

Exercises to Advanced Quantum Mechanics — Sheet 1

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Exercise 1.1 *Pure versus mixed ensembles of qm. states* (3 points)

Consider a hermitian operator A operating on a two-dimensional Hilbert space \mathcal{H} spanned by the two normalised orthogonal states $|1\rangle, |2\rangle$, i.e. A has the matrix representation $A = \sum_{k,l} A_{kl} |k\rangle\langle l|$.

- a) Calculate the expectation value $\langle A \rangle_\psi$ in the pure (normalised) qm. state $|\psi\rangle = c_1|1\rangle + c_2|2\rangle$, $c_1, c_2 \in \mathbb{C}$. Keeping A fixed, show that the extremal values of $\langle A \rangle_\psi$ are the eigenvalues of the operator A .
- b) Calculate the density operator ρ for a mixed ensemble of systems that are all in pure qm. states $|1\rangle$ or $|2\rangle$ with classical probabilities $p_k = |c_k|^2$ for $k = 1, 2$, respectively. Use ρ to determine the expectation value $\langle A \rangle_\rho$ for an A measurement in the ensemble.
- c) Consider the difference $\langle \delta A \rangle = \langle A \rangle_\psi - \langle A \rangle_\rho$. Under which conditions does $\langle \delta A \rangle$ vanish? For which states $|\psi\rangle$ and ensembles ρ is $\langle \delta A \rangle$ extremal?

Exercise 1.2 *System of free electrons* (4 points)

Consider a system of N free electrons whose one-particle states are characterised by fixed wave vectors \vec{k} (we ignore the spin quantum numbers), which are normalised according to $\langle \vec{k}' | \vec{k} \rangle = (2\pi)^3 \delta(\vec{k} - \vec{k}')$.

- a) Construct the position-space wave function $\psi_{\vec{k}_1, \vec{k}_2}(\vec{x}_1, \vec{x}_2)$ for a state $|\vec{k}_1, \vec{k}_2\rangle$ containing two electrons with momenta \vec{k}_1 and \vec{k}_2 . Determine the normalisation of this state by calculating $\langle \vec{k}'_1, \vec{k}'_2 | \vec{k}_1, \vec{k}_2 \rangle$ in two ways and using the completeness relation $\frac{1}{2} \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} |\vec{k}_1, \vec{k}_2\rangle \langle \vec{k}_1, \vec{k}_2| = \mathbb{1}$.
- b) Calculate $|\psi_{\vec{k}_1, \vec{k}_2}(\vec{x}_1, \vec{x}_2)|$ and separately inspect the two limits $\vec{x}_1 \rightarrow \vec{x}_2$ and $\vec{k}_1 \rightarrow \vec{k}_2$. Give physical arguments explaining the two results.
- c) Generalise problem a) to the case of N electrons and consider $\psi_{\vec{k}_1, \dots, \vec{k}_N}(\vec{x}_1, \dots, \vec{x}_N)$ in the limits $\vec{x}_i \rightarrow \vec{x}_j$ and $\vec{k}_i \rightarrow \vec{k}_j$ for a pair of particle indices i, j .
Hint: remember the concept of Slater determinants.
- d) Determine the dependence of $\psi_{\vec{k}_1, \dots, \vec{k}_N}(\vec{x}_1, \dots, \vec{x}_N)$ on the centre-of-mass position \vec{X} upon introducing the new coordinates

$$\vec{X} = \frac{1}{N} \sum_{i=1}^N \vec{x}_i, \quad \vec{x}'_j = \vec{x}_j - \vec{X}, \quad j = 1, \dots, N-1.$$

Please turn over!

Exercise 1.3 *Plane and spherical waves of a free particle* (2 points)

The Hamilton operator $\hat{H} = \frac{\hat{p}^2}{2M}$ of a free particle commutes with the angular momentum operator \vec{L} , i.e. in particular with the operators \vec{L}^2 and L_3 , for which $[\vec{L}^2, L_3] = 0$. A complete set of energy eigenfunctions in position space can, thus, be constructed from the usual spherical harmonics $Y_{lm}(\theta, \varphi)$ containing the angular information and functions $f(r)$ containing the dependence on the radius r in polar coordinates. The functions are easily identified as the *spherical Bessel functions* $j_l(kr)$, where k is related to the energy eigenvalue E by $E = \frac{\hbar^2 k^2}{2M}$. These simultaneous eigenfunctions of \hat{H} , \vec{L}^2 , and L_3 are, thus, of the form

$$\phi_{klm}(r, \theta, \varphi) = j_l(kr)Y_{lm}(\theta, \varphi). \quad (1)$$

On the other hand, plane waves $e^{i\vec{k}\cdot\vec{x}}$ are simultaneous eigenfunctions of \hat{H} and the cartesian momentum operator \hat{p} . For scattering problems, it is useful to express the plane wave solutions in terms of the basis defined in Eq. (1). Consider the case $\vec{k} = k\vec{e}_3$.

- a) Show that the problem is reduced to fixing the coefficients c_l in

$$e^{i\rho u} = \sum_{l=0}^{\infty} c_l j_l(\rho) P_l(u). \quad (2)$$

- b) Show that $c_l = (2l + 1) i^l$.

Hint: One way to determine c_l is to isolate the coefficient of $(\rho u)^l$ on both sides of Eq. (1), making use of the fact that $P_l(u)$ is a polynomial of degree l and $j_l(\rho)$ is a power series in ρ with powers ρ^n , $n \geq l$. Explicitly, P_l and j_l are defined as follows,

$$P_l(u) = \frac{1}{2^l l!} \frac{d^l}{du^l} (u^2 - 1)^l, \\ j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho} \frac{d}{d\rho} \right)^l j_0(\rho), \quad j_0(\rho) = \frac{\sin \rho}{\rho}, \quad l = 0, 1, \dots$$