Exercises to Advanced Quantum Mechanics **Sheet 1**

— Prof. S. Dittmaier, Dr. H. Rzehak, Universität Freiburg, WS14/15 —

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 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 (normalized) 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 characterized by fixed wave-number vectors $\vec{k}$, which are normalized 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 normalization of this state by calculating $\langle \vec{k}_1', \vec{k}_2'|\vec{k}_1, \vec{k}_2\rangle$.

b) Calculate $|\psi_{\vec{k}_1,\vec{k}_2}(\vec{x}_1, \vec{x}_2)|$ and separately inspect the two limits $\vec{x}_1 \to \vec{x}_2$ and $\vec{k}_1 \to \vec{k}_2$. Give physical arguments explaining the two results.

c) Generalize 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 $\vec{x}_i \to \vec{x}_j$ and $\vec{k}_i \to \vec{k}_j$ 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

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

Please turn over!

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

The Hamilton operator $\hat{H} = \frac{\hat{\vec{p}}^2}{2M}$ 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 of 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

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

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

a) Show that for $\vec{k} = k\vec{e}_3$ the problem is reduced to the fixing the coefficients c_l in

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

b) Show that $c_l = (2l+1)\mathrm{i}^l$.

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,

$$\begin{aligned} P_l(u) &= \frac{1}{2^l l!} \frac{\mathrm{d}^l}{\mathrm{d}u^l} (u^2 - 1)^l, \\ j_l(\rho) &= (-\rho)^l \left(\frac{1}{\rho} \frac{\mathrm{d}}{\mathrm{d}\rho} \right)^l j_0(\rho), \qquad j_0(\rho) = \frac{\sin\rho}{\rho}, \qquad l = 0, 1, \ldots. \end{aligned}$$