PHY635, MBQM II-Semester 2022/23, last Assignment 6

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Due-date: email by 14.4.2023

(1) Treating an atom like a degenerate Fermi gas
In heavy atoms, the attraction of electrons towards the heavily charged nucleus might lead to the generation of a "degenerate Fermi gas". Let us assume an atom has a radius R, which roughly stays constant at $R = a_0$ for various species (which it approximately does in fact), and all Z electrons are squeezed into a spherical shell of that radius. We then want to define a local electron density profile $\rho_e(r)$ and want to calculate this profile as a function of distance from the nucleus.

(a) For this to make any sense, we require $k_F R \gg 1$, since otherwise the wavelengths of even the highest occupied electron states is too large to add up to a density profile $\rho_e(r)$. Assuming the electrons are homogeneously distributed in a spherical volume of radius R, evaluate $k_F R$ for 5-6 elements representatively spread accross the periodic table, and discuss for which atoms our degenerate Fermi gas approach might work. [*2 points*]

(b) Now we assume we can define a <u>local</u> Fermi wavenumber k_F, again using the homogenous result for Fermions with spin 1/2, but now allowing the density $\rho_e(\mathbf{x})$ to vary with position $\mathbf{x}$. The same local density approximation and results from the lecture can give you the kinetic energy as a function of r. Combine these with all other energies in the problem, to set up an <u>energy functional</u> $E[\rho(\mathbf{x})]$, which gives you how the total energy of the atom depends on the electron density $\rho_e(\mathbf{x})$. [*4 points*]

(c) Now we add the constraint that the total number of electrons must be $N_e = Z$, by means of a Lagrange multiplier[1] λ to reach the functional

$$H[\rho(\mathbf{x}), \lambda] = E[\rho(\mathbf{x})] - \lambda(N[\rho(\mathbf{x})] - N_e), \tag{1}$$

where $N[\rho(\mathbf{x})]$ is the expression that gives you N_e from $\rho_e(\mathbf{x})$.

Find extrema by the functional differentiation $\delta H[\rho(\mathbf{x}), \lambda]/\delta\rho(\mathbf{x})$ simultaneous with $\partial H[\rho(\mathbf{x}), \lambda]/\partial\lambda = 0$. Discuss the meaning of the two coupled equations obtained. [*2 points*]

(d) In the equations from (c), let us now exploit the spherical symmetry of the atom and use a coordinate $r = |\mathbf{x}|$. Write down the electro-static potential energy $V(r)$ for an electron within the atom, and then define the functions $U(r) = V(r) - \lambda$ and from that $\Phi(r) = -\frac{r}{C}U(r)$ with constant(s) C. Finally show the <u>Thomas-Fermi equation</u>

$$\frac{d^2}{dx^2}\Phi(x) = \frac{1}{\sqrt{x}}\Phi(x)^{3/2}. \tag{2}$$

[1] revise finding minima of functions in higher dimensions with constraints.

when using the right dimensionless radius $x = r/b$ and choice of C. *Hints: Find some physical constraints for solutions, and reasonable initial conditions at* $r = 0$. *One initial condition can be derived and one can be found by trial and error, requiring the total electron charge to be* $Z(-e)$. *Make plots of solutions you find. In the very end test your result by calculations for a selected atom and compare the radial electron distribution with figures found in the internet for the full (Schrödinger's equation) result.* [*4 points*]

(e) To numerically solve Eq. (2) from some infinitesimal ϵ to $x_{\text{max}} = R/b$, we need two initial conditions. You can derive $\Phi(\epsilon)$ from physical principles and just take $\Phi(\epsilon)' = -1.5880710$ for reasons that shall be explained in the solution[2] Then compare a numerical solution for the electron density with an exact literature result for Mercury and discuss. [*3 points*]

(2) Excitations in a Fermi liquid: Calculate the energy of hole and particle excitations in a Fermi liquid (homogeneous system as in lecture) to first order perturbation theory in the interaction between different spin Fermions. Then take their energy relative to the unperturbed Fermi sea. Make a graph of particle/hole energy as a function of k and discuss your results and their interpretation. [*5 points*]

(3) Superfluid current Assume an attractively interacting Fermi gas described by the BdG equations (4.65). Let the order parameter be $\Delta(\mathbf{r}) = \Delta_0 \exp\left[2i\varphi(\mathbf{r})\right]$, in an otherwise homogenous system (no external potential, homogenous density). Find an expression for the superfluid current and superfluid velocity and discuss. [*10 points*]

[2] This picks neutral atoms, as opposed to e.g. positive ions, for which the TF equation is also valid.