

Coulomb interaction in thin semiconductor and semimetal films

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It is shown that the Coulomb interaction in thin films increases strongly with decreasing film thickness, if the film dielectric constant is much larger than that of the substrate. The variation of exciton binding energy and of shallow impurity levels with film thickness and the ratio of the dielectric constants is determined.

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Large values of the dielectric constant $\epsilon \sim 10\text{--}100$ are characteristic of semiconductors and semimetals. Therefore, the Coulomb interaction of free electrons and holes in these substrates is strongly attenuated, and hydrogen-like binding states such as shallow impurity levels and Wannier-Mott excitons have small binding energies E_0 and macroscopically-large effective radii a_0

$$E_0 = \frac{e^4 m}{2 \epsilon^2 \hbar^2} \lesssim 10^{-2} \text{ eV}, \quad a_0 = \frac{\epsilon \hbar^2}{m e^2} \gtrsim 10^{-6} \text{ cm}. \quad (1)$$

Here e and \hbar are the electron charge and Planck's constant, and m is the effective mass. The very fact of the existence of these levels is manifested only at sufficiently low temperatures. However, in thin films the interaction between charges increases with decreasing thickness d , since for distances between charges $\gtrsim d$ the field produced by these charges in the medium surrounding the film begins to play a perceptible role, and if the dielectric constant for this medium is much less than ϵ , the interaction turns out to be significantly larger than in a homogeneous medium with film dielectric constant ϵ .

Assume the film occupies a region of space $-d/2 \leq z \leq d/2$. The half-space $z < -d/2$ (substrate layer) is filled with a medium having a dielectric constant ϵ_1 , and the half-space $z > d/2$ with a medium having a dielectric constant ϵ_2 . The energy of the interaction between the charges e and e' located at the points (ρ, z) and $(0, z')$ ($z \geq z'$; $\rho = (x, y)$) (are the coordinates in the film plane) is equal to

$$V(\vec{\rho}, z, z') = \frac{4 \pi e e'}{\epsilon} \int \frac{d^2 k}{(2\pi)^2} e^{2k\vec{\rho}} \frac{\text{ch} \left[|k| \left(\frac{d}{2} - z \right) + \eta_2 \right] \text{ch} \left[|k| \left(\frac{d}{2} + z' \right) + \eta_1 \right]}{|k| \text{sh} [|k| d + \eta_1 + \eta_2]}$$

$$\eta_{1,2} = \frac{1}{2} \ln \frac{\epsilon + \epsilon_{1,2}}{\epsilon - \epsilon_{1,2}} .$$

We will consider only the most interesting case $\epsilon_{12} \ll \epsilon$ and $d \ll a_0$. For $\rho \gg d$ there exists in the interval \mathbf{k} such that $|\mathbf{k}|d \ll 1$. Moreover, V is independent of z and z' , and can be reduced as follows:

$$V(\vec{\rho}) = \frac{2ee'}{\epsilon d} \int_0^{\infty} \frac{J_0(t) dt}{t + \frac{\epsilon_1 + \epsilon_2}{\epsilon} \frac{\rho}{d}} \quad (2)$$

$$= \frac{\pi ee'}{\epsilon d} \left[\mathcal{H}_0\left(\frac{\epsilon_1 + \epsilon_2}{\epsilon} \frac{\rho}{d}\right) - N_0\left(\frac{\epsilon_1 + \epsilon_2}{\epsilon} \frac{\rho}{d}\right) \right],$$

where $N_0(x)$ and $\mathcal{H}_0(x)$ are the Neumann and Struve functions. In the interval $d \ll \rho \ll \epsilon d / (\epsilon_1 + \epsilon_2)$

$$V(\vec{\rho}) \approx \frac{2ee'}{\epsilon d} \left[\ln\left(\frac{2\epsilon}{\epsilon_1 + \epsilon_2} \frac{d}{\rho}\right) - C \right], \quad (3)$$

$C \approx 0.577$ is the Euler constant, and for $\rho \gg [\epsilon / (\epsilon_1 + \epsilon_2)] d$

$$V(\vec{\rho}) \approx \frac{2ee'}{(\epsilon_1 + \epsilon_2) \rho}. \quad (4)$$

When $d \ll a_0$ the distance between the dimensionally quantized energy levels \hbar^2/md^2 is much larger than the interaction energy of Eqs. (3)–(4). Therefore, the transverse motion of charges relative to the film does not change when interaction is taken into account, and the problem concerning their relative motion becomes two-dimensional

$$-\frac{\hbar^2}{2m} \Delta_{\vec{\rho}} \psi_n(\vec{\rho}) + V(\vec{\rho}) \psi_n(\vec{\rho}) = E_n \psi_n(\vec{\rho}). \quad (5)$$

For films satisfying the condition $a_0 \gg d \gg (\epsilon_1 + \epsilon_2/2\epsilon)^2 a_0$, the effective radii of the fundamental and first excited binding states fall within a range of distances where $V(\rho)$ has the form of Eq. (3), and by substituting $\rho = a\xi$ we transform Eq. (5) as follows:

$$\Delta_{\vec{\xi}} \psi_n(\vec{\xi}) - \ln|\vec{\xi}| \psi_n(\vec{\xi}) = \gamma_n \psi_n(\vec{\xi}), \quad (6)$$

where

$$a = \frac{1}{2} \sqrt{\frac{\epsilon \hbar^2}{m e^2} d} = \frac{1}{2} \sqrt{a_0 d}, \quad (7)$$

$$E_n = - \frac{e^2}{\epsilon d} \left\{ \ln \left[\left(\frac{2\epsilon}{\epsilon_1 + \epsilon_2} \right)^2 \frac{d}{a_0} \right] - 2C - 2\gamma_n \right\}. \quad (8)$$

Equations (7) and (8) determine the effective radii and binding energies of the hydrogenic states in a thin film. Since Eq. (6) contains no parameters, the terms $\gamma_n \sim 1$ are small in comparison with the logarithm which, thus, determines the binding energy of both the ground and the lowest excited states. The spacing between these levels is substantially less than their binding energy.

If the parameters of the film and substrate satisfy the condition

$$\frac{(\epsilon_1 + \epsilon_2)^2}{\epsilon} \times \frac{m_0}{m} \gg 10,$$

where $m_0 \simeq 9 \times 10^{-28}$ g, then the condition

$$d \ll \left(\frac{\epsilon_1 + \epsilon_2}{\epsilon} \right)^2$$

a_0 is consistent with the requirement that the film be macroscopic, i.e., that it contains a large number of atomic layers. For films like this the radius of the bound states lies in the region where $V(\rho)$ has the form of Eq. (4), and the binding energy ceases to increase for a further decrease in d as it acquires a form which is characteristic of the two-dimensional Coulomb problem^(1,2) with a dielectric constant $(\epsilon_1 + \epsilon_2)/2$ ⁽³⁾

$$E_n = \left(\frac{2\epsilon}{\epsilon_1 + \epsilon_2} \right)^2 \frac{4E_0}{(2n+1)^2}. \quad (9)$$

Equation (9) has, however, hardly any region of applicability for $n = 0$, since the small effective masses required for this are usually associated with the narrow forbidden bands E_g in the electron spectrum and with its strong nonparabolicity⁽⁴⁾

$$-E_p = E_{g0} \left[1 + \frac{p^2}{mE_{g0}} \right]^{1/2}.$$

Because of the effect of dimensional quantization, E_g increases in the films along with the effective mass value, so that the condition for the applicability of Eq. (3) for $V(\rho)$ is automatically satisfied. Taking nonparabolicity into account

$$a = \frac{1}{2} \sqrt{a_0 d} \left[1 + \frac{1}{mE_{g0}} \left(\frac{\pi \hbar}{d} \right)^2 \right]^{-1/4} = \frac{1}{2} \sqrt{\epsilon d} \left[\left(\frac{m e^2 d}{\hbar^2} \right)^2 + \pi^2 \frac{e^4 m}{\hbar^2 E_{g0}} \right], \quad (10)$$

$$E_0(d) = - \frac{e^2}{\epsilon d} \ln \left[\left(\frac{2\epsilon}{\epsilon_1 + \epsilon_2} \right)^2 \sqrt{\left(\frac{d}{a_0} \right)^2 + 2\pi^2 \frac{E_0}{E_{g0}}} \right]. \quad (11)$$

The ratio of m and E_{g0} is such⁽⁴⁾ that usually $e^4 m / \hbar^2 E_{g0} \sim 1$, so that Eqs. (10) and (11) are valid for all $d \ll a_0$, providing $4\epsilon / (\epsilon_1 + \epsilon_2)^2 \gg 1$.

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