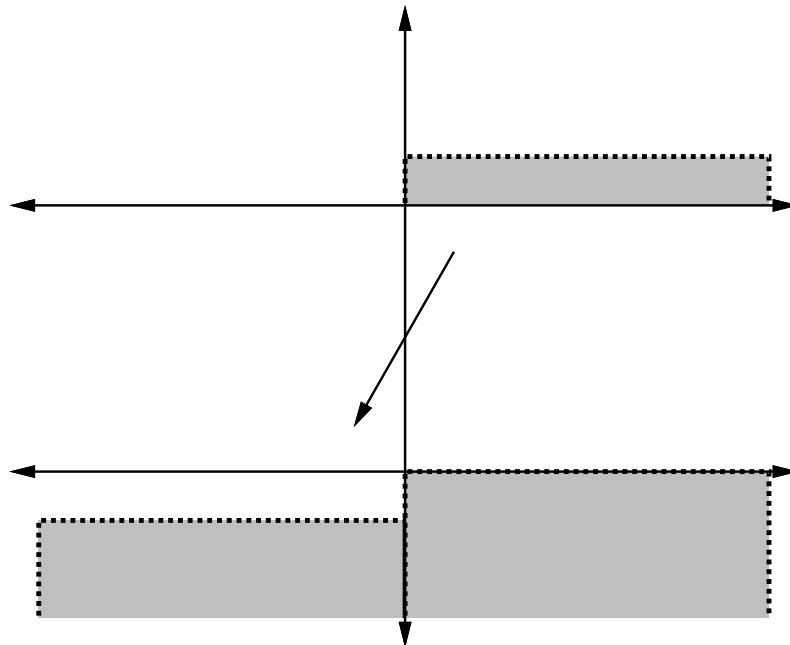


Physics 6: Doped Semi-Conductor Interfaces

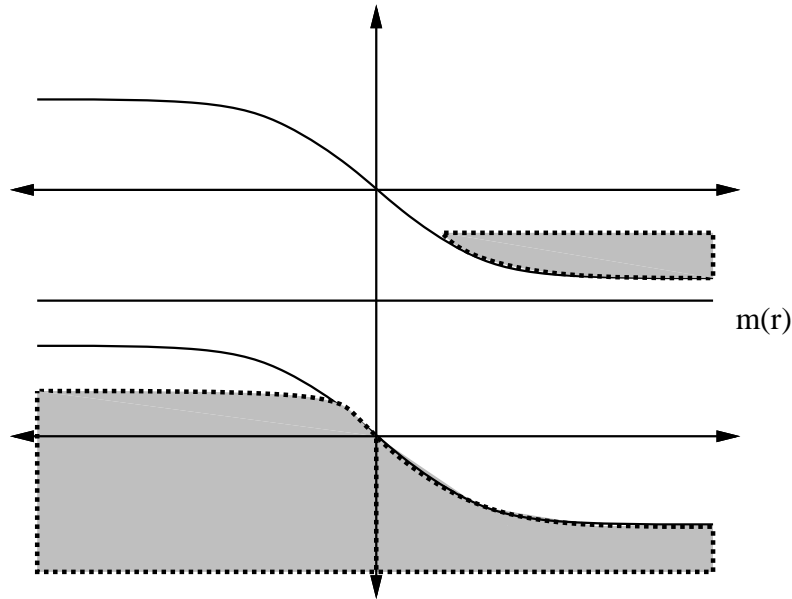
Semi-conductors are insulators at low temperature which can be made to conduct with a combination of doping and temperature. The underlying material is usually Group IV of the periodic table; Si or Ge. Doping is then achieved with holes by a neighbouring Group III element; Al or Ga, and with electrons by a neighbouring Group V element; P or As. A Group III element will look electronically similar to its replacement, achieving four bonds, but only contributing three of the four necessary electrons and hence releasing a hole. Electron doping is analogous. Although the nuclei are *static* charged defects, the released electrons and holes are mobile and can react to electrostatic forces.

A *p-n* junction is formed when two regions of opposite doping are brought together. The mobile electrons in the *n*-type region naturally annihilate partners in the *p*-type region, yielding a small layer between the two blocks which is devoid of either type of carrier: The *depletion layer*. As this region grows, the underlying static background charge is revealed and builds up an electrostatic potential repelling continued flow, until an equilibrium is reached. It is this effect and the conflicting disorder induced by temperature which is the current problem under investigation.

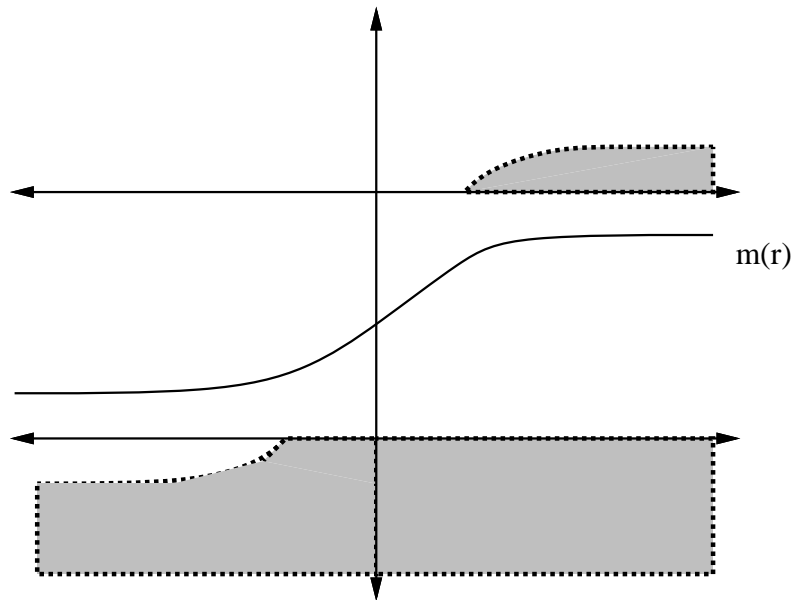
We recognise two types of charges in the system: *Static* charge associated with the nuclei, $\Sigma_s(\mathbf{r})$, and the dynamic charge of the electrons, $\Sigma(\mathbf{r})$. The undoped system has a *gap*, with all the filled levels separated from the unfilled levels. *p*-type doping pushes holes into the lower band and *n*-type doping pushes electrons into the upper band. When a *p-n* junction is made, electrons can drop down locally gaining the gap energy. The electrostatic energy resulting from the build up of charge eventually counteracts the gain, leading to a *depletion layer*.



electrons move from the n -type region into the p -type region:



or equivalently, allowing the chemical potential to mirror the change:



and we use the second representation.

We place the boundary between the n -doped and p -doped material at the origin. In the p -doped region, $x < 0$, we have a *static* negative excess background charge from the dopant nuclei, and in the n -doped region, $x > 0$, we have a static positive excess background charge. We will *not* use this electric charge density, but will use the electron density as our variable at all times, the opposite *sign* for *both* electronic and nuclear charges will therefore be employed, as if electrons were positive. The total background nuclear charge is $\Sigma_s(\mathbf{r})$, and once the reference charge associated with the undoped semi-conductor is subtracted, we are left with the excess nuclear charge, $\sigma_s(\mathbf{r})$. The physical problem involves describing the mobile electronic charge. We could consider

quantum mechanics and Schrodinger's equation, but we will analyse only a *classical* problem under the assumption that the charge fluctuations are *slow* on atomic length scales.

We describe the electrons with a single-particle density of states; $\rho(\epsilon; \mathbf{r})$, which is populated according to a Fermi-occupation number, $n(\epsilon; \mathbf{r})$, with:

$$\Sigma(\mathbf{r}) = \int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) n(\epsilon; \mathbf{r})$$

and $\Sigma(\mathbf{r})$ is the charge density of the electrons. The usual way to incorporate the potential from the redistribution of charges is to introduce a position dependent chemical potential, $\mu(\mathbf{r})$, which measures the electrostatic penalty from building up charge at \mathbf{r} . Provided that this potential varies *slowly* in comparison to atomic length scales, then this assumption is good. The local occupation number is then:

$$n(\epsilon; \mathbf{r}) = \frac{1}{1 + \exp \left[\frac{\epsilon - \mu(\mathbf{r})}{k_B T} \right]}$$

where T is the temperature.

To determine the equilibrium charge configuration for this system, we need to employ statistical physics: The equilibrium charge configuration, $\Sigma(\mathbf{r})$, minimises the free-energy functional. The single-particle energy is:

$$E_1 = \int_{\mathbf{R}^3} d^3 \mathbf{r} \int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) n(\epsilon; \mathbf{r}) \epsilon$$

and the two-particle electrostatic energy from the build up of charge is:

$$E_2 = \frac{1}{2} \int_{\mathbf{R}^3} d^3 \mathbf{r} \int_{\mathbf{R}^3} d^3 \mathbf{r}' [\Sigma_s(\mathbf{r}) + \Sigma(\mathbf{r})] V(\mathbf{r} - \mathbf{r}') [\Sigma_s(\mathbf{r}') + \Sigma(\mathbf{r}')]]$$

where $V(\mathbf{r} - \mathbf{r}')$ is the Coulomb potential. The associated entropy is:

$$S = -k_B \int_{\mathbf{R}^3} d^3 \mathbf{r} \int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) (n(\epsilon; \mathbf{r}) \log n(\epsilon; \mathbf{r}) + [1 - n(\epsilon; \mathbf{r})] \log [1 - n(\epsilon; \mathbf{r})])$$

and so the free-energy is:

$$F = E_1 + E_2 - TS$$

which is minimised by solving:

$$\begin{aligned} 0 = \frac{\delta F}{\delta \mu} &= \int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) \frac{\delta n}{\delta \mu} \left[\epsilon + k_B T \log \left(\frac{n}{1 - n} \right) \right] \\ &+ \int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) \frac{\delta n}{\delta \mu} \int_{\mathbf{R}^3} d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') [\Sigma_s(\mathbf{r}') + \Sigma(\mathbf{r}')]] \end{aligned}$$

and hence:

$$\int_{\mathbf{R}} d\epsilon \rho(\epsilon; \mathbf{r}) \frac{\delta n}{\delta \mu} \left(\mu(\mathbf{r}) + \int_{\mathbf{R}^3} d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') [\Sigma_s(\mathbf{r}') + \Sigma(\mathbf{r}')] \right) = 0$$

leading to:

$$\mu(\mathbf{r}) = - \int_{\mathbf{R}^3} d^3 \mathbf{r}' V(\mathbf{r} - \mathbf{r}') [\Sigma_s(\mathbf{r}') + \Sigma(\mathbf{r}')]]$$

Now the Coulomb potential is intimately related to the Laplacian, ∇^2 , and with a carefully chosen scale we can assume that:

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

and then:

$$\nabla^2 \mu(\mathbf{r}) = \Sigma_s(\mathbf{r}) + \Sigma(\mathbf{r}) \quad (1)$$

(1) is a fairly general classical description for the build up of charge in electrostatic systems. For our semi-conductors we have a *gap* in the single-particle spectrum and we need to use this as a reference, measuring charge-densities as excess to this reference. We split up the energy integral into \mathbf{R}_+ for energies above the gap and \mathbf{R}_- for energies below the gap. We extract the reference using:

$$\Sigma_s(\mathbf{r}) = - \int_{\mathbf{R}_-} d\epsilon \rho(\epsilon; \mathbf{r}) + \sigma_s(\mathbf{r})$$

and:

$$\Sigma(\mathbf{r}) = \int_{\mathbf{R}_-} d\epsilon \rho(\epsilon; \mathbf{r}) + \sigma(\mathbf{r})$$

and so:

$$\nabla^2 \mu(\mathbf{r}) = \sigma_s(\mathbf{r}) + \sigma(\mathbf{r})$$

with:

$$\sigma(\mathbf{r}) = \int_{\mathbf{R}_+} d\epsilon \rho(\epsilon; \mathbf{r}) n(\epsilon; \mathbf{r}) - \int_{\mathbf{R}_-} d\epsilon \rho(\epsilon; \mathbf{r}) [1 - n(\epsilon; \mathbf{r})]$$

and we recognise $1 - n(\epsilon; \mathbf{r})$ as the hole occupation number.

This provides us with the eventual non-linear differential equation for $\mu(\mathbf{r})$:

$$\nabla^2 \mu(\mathbf{r}) = \sigma_s(\mathbf{r}) + \int_{\mathbf{R}_+} d\epsilon \rho(\epsilon; \mathbf{r}) \frac{1}{1 + \exp \left[\frac{\epsilon - \mu(\mathbf{r})}{T} \right]} - \int_{\mathbf{R}_-} d\epsilon \rho(\epsilon; \mathbf{r}) \frac{1}{1 + \exp \left[\frac{\mu(\mathbf{r}) - \epsilon}{T} \right]}$$

in terms of $\sigma_s(\mathbf{r})$, the excess *static* dopant charge, $\rho(\epsilon; \mathbf{r})$ the single-particle density of states and T is the temperature (in units of k_B).