Mathematics 19: Screening

Charged particles interact with each-other via the Coulomb interaction. One might therefore think, that any extraneous impurity charge in a metal could be felt outside the metal, via this long-range Coulomb interaction. In fact, it is not as simple as this. When such a charge is placed in the metal, the electrons in the metal are either attracted to it or repelled from it. Such a build-up of charge around the impurity is known as a *screening charge* and to some extent compensates for the effect of the impurity with respect to more distant charges. In this project the screening of an impurity charge will be investigated as a function of the dimension of the system. The potential between the impurity charge and the other charges wants to build up the screening charge, but there are several competing effects trying to reduce it: Firstly, there is the kinetic energy of the other particles, localising a particle pushes up its kinetic energy through quantum mechanics. Secondly, there is thermodynamics, localising a particle decreases its entropy, and so at high temperature we might expect the screening charge to be 'shaken off'. In this project we will *only* deal with temperature and the competition between screening and entropy.

The problem that we tackle is that of particles interacting with each-other via a *Coulomb Potential.* Unfortunately, if we are dealing in one- or two-dimensions it is not a simple thing to generalise a Coulomb interaction. We will use solutions to Laplace's equation:

$$-\nabla^2 v(\mathbf{r}) = \delta(\mathbf{r})$$

in the presence of a source, in analogy with Electromagnetism. In one-dimension we obtain a linear potential:

$$v(\mathbf{r}) = v_0 - \frac{|\,\mathbf{r}\,|}{2}$$

in two-dimensions we obtain a logarithm:

$$v(\mathbf{r}) = v_0 - \frac{\log(|\,\mathbf{r}\,|)}{2\pi}$$

and in three-dimensions we obtain the standard Coulomb interaction:

$$v(\mathbf{r}) = v_0 + \frac{1}{4\pi\,|\,\mathbf{r}\,|}$$

The energy of our distribution of charges is described by a charge density, $\rho(\mathbf{r})$ say, in terms of which:

$$E(\rho) = \frac{1}{2}\int_V d^d\mathbf{r}\rho(\mathbf{r})\int_V d^d\mathbf{r}'\rho(\mathbf{r}')v(\mathbf{r}-\mathbf{r}') - \int_V d^d\mathbf{r}\rho(\mathbf{r})\int_V d^d\mathbf{r}'\rho_\infty v(\mathbf{r}-\mathbf{r}') - \int_V d^d\mathbf{r}\rho(\mathbf{r})v(\mathbf{r})$$

where the first term is the particles interacting with each-other, the second term is an interaction with a uniform background (to preserve neutrality), ρ_∞, and the last term is the impurity potential, attractive and placed at the origin. The Free-energy also includes the entropy:

$$F = E - TS = E + k_B T\int_V d^d\mathbf{r}\rho(\mathbf{r})\left[\log\rho(\mathbf{r}) - 1\right]$$

and is minimised to provide thermodynamic equilibrium. Note that there has been some 'scaling' of variables. The minimisation yields:

$$\int_V d^d\mathbf{r}'\rho(\mathbf{r}')v(\mathbf{r}-\mathbf{r}') - \rho_\infty \int_V d^d\mathbf{r}'v(\mathbf{r}-\mathbf{r}') - v(\mathbf{r}) + k_B T \log \rho(\mathbf{r}) = 0 \qquad (*)$$

which needs to be self-consistently solved for $\rho(\mathbf{r})$. This is best done by setting:

$$\rho(\mathbf{r}) = \exp\left(-\frac{\epsilon(\mathbf{r})}{k_B T}\right)$$

in terms of the screened potential $\epsilon(\mathbf{r})$, and then by applying $-\nabla^2$ to the above equation (*), we obtain:

$$\nabla^2\epsilon(\mathbf{r}) + \exp\left(-\frac{\epsilon(\mathbf{r})}{k_B T}\right) - 1 = \delta(\mathbf{r})$$

where we have used the fact that $\rho_\infty = 1$. It is this equation that we desire to solve in one- two- and three-dimensions.