Mathematisches Institut der Universität München

Prof. Dr. S. Bachmann
Dr. R. Helling

WiSe 2015/16 **Mathematical Quantum Mechanics** 17.11.2015

Problem Sheet 6

Hand-in deadline: 24.11.2015 before 12:00 in the designated MQM box (1st floor, next to the library).

Ex. 1: Let $\mathcal{H}$ be a complex Hilbert space. Recall that for a bounded self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$ we write $A \geq 0$ if $\langle \psi, A\psi \rangle \geq 0$ for every $\psi \in \mathcal{H}$. Similarly, we write $A \leq B$ for two self-adjoint operators $A, B : \mathcal{H} \to \mathcal{H}$ whenever $B - A \geq 0$.

(i) Assume that $A \geq I$ (I being the identity on $\mathcal{H}$). Prove that A is invertible and that $0 \leq A^{-1} \leq I$.

(ii) Assume that $0 \leq A \leq B$. Show that for any $\lambda > 0$, the operators $A + \lambda I$ and $B + \lambda I$ are invertible and that $(B + \lambda I)^{-1} \leq (A + \lambda I)^{-1}$.

(iii) Assume that $0 \leq A \leq B$. Show that $\sqrt{A} \leq \sqrt{B}$. You may use the representation

$$\sqrt{A} = \int_0^\infty \frac{\mathrm{d}\lambda}{\sqrt{\lambda}} \left(I - \lambda (A + \lambda I)^{-1} \right)$$

where the integral is understood in the sense of Riemann integrals for operator-valued functions.

(iv) Assume that $0 \leq A \leq B$. Show that in general this does neither imply $A^2 \leq B^2$ nor $AB \geq 0$. (*Hint:* You might want to try the simplest possible counterexaples where A, B are 2×2 matrices.)

Ex. 2: (i) Let $k \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$. Prove that

$$(A\psi)(x) := \int_{\mathbb{R}^d} k(x, y)\psi(y)\,\mathrm{d}y, \quad \psi \in L^2(\mathbb{R}^d), \tag{1}$$

defines a bounded operator $A : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ with $\|A\| \leq \|k\|_{L^2(\mathbb{R}^d \times \mathbb{R}^d)}$.

(ii) Let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ be a measurable function such that the functions k_1 and k_2 defined by $k_1(x) := \int_{\mathbb{R}^d} |k(x, y)|\,\mathrm{d}y$ and $k_2(y) := \int_{\mathbb{R}^d} |k(x, y)|\,\mathrm{d}x$ both belong to $L^\infty(\mathbb{R}^d)$. Show that (1) defines a bounded operator on $L^2(\mathbb{R}^d)$ with $\|A\| \leq \|k_1\|_{L^\infty(\mathbb{R}^d)}^{1/2} \|k_2\|_{L^\infty(\mathbb{R}^d)}^{1/2}$.

Ex. 3: For $\psi \in \bigwedge^N L^2(\mathbb{R}^3)$ with $\|\psi\| = 1$, we define its *reduced k-particle density matrix* by

$$\gamma_\psi^{(k)}(x_1, \dots x_k, y_1, \dots y_k) := \frac{N!}{(N-k)!} \times \int_{\mathbb{R}^{6(N-k)}} \psi(x_1, \dots x_k, z_{k+1}, \dots, z_N) \overline{\psi(y_1, \dots y_k, z_{k+1}, \dots, z_N)} dz_{k+1} \cdots dz_N$$

Let $\gamma_\psi^{(1)}$ be the integral operator on $L^2(\mathbb{R}^3)$ with kernel $\gamma_\psi^{(1)}(x, y)$, see Ex. 2.

(i) Let $\rho_\psi(x) := \gamma_\psi^{(1)}(x, x)$. Show that $\rho_\psi \in L^1(\mathbb{R}^3)$ with $\|\rho_\psi\|_1 = N$.

(ii) Prove that $0 \leq \langle \varphi, \gamma_\psi^{(1)} \varphi \rangle \leq \langle \varphi, \varphi \rangle$ for all $\varphi \in L^2(\mathbb{R}^3)$.

(iii) Assume that ψ is a Slater determinant, $\psi = f_1 \wedge \cdots \wedge f_N$, where $\{f_i\}_{i=1}^N$ is an orthonormal set in $L^2(\mathbb{R}^3)$. Show that

$$\gamma_\psi^{(1)}(x, y) = \sum_{i=1}^N f_i(x) \overline{f_i(y)}.$$

(iv) Let $H = \sum_{i=1}^N (-\Delta_{x_i}) + \sum_{1 \leq i < j \leq N} V(x_i, x_j)$ acting on $L^2(\mathbb{R}^{3N})$. Show that, for any $\psi \in \mathcal{D}(H) \cap \bigwedge^N L^2(\mathbb{R}^3)$,

$$\langle \psi, H\psi \rangle = \mathrm{Tr}((-\Delta)\gamma_\psi^{(1)}) + \frac{1}{2} \mathrm{Tr}(V \gamma_\psi^{(2)}),$$

where $\mathrm{Tr}(A) := \int k(x, x) dx$ for an integral operator A with kernel $k(x, y)$.

Ex. 4: [Virial theorem] Consider the Schrödinger operator $H = -\Delta + V$ in d dimensions. Assume that $U_{-t} V U_t = \mathrm{e}^{-t} V$ for all $t \in \mathbb{R}$, where $U(t) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is defined by $(U_t \psi)(x) := \mathrm{e}^{-td/2} \psi(\mathrm{e}^{-t} x)$.

(i) Prove that $\{U(t)\}_{t \in \mathbb{R}}$ is a strongly continuous unitary group.

(ii) Let $\psi \in L^2(\mathbb{R}^d)$, $\|\psi\| = 1$. Assume that $\Delta\psi \in L^2(\mathbb{R}^d)$, $V\psi \in L^2(\mathbb{R}^d)$ and $H\psi = E\psi$ (in L^2) for some $E \in \mathbb{R}$. Prove that

$$E = -\langle \psi, (-\Delta)\psi \rangle = \frac{1}{2} \langle \psi, V\psi \rangle$$

and therefore $E \leq 0$. (*Hint:* Compute the commutator of H and U_t.)

Jean-Claude Cuenin