WISE 2015/16 Mathematical Quantum Mechanics 24.11.2015 Problem Sheet 7

Hand-in deadline: 01.12.2015 before 12:00 in the designated MQM box (1st floor, next to the library).

Ex. 1: (i) Let $\psi \in H^{1/2}(\mathbb{R}^d)$, with $d \ge 2$, and let

$$T_{\rm rel}(\psi) := \langle \psi, |p|\psi \rangle = \int_{\mathbb{R}^d} |k| |\widehat{\psi}(k)|^2 dk$$

be the relativistic kinetic energy. By considering the scaling $\psi_{\lambda}(x) := \psi(\lambda x)$ for an arbitrary $\psi \in \mathcal{S}(\mathbb{R}^d)$ and $\lambda > 0$, show that $q = \frac{2d}{d-1}$ is the only possible value for which the following inequality may hold:

$$\langle \psi, |p|\psi \rangle \ge C_d \|\psi\|_q^2. \tag{1}$$

Remark: If $\psi \in H^{1/2}(\mathbb{R}^d)$ and vanishes at infinity, then $\psi \in L^q(\mathbb{R}^d)$ and (1) indeed holds, a fact you may use in the following.

(ii) Let $V \in L^d(\mathbb{R}^d)$, and $V(\psi) = \int_{\mathbb{R}^d} V(x) |\psi(x)|^2 dx$. Show that for $||V||_d$ small enough,

$$T_{\rm rel}(\psi) + V(\psi) \ge 0.$$

(iii) The operator on $L^2(\mathbb{R}^d)$ defined by

$$\left(\mathrm{e}^{-t|p|}\psi\right)(x) := \left(\mathrm{e}^{-t|\cdot|}\widehat{\psi}\right)^{\vee}(x)$$

is bounded (why?) and is given by an integral kernel: $\left(e^{-t|p|}\psi\right)(x) = \int_{\mathbb{R}^d} k(x,y)\psi(y)dy$. Compute k(x,y) for d = 3.

(iv) Prove that

$$T_{\rm rel}(\psi) = \frac{\Gamma((d+1)/2)}{2\pi^{(d+1)/2}} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{|\psi(x) - \psi(y)|^2}{|x - y|^{d+1}} dx dy$$

in the case d = 3 (*Hint*: Use the fact that $|p| = \lim_{t \to 0} \frac{1}{t} (1 - \exp(-t|p|))$).

Ex. 2: (i) Let \mathcal{H} be a separable Hilbert space and let $A : \mathcal{H} \to \mathcal{H}$ 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

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

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

(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 $||A||_{\mathrm{HS}} = ||k_A||_{L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)}$.

(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 $\frac{e^{-\sqrt{e}|\cdot|}}{4\pi|\cdot|}$).

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

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

Ex. 3: (i) Let $(f_j)_{j=1}^N$ be orthonormal functions such that $f_i \in H^1(\mathbb{R}^d)$ for $1 \leq i \leq N$. Let $\psi = f_1 \wedge \cdots \wedge f_N$, and $\rho_{\psi}(x) = \gamma_{\psi}^{(1)}(x, x)$. Show that there exists $K_d > 0$ such that

$$T(\psi) \ge K_d \int_{\mathbb{R}^d} \rho_{\psi}(x)^{1+\frac{2}{d}} dx$$

where $T(\psi) = \sum_{i=1}^{N} \int |\nabla_{x_i} \psi|^2$ (*Hint:* Consider the 'potential' $U(x) = c\rho_{\psi}(x)^{\frac{2}{d}}$ and use the Lieb-Thirring inequality).

(ii) Consider the Laplacian in the box $\Lambda_L := [-L/2, L/2]^3$ with periodic boundary conditions. Let ψ_k be its eigenvectors and ϵ_k its eigenvalues for $k \in \mathbb{Z}^3$. The corresponding fermionic N-body Hamiltonian $H := \sum_{i=1}^N (-\Delta_{x_i})$ acts on $\bigwedge^N L^2(\Lambda_L)$. Let $\psi := \bigwedge_{k=1}^N \psi_k$ be its ground state and $\rho_{\psi}(x)$ its associated density. Show that the (kinetic) energy can be written as a *density* functional, namely that there is a function $F : \mathbb{R} \to \mathbb{R}$ such that

$$\lim_{\substack{N,L\to\infty\\N/L^3=:\rho \text{ constant}}} L^{-3}\left(\langle\psi,H\psi\rangle - \int_{\Lambda_L} F(\rho_\psi(x))dx\right) = 0.$$

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Remarks.

ad 1(ii). This could of course be extended to prove stability of the first kind for any $V \in L^d(\mathbb{R}^d) + L^{\infty}(\mathbb{R}^d)$. The Coulomb singularity is borderline in d = 3 in this case: $|\cdot|^{-1} \notin L^3_{loc}(\mathbb{R}^3)$, while $|\cdot|^{-1} \in L^{3-\epsilon}_{loc}(\mathbb{R}^3)$ for any $\epsilon > 0$. This is related to the fact that relativistic matter is stable only if $Z\alpha$ is small enough.

ad 3(ii). This is the heuristic motivation for the *Thomas-Fermi model* that assumes that over regions small with respect to the typical scale of the potential, the electrons are essentially free and a local version of the above holds. The Lieb-Thirring inequality provides a proof of this fact, at least as a lower bound valid for any N, see 3(i).

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