Solutions for stability of matter problems, Physics 623, Spring 2010, O.W. Greenberg

1.a. The stability of a single atom depends on an inequality that shows the dominance of kinetic energy over the short-distance Coulomb potential. The Sobolev inequality suffices, but the Heisenberg uncertainty inequality does not.
b. The stability of bulk matter requires the Pauli principle for fermions. Boson matter would collapse.
c. Thermodynamic limit for bulk matter requires that the long-distance Coulomb interaction be canceled by having matter be charge neutral.

2. Construct a trial wave function that obeys the Heisenberg-Weyl inequality

$$T_\psi < |x]^2 >_\psi \geq 9/4, \tag{1}$$

where $T_\psi = \int[\nabla\psi(x)]^2 dx$, $< |x]^2 >_\psi = \int[x]^2[\psi(x)]^2 dx$, subject to $\int[\psi(x)]^2 dx = 1$, and yet allows the energy of a single-electron atom to be unbounded below. Following Lieb in RMP, choose ψ to be concentrated inside a radius R near the origin with probability 1/2 and in a thin shell at distance L away from the origin also with probability 1/2. The expectation of the energy is,

$$\langle H \rangle = T_\psi - Z\langle|\mathbf{x}|^{-1}\rangle_\psi \tag{2}$$

(Following Lieb, the x's are three dimensional vectors.) Note that the Sobolev inequality depends on the dimension of space, unlike the Heisenberg-Weyl inequality. We would like to get T_ψ very large from the Heisenberg uncertainty princple inequality so as to prevent the energy getting very negative. Unfortunately, the Heisenberg uncertainty principle factor goes in the denominator, so we get

$$\langle H \rangle \geq (9/4)(2/L^2) - (Z^2/2R) \to -\infty \tag{3}$$

for L large enough and R small enough, even though we used the Heisenberg uncertainty princple.
3. Use the Sobolev inequality

$$T_\psi \geq K_s[\int[\psi(x)]^6 dx]^{1/3} \tag{4}$$

to find a finite lower bound for the energy of a single-electron atom.
K_s is a positive number whose value is not needed.
Again following Lieb, we want to minimize the expectation value of the Hamiltonian,

$$\langle H \rangle = T_\psi - Z \int |x|^{-1} \rho dx \equiv h(\rho) \tag{5}$$

subject to $\int \rho dx = 1$. We defined $\rho = |\psi|^2$. Put in the constraint as a Lagrange multiplier by adding $\lambda(\int \rho dx - 1)$ to $h(\rho)$.

$$\frac{\delta}{\delta \rho(x)}[h(\rho) + \lambda(\int \rho dx - 1)] = K_s[\int \rho^3 dx]^{-2/3} \rho(x) - \frac{Z}{|x|} + \lambda = 0 \tag{6}$$

$$\frac{\delta}{\delta \lambda} \Longrightarrow \int \rho dx = 1 \tag{7}$$

We find

$$\rho(x) = \sqrt{\frac{Z}{K_s}}[\int \rho^3 dx]^{1/3} \sqrt{\frac{1}{|x|} - \frac{\lambda}{Z}} \tag{8}$$

Since ρ must be positive or zero, we need $\frac{1}{|x|} - \frac{\lambda}{Z} \geq 0$, or $|x| \leq \frac{Z}{\lambda} \equiv R$. Then

$$\rho_{min} = \begin{cases} \alpha \sqrt{\frac{1}{|x|} - \frac{1}{R}}, & |x| \leq R \\ 0, & |x| > R \end{cases} \tag{9}$$

where from Eq.(8) $\alpha = \sqrt{\frac{Z}{K_s}}[\int \rho^3 dx]^{1/3}$. Mathematica gives this as a finite expression. The value of R follows from $\int \rho dx = 1$. Mathematica also gives this as a finite expression, $\alpha = (\pi^2/4)^{2/3}(RZ^2/K_s)$. Inserting ρ_{min} into $h(\rho)$ then gives a finite lower bound for the energy.