I. MOTT TRANSITION IN SILICON

A sample of silicon is cooled to low temperature. At this temperature the silicon is insulating. Light falls on silicon and creates excitons.

Describe this Excitons

Excitons are a bound state of electron and hole attracted to each other by Coulomb attraction. They follow a Bose statistic. There are two limiting cases of excitons:

<table>
<thead>
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<th>Binding Energy (eV)</th>
<th>Exciton Radius</th>
</tr>
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<tbody>
<tr>
<td>Frenkel</td>
<td>0.1 . . . 1</td>
<td>≈ 10 Å</td>
</tr>
<tr>
<td>Wannier-Mott</td>
<td>≤ 0.01</td>
<td>≈ 100 Å</td>
</tr>
</tbody>
</table>

The binding energy is inversely proportional to the relative dielectric constant which is usually high (about 11.9 in the case of silicon) in semiconductors. This explains why we expect Wannier-Excitons in our case.

Insulator-Metal Transition

At a critical exciton density the silicon becomes conducting. What is this critical exciton density and why does the silicon become conducting? Such a transition is known as Mott transition. It can be understood as an overlap of the exciton wavefunctions. The bound exciton state is dissociated into unbound electrons and holes.

We know that in solids that consists of atoms with an odd number of valence electrons the upper band is half filled and forms a metallic state, apparently independent of the interatomic distance. This is counterintuitive however and in fact not true, since we neglected electron-electron interaction of the form $-e^2/\varepsilon_0 r_{12}$. If other electrons screen the coulomb potential this will result in a reduced potential $-e/(\varepsilon_0 r) \exp(-q r)$.

It is common to define a Thomas-Fermi wave vector (similar to the Fermi wave vector $k_f$):

$$k_s^2 = \frac{D(E_F) e^2}{\varepsilon_0} = \frac{3}{2} \frac{n}{\varepsilon_0} \frac{e^2}{\varepsilon_0} = \frac{\frac{3}{2} (\hbar^2/2m)(3\pi^2 n)^{2/3}}{\varepsilon_0} e^2 = 3.939 \frac{n^{1/3}}{a_B},$$

here we used the Fermi-energy of the free electron gas ($E_F = \hbar^2 (3\pi^2 n)^{2/3}/2m$) and the Bohr radius ($a_B = 4\pi\varepsilon_0\hbar^2/m e^2$). It can be shown [2] (though this is a longer calculation) that only screening lengths that satisfy $k_s \leq 1.19/a_B$ allow a bound solution.

By using above derived formula that results in:

$$3.939 \frac{n^{1/3}}{a_B} \leq \left( \frac{1.19}{a_B} \right)^2,$$

Figure 1. Screened Coulomb potential
where $n$ describes the electron concentration. This is called the **Mott criterion** and is sometimes written differently in the form:

$$n^{-1/3} \leq C a^*_0,$$

where $C$ absorbs all the numerical constants and lies between 2.0 and 4.5 (the latter one being the original estimate by N.F. Mott [1]) and $a^*_0$ describing the effective bohr radius (note that for semiconductors effective masses can deviate significantly from the free electron mass).

### Results for Silicon

In this last section we want to present results obtained for silicon [3]. The Mott density is numerically fitted ($m_{el} = 0.1905m_e$, $m_{el} = 0.916m_e$ and $\varepsilon = 11.4$) and one obtains:

$$n_{Mott} = (0.2414 + 0.1260 \exp(-0.1302T) + 0.01641T) \times 10^{17}$$

in units of cm$^{-3}$ and $T$ in Kelvin. $n_{Mott}$ is the density of electron-hole pairs (excitons) now as a function of temperature. If we evaluate this at 0 K (this is done for reasons of comparison) we obtain $n_{Mott} = 3.6 \times 10^{17}$.

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