Note! The last exercise session is on Tuesday 7.4 10:15-12:00.

1. **Variational analysis**
   a) A function of two real variables, $g(x,y)$, can be represented also in the form $f(z,z^*) \equiv g(\Re\mathrm{e}\, z, \Im\mathrm{m}\, z)$ with $z = x+iy$. Show that in case $\frac{\partial g}{\partial x} = \frac{\partial g}{\partial y} = 0$, also $\frac{\partial f}{\partial z} = \frac{\partial f}{\partial z^*} = 0$.
   b) Justify, in the case of one particle with the Hamiltonian $\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$, that the functional

$$\frac{\int d\vec{r}\psi^*(\vec{r})\hat{\mathcal{H}}\psi(\vec{r})}{\int d\vec{r}|\psi(\vec{r})|^2}$$

   has an extremum in case ψ is an eigenstate of $\hat{\mathcal{H}}$.
   c) Repeat the analysis by minimizing $\int d\vec{r}\psi^*(\vec{r})\hat{\mathcal{H}}\psi(\vec{r})$ with the constraint $\int d\vec{r}|\psi(\vec{r})|^2 = 1$ taken into account with a Lagrange multiplier.

2. **Hartree equations**
   a) Find the expectation value F_{H} of

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{l=1}^{N}\nabla_l^2 + \sum_{l=1}^{N}U_{\mathrm{ion}}(\vec{r}_l) + \sum_{l<l'}\frac{e^2}{|\vec{r}_l - \vec{r}_{l'}|}$$

   in a state of the form $\Psi = \prod_{l=1}^{N}\psi_l(\vec{r}_l)$ where the $\psi_l(\vec{r}_l)$ are orthonormal.
   b) Take the variation of F_{H}, subject to the constraint that each ψ be normalized:

$$\frac{\delta F_{\mathrm{H}}}{\delta\psi_l(\vec{r})} - \frac{\delta}{\delta\psi_l(\vec{r})}\sum_j \mathcal{E}_j \int d\vec{r}'\,\psi_j^*(\vec{r}')\psi_j(\vec{r}') = 0\,.$$

   c) Add one extra term (without much justification apart from simplicity) so that the Coulomb interaction term of the Hamiltonian becomes the same for all wave functions. In this way, recover the Hartree equations. Notice that demanding that each ψ_l be normalized is sufficient to result in an orthonormal set of functions.

3. **Lindhard dielectric function**
   By direct integration, show that

$$\int_{k'\le k_F} d\vec{k}'\,\frac{1}{|\vec{k}-\vec{k}'|^2} = 4\pi k_F F\left(\frac{k}{k_F}\right)$$

where

$$F(x) = \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| + \frac{1}{2}\,.$$

4. **Hartree–Fock energy for jellium**

Show that the Hartree–Fock energy for jellium

$$\mathcal{E} = \sum_{\vec{k},\sigma} \left[\frac{\hbar^2 k^2}{2m} - \frac{e^2}{\pi} k_F F\left(\frac{k}{k_F}\right)\right]$$

can also be given in the form

$$\mathcal{E} = N\left[\frac{3}{5}\mathcal{E}_F - \frac{3}{4}\frac{e^2 k_F}{\pi}\right]\,.$$

Sketch $\mathcal{E}/N$ as a function of k_F, and find the equilibrium density.