

# Application of Fourier transform in Problem 1 of Homework Set 6.

**Problem 1.** The idea of screening comes originally from electrolytic solutions. Imagine placing a charged ion into such solution. At first the potential due to the added ion extends its influence to the far reaches of the system, dying slowly off as  $1/r$ . However, mobile ions nearby rapidly react to the intruder, and the motions they make in response have the effect of almost completely canceling out its electric field, except within a characteristic distance called the *screening length*. Because the phenomenon occurs generally for any assembly of charged particles, it can be studied in the context of Thomas-Fermi theory which yields the following equation

$$\frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3}(\mathbf{r}) + U(\mathbf{r}) + \int d\mathbf{r}' \frac{e^2 n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \left(\frac{3}{\pi}\right)^{1/3} e^2 n^{1/3}(\mathbf{r}) = \mu$$

where  $n(\mathbf{r})$  is the density of particles and  $\mu$  is the chemical potential characterizing the equilibrium state.

(a) Consider this Thomas-Fermi equation where the last term on the left-hand side (resulting from the exchange interaction) is omitted for simplicity. Suppose that  $n_0$  is the solution of this equation when the potential  $U(\mathbf{r})$  vanishes  $U(\mathbf{r}) \rightarrow 0$ . If now a small potential  $U(\mathbf{r})$  is added, find the equation governing deviations  $\delta n(\mathbf{r})$  of the density from perfect uniformity to first order in  $U$ .

(b) Consider adding one extra electron to the uniform electron gas and therefore specializing to the case  $U(\mathbf{r}) = e^2/r$ . Solve the linearized equation for  $\delta n(\mathbf{r})$  by use of Fourier *transform*. The answer should be of the form  $\delta n \sim \frac{e^{-r/\xi}}{r}$ . Identify the screening length  $\xi$  and express it in terms of the Bohr radius and the average volume per particle of the original uniform electron gas.

(c) Estimate the screening length for aluminum and copper.

**HINT:** The problem deals with more exact (Thomas-Fermi) theory of screening, which, nevertheless, leads to similar screening length as derived in the class (up to numerical factors of order one). It also introduces Fourier transform as a tool to solve integral (or, in general, integro-differential equations) by converting them into algebraic ones.

The first step is to write the TF equation in the absence of impurity potential  $U(\mathbf{r})$  and by neglecting the exchange interaction term (due to Pauli principle)

$$\frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3} + \int d\mathbf{r}' \frac{e^2 n}{|\mathbf{r} - \mathbf{r}'|} = \mu \quad (1)$$

If we now introduce charged impurity with potential  $U(\mathbf{r})$ , the charge density will change to  $n \rightarrow n + \delta n(\mathbf{r})$  so that the chemical potential remains the same throughout the system (in equilibrium)

$$\frac{\hbar^2}{2m} (3\pi^2)^{2/3} [n + \delta n(\mathbf{r})]^{2/3} + U(\mathbf{r}) + \int d\mathbf{r}' \frac{e^2 [n + \delta n(\mathbf{r}')] }{|\mathbf{r} - \mathbf{r}'|} = \mu \quad (2)$$

By expanding functions of  $\delta n(\mathbf{r})$  into a Taylor series, retaining only linear in  $\delta n(\mathbf{r})$  terms for small deviations, and using Eq. (1) one arrives at an equation which contains only  $\delta n(\mathbf{r})$ . At first sight this equation is rather complicated since it will contain the term

$$\int d\mathbf{r}' \frac{e^2 \delta n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (3)$$

where unknown function  $\delta n(\mathbf{r})$  appears inside the integral [therefore, we have to deal with the integral equation for  $\delta n(\mathbf{r})$ !].

At this point we invoke the Fourier transform technique, over the spatial coordinates

$$\text{FT}[f(\mathbf{r})] \equiv f_{\mathbf{k}} = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{+\infty} d\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (4)$$

The Fourier transform of the derivative of a function is  $\text{FT}[\partial f(\mathbf{r})/\partial x] = ik_x f_{\mathbf{k}}$ , meaning that differential operator  $\nabla$  after Fourier transform becomes just a  $\mathbf{k}$ -vector multiplying the corresponding function  $\nabla \rightarrow i\mathbf{k}$ . This allows one to convert partial differential equations for function  $f(\mathbf{r})$  into algebraic ones for its Fourier transform  $f_{\mathbf{k}}$ . Another useful property of the Fourier transform is its action on the convolution of two functions

$$\text{FT}[f(\mathbf{r}) * g(\mathbf{r})] \equiv \text{FT} \left[ \int f(\mathbf{r})g(\mathbf{r} + \mathbf{r}')d\mathbf{r} \right] = f_{\mathbf{k}}g_{\mathbf{k}} \quad (5)$$

which yields just a product of their Fourier transforms. Thus, Fourier transform of the integral in Eq. (3) is simply

$$\text{FT} \left[ \int d\mathbf{r}' \frac{e^2 \delta n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] = e^2 \frac{4\pi}{\mathbf{k}^2} \delta n_{\mathbf{k}} \quad (6)$$

where  $4\pi/\mathbf{k}^2$  is the Fourier transform of  $g(\mathbf{r}) = 1/|\mathbf{r}|$  [the same Fourier transform applies to the Coulomb potential  $U(\mathbf{r})$  in (b)]. After solving algebraic equation for  $\delta n_{\mathbf{k}}$ , one only has to find its inverse FT to obtain the corresponding function in real space  $\delta n(\mathbf{r}) \sim e^{-r/\xi}$  where  $\xi$  is the screening length (appearing already in the algebraic equation for  $\delta n_{\mathbf{k}}$ ).

Note that the inverse FT

$$\text{FT}^{-1}[f_{\mathbf{k}}] \equiv f(\mathbf{r}) = \iiint_{-\infty}^{+\infty} d\mathbf{k} f_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (7)$$

into which the intricacy of the original integral equation is transferred, does not really require to do any triple integration manually. Instead, just look at the table of the Fourier transforms or use Mathematica or Maple. Example of usage of the inverse Fourier transform in Maple is

```
>with(inttrans);
>assume(xi>0);
>assume(k>0);
>invfourier(1/(1+xi^2*k^2),k,r);
```

To understand parameters in these commands just type `help(invfourier)` from the command line of Maple.