Response to "Screening of a point charge in semiconductors and insulators"

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A new Thomas-Fermi treatment of electronic screening in an insulator, applied to screening of a positive point charge in an insulator, was recently developed by the present author [Phys. Rev. B **35**, 3431 (1987)]. The general form and near impurity behavior of the potential for this case are discussed in response to the preceding Comment [Resta, Phys. Rev. B **38**, 818 (1988)].

A new Thomas-Fermi (TF) theoretic treatment of electronic screening response in semiconductors and insulators was recently put forward by the present author.[1] This approach differs from earlier TF studies in that the noninteracting internal chemical potential functional of the electron density,[2] a main input in TF approaches, directly builds in the insulator band structure, i.e., with gap. In earlier TF approaches the internal chemical potential is that of free electrons, i.e., with a single parabolic band. This new version of TF was applied in Ref. 1 to the case of screening of a point-positive charge in an insulator or semiconductor.

The preceding Comment[3] makes a number of criticisms of the work of Ref. 1. A response is now given:

First, Ref. 3 claims that the TF approach of Ref. 1 yields for the potential ϕ for a positive point charge Q in an insulator the form, $\phi(r) \approx Q/\epsilon r$ for *any* distance r from the point charge. It is moreover implied in Ref. 3 that the constant ϵ here is the macroscopic dielectric constant.[4] Reference 3 then points out that this (claimed) behavior is incorrect. In fact, the form for $\phi(r)$ is *not* the form of $\phi(r)$ developed in Ref. 1 for this problem [see Eqs. (8a) and (8b) of Ref. 1]. Specifically, it is clearly stated in Ref. 1 that the small r and large r behaviors of the potential are $\phi(r) \approx Q/\epsilon r$ $(r \to 0)$ and $\phi(r) \approx Q/\epsilon_0 r$ $(r \to \infty)$ where ϵ_0 $(\neq \epsilon)$ is a constant. (The departure of ϵ_0 from ϵ reflects the "pile up" of electrons near the impurity into an effectively shifted local conduction band.[1]) Furthermore, for intermediate r, Ref. 1 gives a form for $\phi(r)$ which connects these two limiting forms and which is necessarily different from the form claimed in Ref. 3 (see, e.g., Fig. 7 of Ref. 1).

It is also argued in Ref. 3 that the form for $\phi(r)$ for $r \to 0$ of Ref. 1 [i.e., $\phi(r) \approx Q/\epsilon r$] should be replaced by $\phi(r) \approx Q/r$. We point out though that the form of Ref. 1 was motivated by the desire to take some account of the effect of screening by the "background,"[5] which is not explicitly taken into account in the TF framework. It is more appropriate to replace ϵ by unity in $\phi(r)$ *very* near the point charge, but allowing $\epsilon \neq 1$ here gives some idea of the otherwise neglected effect of the "background" screening for larger r. In any case a modification in the small r limit of $\phi(r)$ could be very simply incorporated within our overall approach through a change of boundary condition. It should be noted that this concern does not pertain to the overall TF idea developed in Ref. 1.

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[1] J. Oliva, Phys. Rev. B **35**, 3431 (1987).

[2] The internal chemical potential is here the difference between the chemical potential and the electrostatic potential energy of a particle at a given location.

[3] R. Resta, preceding paper, Phys. Rev. B **38**, 818 (1988).

[4] The symbol ϵ used here and in Ref. 3 corresponds to the symbol ϵ_x of Ref. 1.

[5] For a positive point charge the TF screening response involves only electrons present in the locally shifted conduction band. The valence electrons and ion cores then constitute the "background."

