Comment on "Electrostatic screening near semiconductor surfaces"

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(Received 29 January 2001; published 26 December 2001)

A recent paper [Phys. Rev. B **61**, 13 821 (2000)] addressed the problem of surface screening in a doped semiconductor at finite temperature and proposed a model solution. We discuss the bulk limit of this solution, where well established models are available.

DOI: 10.1103/PhysRevB.65.047301 PACS number(s): 73.20.−r, 41.20.Cv, 71.10.Ca

The problem of electrostatic screening near the surface of a doped semiconductor at finite temperature has been studied in a recent paper by Krčmar *et al.*[1] The purpose of this Comment is to clarify some issues that remain somewhat obscure in the paper. The model solution proposed by the authors has a well defined bulk limit, where their theory can be discussed in comparison to previous work and to well-established models,[2–6] ignored in Ref. 1. This comparison is briefly provided here: Although we limit ourselves to pure bulk screening, the same concepts apply to surface screening as well, although the resulting mathematics may of course be more involved.

Quite generally, screening can be defined as the effect of the competition between electrical forces and some kind of hindering mechanism. In the abovementioned screening problem, the relevant hindering mechanisms are actually two, resulting from Pauli principle and thermal agitation. To these two qualitatively different mechanisms correspond two very different screening lengths. In order to see how the two different mechanisms arise, it is sufficient to consider first the ideal undoped semiconductor at zero temperature. In this case, electric perturbations are screened, albeit incompletely, by the electrons of the completely filled valence bands. Quantum mechanics provides a microscopic description of the phenomenon, and satisfactory models are well established.[2–4] In all these models, the role of the Pauli principle is essential: The corresponding screening length a, schematically shown in Fig. 1 of Ref. 1, is of the order of one bond length in the simplest semiconductors. Imagine now that we "switch on" doping and temperature in this medium: We then additionally have a plasma of free carriers, whose screening features are dominated by thermal agitation. A Boltzmann distribution is appropriate to deal with the equilibrium situation. Screening by free carriers is *complete*, that is, metallic; the pertinent screening length is the Debye–Hückel screening length, called R_b in Ref. 1. Typically one has $R_b \gg a$, and the model of Krčmar *et al.* is appropriate to describe the $a \to 0$ limit.

The authors use (both in the abstract and in the main text) Debye–Hückel essentially as a synonym of Thomas–Fermi. In fact, the physical basis of Debye–Hückel screening is qualitatively different from the main concepts of the Thomas–Fermi model, and the former may be viewed as the classical limit of the latter only in the particular situation of complete screening, which may be appropriate to the standard metallic electron gas of free carriers, in our case. However, a model homogenous and isotropic semiconductor can be viewed as a "semiconducting electron gas" where screening of a perturbing point charge is *incomplete*.[2] Application of Thomas–Fermi concepts to the problem of (zero temperature) linear screening in this semiconducting electron gas is well known,[3,4] and leads to a mathematics which is quite different from the case of complete screening.

As far as bulk screening is concerned, the problem of incorporating both mechanisms in a single screening model has already been solved in Refs. 5–7. Therein, a simple model dielectric function accounts for both the incomplete screening due to the "semiconducting electron gas" of the valence electrons and for the Debye–Hückel complete screening due to the plasma of free carriers. The two different screening lengths a and R_b emerge naturally within that theory. Adopting units where $4\pi\varepsilon_0 = 1$, and calling for the sake of clarity ε_∞ the macroscopic dielectric constant (which is simply called ε by Krčmar *et al.*), the theory of Refs. 5,6 provides the Fourier transform of the screened potential $\phi(r)$ generated by a perturbing point charge q as

$$\tilde{\phi}(k) = \frac{4\pi q}{k^2 \varepsilon(k) + R_b^{-2} \varepsilon_\infty}, \tag{1}$$

where $\varepsilon(k)$ is any zero-temperature model dielectric function,[2] such as the Thomas–Fermi result of Ref. 3. The potential $\phi(r)$ for $r \gg a$ is then determined by its Fourier transform at $k \ll 1/a$. Since, at small k, one has $\varepsilon(k) \to \varepsilon_\infty$, replacement of this limit into Eq. (1) yields

$$\tilde{\phi}(k) = \frac{4\pi q}{\varepsilon_\infty (k^2 + R_b^{-2})}. \tag{2}$$

This coincides with the Fourier transform of Eq. (2) in Krčmar *et al.*, which is indeed appropriate in the given limit. We believe that these results generalize to the problem of surface screening as well.

This work has been supported by the Office of Naval Research, through Grant No. N00014-96-1-0689.

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