Mathematical Quantum Mechanics, 2014/15 Homework Problems, LMU

Issued: November 18, 2014; deadline for handing in the solutions: November 25, 2014, 4 pm

20. Let γ_ψ denote the one-particle reduced density matrix associated to the state ψ, and let $T^{(N)} = T\otimes 1\otimes \ldots \otimes 1 + 1\otimes T\otimes 1\otimes \ldots \otimes 1 + \ldots + 1\otimes 1\otimes \ldots \otimes T$ be a one-particle operator with $\psi \in \mathcal{D}(T^{(N)})$.

(i) Show that $\langle \psi,\, T^{(N)}\psi\rangle = \mathrm{tr}\,\{T\gamma_\psi\}$.

(ii) If $\psi(x_1,\ldots,x_N) = (N!)^{-1/2}\,|\phi_1(x_1)\ldots\phi_N(x_N)|$ is of determinantel form, i.e., $|\phi_1(x_1)\ldots\phi_N(x_N)| = \sum_{\pi\in S_N} \mathrm{sign}(\pi)\phi_1(x_{\pi(1)})\ldots\phi_N(x_{\pi(N)})$ with the sum running over all permutations π, and where $\{\phi_j\}$ is an orthonormal set, prove that $\gamma_\psi(x,y) = \sum_{j=1}^N \phi_j(x)\overline{\phi}_j(y)$.

21. Use the Hardy inequality to demonstrate that the (distributional) Laplacian obeys the inequality $|x|(-\Delta)+(-\Delta)|x| \geq 0$. Infer that this implies $\mathrm{Re}\,\langle |x|\psi,\, -\Delta\psi\rangle \geq 0$ for all $\psi \in \mathcal{D}(-\Delta)\cap\mathcal{D}(|x|)$.

22. Consider the modified atomic functional $\mathcal{E}(\rho) = \int (\nabla\sqrt{\rho})^2 d^3x + (3/5)\gamma_{\mathrm{TF}}\int \rho(x)^{5/3}d^3x - \int Z|x|^{-1}\rho(x)d^3x + D(\rho,\rho)$ defined on $\mathcal{D}_{\mathcal{E}} = \{\rho \in L^{5/3}(\mathbb{R}^3),\, \nabla\sqrt{\rho} \in L^2(\mathbb{R}^3),\, D(\rho,\rho) < \infty, \rho > 0\}$. Assume that $\mathcal{E}$ enjoys a unique minimizer (For enthusiasts (and extra points): Prove this).

(i) Show that this minimizer solves the Euler equation (expressed with the help of $\psi = \sqrt{\rho}$) associated with $\mathcal{E}$, viz.,

$$-\Delta\psi(x) + \gamma\psi^{7/3}(x) - \frac{Z}{|x|}\psi(x) + \int \frac{\psi(y)^2}{|x-y|}\psi(x) = 0. \qquad (20)$$

(ii) Prove that the validity of (20) implies the bound $N < 2Z$ for $\int \rho = N$. (Hint: Take the inner product of (20) with $|x|\psi$ and employ the results of problem 21.)