Mathematical Quantum Mechanics, 2014/15 Homework Problems, LMU

Issued: December 9, 2014; deadline for handing in the solutions: December 16, 2014, 4 pm

27. Compute for the Gaussian coherent states

$$\psi_{p,q}(x) = e^{\mathrm{i}\hbar^{-1}px} e^{-a(x-q)^2} \tag{28}$$

the convolution $\psi_{p_1,q_1} \star \psi_{p_2,q_2}$ with $q_j, p_j \in \mathbb{R}$, $j = 1, 2$, $a > 0$. Is this again a coherent state?

28. For a given charge $Z > 0$, assume an electronic density

$$\rho_{\tau,R}(x) = \tau \chi_{|x| \leq R}(x) \tag{29}$$

with $\tau > 0$ and where $\chi_{|x|\leq R}$ stands for the indicator function of the ball of radius $R > 0$.

(i) Prove that the resulting Thomas-Fermi energy is given by

$$\mathcal{E}_{\mathrm{TF}}(\rho_{\tau,R}) = \frac{4\pi}{5}\gamma_{\mathrm{TF}}\tau^{5/3}R^3 - 2\pi Z\tau R^2 + \frac{16}{15}\pi^2\tau^2 R^5. \tag{30}$$

(ii) Employ the condition $\int \rho_{\tau,R} = Z$ to derive a relation between the parameters τ and R. After eliminating τ, minimize $\mathcal{E}_{\mathrm{TF}}(\rho_R)$ with respect to R and compute $\inf_{R>0} \mathcal{E}_{\mathrm{TF}}(\rho_R)$.

(iii) Use the functional $\mathcal{E}(\psi) = -(1/(8\pi)) \int |\nabla\psi(x)|^2 d^3x - (2/5)\gamma_{\mathrm{TF}}^{-3/2} \int [V(x) - \psi(x)]_+^{5/2} d^3x$ of problem 26 and the relation between the corresponding ψ and ρ_R, viz.,

$$\psi_R(x) = \int \frac{\rho_R(y)}{|x-y|}, \tag{31}$$

to obtain a lower bound on the Thomas-Fermi energy, i.e., maximize $\mathcal{E}(\psi_R)$ with respect to $R > 0$ and compute $\sup_{R>0} \mathcal{E}(\psi_R)$. Hint: You may use that

$$\int_0^1 t^2 \Big(\frac{t^2}{2} + \frac{1}{t} - \frac{3}{2}\Big)^{5/2} dt = \frac{531}{2^8\sqrt{2}} \Big(\frac{205}{59} \mathrm{csch}^{-1}\sqrt{2} - \sqrt{3}\Big). \tag{32}$$

29. Provide a counterexample to the positivity of

$$\rho_\gamma(x)\rho_\gamma(y) - \sum_{\sigma,\sigma'}^{q} |\gamma^{1/2}(x,y)|^2 \geq 0 \tag{33}$$

in the Müller functional discussed in the lecture.

30. Prove that a density of the form $c|x|^{-a}$ obeys the neutral atomic Thomas-Fermi equation

$$-\Delta\phi_{\mathrm{TF}} = -4\pi(\phi_{\mathrm{TF}}/\gamma_{\mathrm{TF}})^{3/2} \tag{34}$$

for $x \neq 0$ and a certain c and $a > 0$.