Mathematisches Institut
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Mathematical Quantum Mechanics

Problem Sheet 8

Hand-in deadline: 12/16/2016 before noon in the designated MQM box (1st floor, next to the library).

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

$$\gamma_\psi^{(k)}(x_1, \dots x_k; y_1, \dots y_k) := \binom{N}{k}$$
$$\int_{\mathbb{R}^{d(N-k)}} \overline{\psi(x_1, \dots x_k, z_{k+1}, \dots, z_N)} \psi(y_1, \dots y_k, z_{k+1}, \dots, z_N) dz_{k+1} \cdots dz_N.$$

Let $\gamma_\psi^{(k)}$ be the integral operator on $L^2(\mathbb{R}^{dk})$ with kernel $\gamma_\psi^{(k)}(x_1, \dots x_k; y_1, \dots y_k)$, and let Let $\rho_\psi^{(k)}(x)$ be the corresponding density.

(i) Show that $\rho_\psi^{(1)} \in L^1(\mathbb{R}^d)$ with $\|\rho_\psi^{(1)}\|_1 = N$.

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

$$\gamma_\psi^{(1)}(x; y) = \sum_{i=1}^N \overline{f_i}(x) f_i(y),$$
$$\rho_\psi^{(2)} = \rho_\psi^{(1)}(x_1)\rho_\psi^{(1)}(x_2) - |\gamma_\psi^{(1)}(x_1; x_2)|^2.$$

(iii) Let $H = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \sum_{1 \le i < j \le N} W(x_i, x_j)$ acting on $L^2(\mathbb{R}^{dN})$, with V, W bounded and with $W(x, y) = W(y, x)$. Show that, for any $\psi \in H^2(\mathbb{R}^d) \cap \bigwedge^N L^2(\mathbb{R}^d)$,

$$\langle \psi, H\psi \rangle = \operatorname{tr}((-\Delta + V)\gamma_\psi^{(1)}) + \operatorname{tr}(W\gamma_\psi^{(2)}).$$

Ex. 2: (i) Let $\mathfrak{h}$ be a separable Hilbert space and let $A : \mathfrak{h} \to \mathfrak{h}$ be a bounded operator. A is called a *Hilbert-Schmidt operator* if there exists an orthonormal basis $\{\phi_n\}_{n \in \mathbb{N}}$ such that

$$\|A\|_{\mathfrak{S}^2}^2 := \sum_{n \in \mathbb{N}} \|A\phi_n\|^2 < \infty.$$

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Prove that this definition is independent of the choice of the orthonormal basis $\{\phi_n\}_{n\in\mathbb{N}}$. Moreover, prove that $\|A\|_{\mathfrak{S}^2} \geq \|A\|$.

(ii) Let $A : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ be the integral operator

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

with kernel $k_A \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$. Prove that A is a Hilbert-Schmidt operator with $\|A\|_{\mathfrak{S}^2} = \|k_A\|_{L^2(\mathbb{R}^d)\times L^2(\mathbb{R}^d)}$.

(iii) Let $e > 0$, and let $K_e := \sqrt{V_-}(-\Delta + e)^{-1}\sqrt{V_-}$ be the Birman-Schwinger operator on $L^2(\mathbb{R}^3)$. Show that K_e is an integral operator and determine its kernel. (*Hint:* You may use the fact that the inverse Fourier transform of $(|\cdot|^2 + e)^{-1}$ is given by $\frac{\mathrm{e}^{-\sqrt{e}|\cdot|}}{4\pi|\cdot|}$).

(iv) Assume that $V_- \in L^2(\mathbb{R}^3)$. Prove that K_e is a Hilbert-Schmidt operator and

$$\|K_e\| \leq Ce^{-1/4}\|V_-\|_2.$$

Ex. 3: Let γ be a finite rank projection and let A be a bounded operator on some Hilbert space. Prove that the Riesz projection P_ε corresponding to $\gamma_\varepsilon := \gamma + \varepsilon A$, $\varepsilon > 0$, satisfies

$$P_\varepsilon := \frac{1}{2\pi i}\oint_{|z-1|=\frac{1}{2}} (z - \gamma_\epsilon)^{-1}\mathrm{d}z = \gamma + \varepsilon(\gamma A\gamma^\perp + \gamma^\perp A\gamma) + \varepsilon^2 R$$

for ε sufficiently small. Here, R is some bounded operator.