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# Influence of a bound electron on the screening of a test charge by an electron gas

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**Abstract.** – By including the contribution of a bound electron to the potential to be screened, it is shown that the screening cloud around a Coulomb charge is repelled so as to enable the formation of a persistent localized state. This result is obtained either with Thomas-Fermi or Lindhard screening, and is applied to the determination of Mott's critical density.

*Introduction.* – The bound states induced by a test charge screened by an electron gas have already been the subject of numerous papers. Their determination was primarily of interest in the study of the Metal-Insulator Transition (MIT) (see, *e.g.*, [1-4]). Screened potentials are also known for exhibiting specific features such as Friedel oscillations, either in three-dimensional [5] or two-dimensional systems [6]. More recently, some authors also investigated the possibility of occurrence of a bound state in the attractive part of such oscillating potentials, either attractive or repulsive [7]. In all the cases I am aware of, an important property of such bound systems seems to have remained unnoticed: In contrast to the stationary states induced by an unscreened potential, as, for instance, with a hydrogen atom in vacuum or an impurity in a low-doped semiconductor, the potential felt by the trapped electron is not the same as the one which exists in the absence of such an electron. In other words, the screening of the test charge is also a function of the potential induced by the wave function of the bound particle. That the localized electron tends to repel the screening cloud should indeed be a trivial remark. But I wish to show that this may have major consequences, since this implies that the binding energy is not the same, depending on whether an electron was present or not in the site before switching on electron screening. Indeed, we shall see that even when the increase in electron density is such that there is no longer an empty state, the binding energy of the occupied state never vanishes. For the sake of clarity (and brevity), in this letter, I only intend to provide the simplest comprehensive example of such a phenomenon, in a three-dimensional system. I have therefore chosen to treat the case of an occupied bound state with a positive test charge, the screening of which is accounted for by introducing either the Lindhard or the Thomas-Fermi

(TF) dielectric function. Besides, I shall only be concerned with the ground state and I shall not treat many-body effects as, *e.g.*, in refs. [7,8], where the authors have put to good use the local field correction approach. Nevertheless, I do not expect any of the qualitative conclusions exposed in this letter to be caught out once such effects are taken into account.

*Model.* – The case of the empty site has been thoroughly studied in many papers and here only the calculation details of the occupied case are given. Besides, I have already treated in detail elsewhere the case of the TF approximation, with an emphasis put on scattering phenomena [9]. I shall therefore focus on Lindhard screening, treated in reciprocal space. The bound electron wave function is assumed to be hydrogenic. One might indeed make use of improved variational forms (see, *e.g.*, [8]), but for our purpose we do not require an extreme accuracy. All formulae are in SI units and the Fourier transform $\varphi(\vec{q})$ of a function $\varphi(\vec{r})$ is defined as $\varphi(\vec{q}) = \int \varphi(\vec{r}) \exp[-2i\pi\vec{q}\vec{r}]\mathrm{d}^3\vec{r}$. In $q$-space the total electrostatic potential to be screened (fixed impurity $V_{\mathrm{bare}}^{\mathrm{imp}}(\vec{q})+$ bound electron $V_{\mathrm{bare}}^{\mathrm{e}}(\vec{q})$) has the same form as that of a hydrogen atom in the ground $1s$ state [10]:

$$V_{\mathrm{bare}}(\vec{q}) = \frac{-e}{4\kappa} \left( \frac{1}{a^2 + \pi^2 q^2} + \frac{a^2}{(a^2 + \pi^2 q^2)^2} \right), \tag{1}$$

where $\kappa$ is the static dielectric constant of the medium and $e$ is the electron charge. $a$ is the reciprocal Bohr radius of the bound electron. Screening is taken into account by dividing this potential by the Lindhard dielectric function [11]:

$$\varepsilon(\vec{q}) = 1 + \frac{k_{\mathrm{F}}}{\pi^3 a_0 q^2} \left( \frac{1}{2} + \frac{k_{\mathrm{F}}^2 - \pi^2 q^2}{4\pi k_{\mathrm{F}} q} \ln \left| \frac{\pi q + k_{\mathrm{F}}}{\pi q - k_{\mathrm{F}}} \right| \right), \tag{2}$$

where $k_{\mathrm{F}}$ is the Fermi momentum and $a_0$ is the unscreened Bohr radius. In real space, the total potential $V(\vec{r})$ (*i.e.* the inverse Fourier transform of $V_{\mathrm{bare}}(\vec{q})/\varepsilon(\vec{q})$) exhibits Friedel oscillations, as for a simple test charge, and using a theorem due to Lighthill [12], it can be shown that the singularity in the derivative at $k_{\mathrm{F}}/\pi$ gives rise to oscillations the asymptotic form of which is

$$V(\vec{r}) \cong \frac{2a^2 + k_{\mathrm{F}}^2}{(a^2 + k_{\mathrm{F}}^2)^2} \frac{ea_0 k_{\mathrm{F}}}{4\kappa(1 + 2\pi a_0 k_{\mathrm{F}})^2} \frac{\cos(2k_{\mathrm{F}} r)}{r^3}. \tag{3}$$

In $q$-space, the potential felt by the bound electron is

$$V_{\mathrm{e}}(\vec{q}) = \frac{V_{\mathrm{bare}}(\vec{q})}{\varepsilon(\vec{q})} - V_{\mathrm{bare}}^{\mathrm{e}}(\vec{q}) = V_{\mathrm{bare}}^{\mathrm{imp}}(\vec{q}) + \left( \frac{1}{\varepsilon(\vec{q})} - 1 \right) V_{\mathrm{bare}}(\vec{q}). \tag{4}$$

With TF screening this potential can be expressed analytically in real space [9], but with Lindhard screening it is much easier to solve the Schrödinger equation in $q$-space. The kinetic energy part is $\langle T \rangle = \hbar^2 a^2/2m$, $m$ being an effective mass, and the potential energy is [3]

$$\langle W_{\mathrm{e}} \rangle = \int eV_{\mathrm{e}}(\vec{q})G(\vec{q})\mathrm{d}^3\vec{q}, \tag{5}$$

where $G(\vec{q})$, the Fourier transform of the electron wave function product $\varphi(\vec{r})\varphi^*(\vec{r})$, is given by

$$G(\vec{q}) = \frac{a^4}{(a^2 + \pi^2 q^2)^2}. \tag{6}$$

Minimizing $\langle T + W_{\mathrm{e}} \rangle$ can be easily achieved numerically, and one then obtains the dependence of the binding energy $E_{\mathrm{bound}}$ and reciprocal Bohr radius on $k_{\mathrm{F}}$. This dependence has been
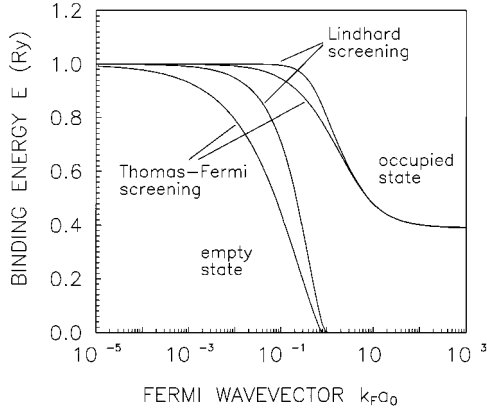
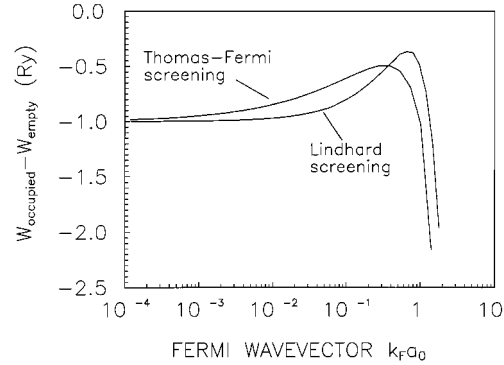Fig. 1                                                    Fig. 2

Fig. 1. – Graph of the binding energy *vs.* the Fermi wave vector, both for Thomas-Fermi and Lindhard screening. The two upper curves are for an occupied site, and the two lower ones are for an empty site.

Fig. 2. – Graph of the difference in electron energy separating a screened occupied impurity from a screened empty site.

plotted in fig. 1, both for Lindhard and TF screening. As is well known, the binding energy of the empty state vanishes above a critical value of $k_F$ [2-4]. But fig. 1 also demonstrates that there is always an occupied bound state, whatever is the free-electron concentration. Besides, the binding energy in the occupied case tends to a limit which is about the same for both kinds of screening, around 0.39 Ry. Obviously, the correct way of treating a number of problems related to screened potentials, either theoretical or experimental, should be affected by such a result. I shall end this letter by addressing one of them, which is the determination of Mott's critical density.

Going from the high-concentration range, Mott's critical density $n_c$ is attained when an electron gas cannot sustain itself because electron screening is lowered so as to enable the formation of bound states. It is a widespread practice to consider only the empty case, and $n_c$ is assumed to be the concentration at which the binding energy vanishes. However, it is clear from fig. 1 that this is *a priori* not the correct way to assess $n_c$. One should indeed determine it as the value for which the total gain in electron energy brought by the impurity is the same, both in the empty and occupied cases. We shall note these two energies as $W_{empty}$ and $W_{occupied}$. Firstly, I would like to point out that in both cases, exactly one negative elementary charge is induced in the electron assembly by the positive point charge. In the occupied case, there is indeed a deficit of free electrons close to the impurity, and a local positive charge is formed from the fixed positive jellium; it is not difficult to show that the net screening charge is equal to zero. One can calculate the total energy in each case by using the linear response approach. In the empty case, the total energy is calculated pertrubatively from the energy $E(N + 1)$ of a system of $(N + 1)$ electrons in which one withdraws an amount equal to one elementary charge from the uniform positive background, and introduces the positive point charge. In the occupied case, one calculates the perturbation induced by the system composed of the point charge and the bound electron on an assembly of $N$ free electrons with initial energy $E(N)$. In this last case, one must also add the quantized energy $E_{bound}$ of the bound electron to the energy perturbation brought to the electron gas. It is worth noting that the

initial number of free electrons is $N$ rather than $N+1$ in the occupied case, since in this scheme the bound electron is considered as an entity distinct from the electron assembly. The energy of the bound electron omitted, in both cases, the change in energy is the sum of the Coulomb interaction between the screening cloud and the localized charge, and the electrostatic and kinetic energies of the screening cloud. By virtue of the Hellman-Feynman theorem, it can be demonstrated that the addition of all these three terms is indeed equal to half the interaction energy of the screening cloud with the localized charge (point charge or point charge + bound electron) [13,14]. Noting as $\rho_s^{\text{empty}}(\vec{q})$ and $\rho_s^{\text{occupied}}(\vec{q})$ the screening charge distributions in the empty and occupied cases, respectively, the difference $\Delta W = W_{\text{occupied}} - W_{\text{empty}}$ is therefore given by

$$\Delta W = \frac{1}{2} \int_V \rho_s^{\text{occupied}}(\vec{q})(V_{\text{bare}}^{\text{imp}}(\vec{q}) + V_{\text{bare}}^{\text{e}}(\vec{q}))\mathrm{d}^3\vec{q} - E(N+1) + E(N) -$$
$$-\frac{1}{2}\int_V \rho_s^{\text{empty}}(\vec{q})V_{\text{bare}}^{\text{imp}}(\vec{q})\mathrm{d}^3\vec{q} + E_{\text{bound}}\,, \tag{7}$$

which can be put in the form

$$\Delta W = 16\pi^3 e\kappa \int_0^\infty q^4 \left(1 - \frac{1}{\varepsilon(\vec{q})}\right) V_{\text{bare}}^{\text{e}}(\vec{q})(V_{\text{bare}}^{\text{e}}(\vec{q}) - 2V_{\text{bare}}^{\text{imp}}(\vec{q}))\mathrm{d}q -$$
$$-E_0\left((k_{\text{F}}a_0)^2 - \frac{2}{\pi}k_{\text{F}}a_0\right) + E_{\text{bound}}\,, \tag{8}$$

by noting that the screening charge distributions can be replaced by the corresponding potentials through the Poisson equation written in reciprocal space. The difference $E(N+1)-E(N)$ has been approximated by summing the kinetic and exchange terms [15]. $E_0$ is equal to one Rydberg.

In the Thomas-Fermi case, we directly calculate and sum all electrostatic and kinetic energy terms, considering the screening cloud as a smooth and continuous distribution of charges (mean-field approximation). The electrostatic terms have already been explicited in ref. [9,16]. The kinetic energy terms of the screening cloud which must be subtracted from one another are of the form [14]

$$\langle T \rangle = \frac{3\hbar^2}{40\pi^2 m}\left(\frac{3}{8\pi}\right)^{\frac{2}{3}} \int \left(\left(\frac{\rho_s(\vec{r})}{e}\right)^{\frac{5}{3}} - n_{\text{F}}^{\frac{5}{3}}\right)\mathrm{d}^3\vec{r}, \tag{9}$$

where $n_{\text{F}}$ is the free-carrier density. $\Delta W$ has been numerically integrated and plotted in fig. 2. A rather alarming feature arises both in the TF and Lindhard cases: from fig. 2 it is clear that the configuration with the bound state is always energetically more favorable. In this scheme, it therefore seems that stable screening cannot be ensured by a Fermi gas without electron bonding to the positive test charge. I note that such a conclusion is in qualitative agreement with much earlier and somewhat different considerations by Friedel [17]. When the empty case is considered alone, it is well known that Mott's transition occurs for $n_c^{1/3}a_0 = \gamma$ with $\gamma \cong 0.36$ or $0.4$ for Thomas-Fermi or Lindhard screening, respectively [3] (experimentally, the practical value is close to $\gamma = 0.26$ for many different materials [18]). It is now well established that a correct modelling of the Metal-Insulator transition must involve the local correlations between the electrons occupying the various impurity sites, using tight-binding models of the Hubbard form [19]. The fact that the screening approach derived in this letter does not predict a conducting phase clearly indicates that such a scheme can only be used for giving an introductory and qualitative account of the transition. Coming back to more recent work [7], it would certainly be interesting to see whether the conclusions developed by

the authors still apply if they include the contribution of the bound electron to the potential to be screened. It is also worth noticing that introducing the calculated dependence of $a$ on electron concentration in eq. (3) shows that the amplitude of the Friedel oscillations goes through a maximum which precisely lies in the range of metallic densities. It would therefore be interesting to check whether such a prediction might have some impact in real experimental systems.

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