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Screening of a point charge in semiconductors and insulators

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A recently proposed model [Phys. Rev. B **35**, 3431 (1987)] for screening in semiconductors and insulators gives results in disagreement with the most obvious features of microscopic electronic response in solids.

The model homogeneous and isotropic semiconductor was introduced a long time ago[1] to describe the main features of dielectric screening in real materials. I specify the subject here to be electronic microscopic screening in pure materials at $T=0$. Given that a homogeneous and isotropic many-electron system in a background is a metal,[2] some prescription to get semiconductorlike behavior has to be introduced *ad hoc*. Although almost any prescription can be mathematically justified, a physical model is acceptable only when its results agree with common sense, experiment, and first-principles theory (whichever available). In a recent paper Oliva[3] proposes a model for dielectric screening in semiconductors which does not meet such criteria, as it will be shown in the following Comment.

Several theories for screening in a model semiconductor have been proposed over the years. They all start from an electron-gas formulation, and they differ in the *ad hoc* prescription, which is adopted to simulate semiconducting behavior. The most successful results came from essentially three models: the Penn[4] model, put in workable form by Srinivasan[5] and Grimes and Cowley[6]; the Tosatti-Pastori[7] model, improved by Levine and Louie[8]; and the Resta[9] model. The prescription proposed in Ref. 3 yields results in strong qualitative disagreement with all of the above mentioned papers, which, in fact, agree in the main results.

Let us consider the screened potential $\phi(r)$ of a point charge Q in a dielectric medium. Although some of the papers do not explicitly consider this problem, all of them[4-9] imply that $\phi(r)\simeq Q/r$ at small r and $\phi(r)\simeq Q/\epsilon r$ at large r. The results of Oliva,[3] on the contrary, give in the linear regime basically $\phi(r)\simeq Q/\epsilon r$ for any r (see Fig. 8 in Ref. 3). The fact that at short distances from the impurity $\phi(r)\simeq Q/r$ does not mean, as erroneously stated by Oliva, that the electronic screening is metalliclike at short r; on the contrary, such behavior simply means that the electronic screening charge, when described at a microscopic scale, has a finite extent. Incidentally, the popular models of Refs. 4–9 basically predict (even quantitatively) the same spatial extent of the order of one bond length in covalent materials.

When comparing such models to real materials, the first obvious difference is that a solid is not homogeneous and isotropic on a microscopic scale. First-principles theory has been used in recent years to study electronic screening in the simplest semiconductors.[10,11] The validity of the simple and popular models[4-9] in describing the main physical features has been strongly confirmed by comparison of the results (see Refs. 10 and 11 for a thorough discussion).

A final comment about insulators. A semiconductor at $T=0$ is an insulator, but a special kind of one, having a high value of the electronic dielectric constant, a small energy gap, and a valence electronic distribution that is not too inhomogeneous. It is therefore, in a sense, "close" to a metal, which makes the concept of "semiconducting" electron gas that underlies the popular models, valuable.[4-9] For a strong insulator, instead, the homogeneous and isotropic model is not appropriate at all; the Clausius-Mossotti model is a microscopic model much closer to physical reality, in this case.[10,11]

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[2] Strictly speaking, the statement applies to (a) the densities of interest here, and (b) a local background potential.
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