similarly, show that $S(\rho) \leq S(\rho_{GK})$ for all density operators ρ with $\text{Tr}\rho = 1$, $\text{Tr}(\rho\hat{H}) = E$ and $\text{Tr}(\rho\hat{N}) = N$ (ρ_{GK} the grand canonical ensemble).
- d) Let ρ be a density operator in the product Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and denote with $\rho_1 \equiv \text{Tr}_{\mathcal{H}_2}(\rho)$, $\rho_2 \equiv \text{Tr}_{\mathcal{H}_1}(\rho)$ the reduced states in the two spaces \mathcal{H}_1 and \mathcal{H}_2 . Show with a) that $S(\rho_1) + S(\rho_2) \geq S(\rho)$. When does equality hold?

Coherent states and shift operator

Let b, b^+ be bosonic annihilation and creation operators such that $[b, b^+] = 1$, and let β be a complex number. The unitary *shift operator* $D(\beta) = e^{\beta b^+ - \beta^* b}$ allows us to define coherent states as shifted vacua: $|\beta\rangle \equiv D(\beta)|0\rangle$.

- a) What is the effect of two shift operations $D(\beta)D(\gamma)$?
- b) Define two operators $q := (b + b^+)/\sqrt{2}$ and $p := -i(b - b^+)/\sqrt{2}$. Determine the commutator $[q, p]$ and the expectation values $\langle q \rangle = \langle \beta|q|\beta \rangle$, $\langle p \rangle$, $\langle q^2 \rangle$, $\langle p^2 \rangle$ and $\langle qp + pq \rangle$. Compute the uncertainties $\Delta q = \sqrt{\langle (q - \langle q \rangle)^2 \rangle}$, $\Delta p = \sqrt{\langle (p - \langle p \rangle)^2 \rangle}$, and thus show that the states $|\beta\rangle$ have minimum uncertainty: $\Delta q \Delta p = \frac{1}{2}$.
- c) Determine the wave function $\langle q|\beta \rangle$ in “position” representation.

[Hint: in order to determine $\langle q|\beta \rangle$ (as a function of q for fixed β) find a differential equation for $\langle q|\beta \rangle$ (as a function of β for fixed q) and integrate.]

Please turn over!

Second Quantisation

Consider a system of massive bosons (spin 0) with external potential $V(\vec{r})$ and interaction potential $U(\vec{r}, \vec{r}')$ in second quantisation. We use field operators $\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r})$ with $[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}')] = \delta(\vec{r} - \vec{r}')$ to describe the system. The Hamiltonian reads

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) \right) \hat{\psi}(\vec{r}) + \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}') U(\vec{r}, \vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}),$$

and the number operator $\hat{N} = \int d^3r \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r})$. We also define single-particle states $|\phi_1\rangle := \int d^3r \phi_1(\vec{r}) \hat{\psi}^\dagger(\vec{r}) |0\rangle$ and two-particle states $|\phi_2\rangle := \frac{1}{\sqrt{2}} \int d^3r \int d^3r' \phi_2(\vec{r}, \vec{r}') \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}') |0\rangle$.

- Show that $[\hat{N}, \hat{H}] = 0$ (interpretation?).
- Show: $\hat{N}|\phi_1\rangle = |\phi_1\rangle$ and $\hat{N}|\phi_2\rangle = 2|\phi_2\rangle$ (interpretation?).
- Determine the expectation value of the particle density $\hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r})$ using the one- and two-particle states: $\langle \phi_1 | \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) | \phi_1 \rangle$ and $\langle \phi_2 | \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) | \phi_2 \rangle$.
- In second quantisation the position operator is given by $\hat{\vec{r}} = \int d^3r \hat{\psi}^\dagger(\vec{r}) \vec{r} \hat{\psi}(\vec{r})$. Confirm that $\langle \phi_1 | \hat{\vec{r}} | \phi_1 \rangle$ meets our expectations from a first-quantised approach.
- Determine the expectation value of the interaction energy

$$\frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}') U(\vec{r}, \vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}),$$

using the one- and two-particle states.