Mathematical Quantum Mechanics, 2014/15 Homework Problems, LMU

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13. Show that the expectation value $\langle\psi, \sum_{j=1}^N V_j\psi\rangle$ of a sum of one-body potentials V_j can be expressed by means of the N-electron density ρ as $\langle\psi, \sum_{j=1}^N V_j\psi\rangle = \int_{\mathbb{R}^3}\sum_{j=1}^N V_j(x)\rho(x)d^3x$.

14. We study a hydrogen atom within a magnetic field $B = \nabla\wedge A$ that is described by a vector potential A such that the corresponding Hamilton operator $H_A = (-\mathrm{i}\nabla + eA)^2 + eV$ with $V(x) = -|x|^{-1}$ (e =electronic charge) is self-adjoint on the Sobolev space $H^2(\mathbb{R}^3)$. Show that such a magnetic field causes a diamagnetic effect for the ground state of the hydrogen atom, i.e., show that $E_{\mathrm{gs}}(A) \geq E_{\mathrm{gs}}(0)$ holds for the ground state energy $E_{\mathrm{gs}}(A) = \inf\sigma(H_A)$ of H_A. (Hint: Use an appropriate factorization of the wave function.) Could the argumentation be generalized to atoms with $N > 1$ electrons?

15. The potential of a charge distribution $\rho : \mathbb{R}^3 \to \mathbb{R}$ is given by

$$V(x) = \int \frac{\rho(y)}{|x-y|}d^3y. \tag{15}$$

(i) Assuming that ρ is spherically symmetric, prove that then also V is spherically symmetric and has the form

$$V(x) = v(r) = \int_{|y|>r}\frac{\rho(y)}{|y|}d^3y + \frac{1}{r}\int_{|y|<r}\rho(y)d^3y, \tag{16}$$

where $r = |x|$.

(ii) Determine v for the particular charge distribution

$$\rho(x) = \begin{cases} 4\pi r_0^3/3 & \text{if } |x| < r_0 \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

with $r_0 > 0$.

16. If the vector potential A and the electrostatic potential V are such that the Dirac operator $D_{A,V}(e) = \alpha \cdot (-\mathrm{i}\nabla - eA) + eV$ is self-adjoint on $\mathcal{D}(D_{A,V}) = H^1(\mathbb{R}^3, \mathbb{C}^4) \subset \mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, then using again the conjugation operator $\tau : \mathfrak{H} \to \mathfrak{H}$ with $\tau\psi := \overline{\psi}$, we construct the operator $C_c : \mathfrak{H} \to \mathfrak{H}$ ("charge conjugation") by

$$C_c = \mathrm{i}\beta \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} \tau. \tag{18}$$

(i) Prove that C_c is an antiunitary operator.

(ii) Show that $C_c D_{A,V}(e) C_c^{-1} = -D_{A,V}(-e)$. What does this imply for the relation between positive and negative energy solutions of the Dirac equation?