Comment on "Shallow donor states near a semiconductor-insulator-metal interface"

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In a recent paper Hao et al. [Phys. Rev. B 80, 035329 (2009)] reported variational calculations of energy spectrum for shallow hydrogenic donor in the structure of semiconductor/insulator/metal with a new type of trial wave function. They also performed calculations for semiconductor/insulator system and found that their method gives energy values lower than those obtained by MacMillen and Landman [Phys. Rev. B 29, 4524 (1984)]. As follows from these results MacMillen and Landman have got much larger errors in energy values than they expected. However we confirm that the theoretical approach suggested by MacMillen and Landman gives rather accurate energy values for the system of hydrogenic donor near the interface between semiconductor and insulator.

In a recent paper Hao et al. (HDAP) reported variational calculations of energy spectrum for shallow hydrogenic donor in the structure of semiconductor/insulator/metal with a new type of trial wave function. To evaluate the quality of the suggested trial function HDAP compared the calculated ground state energies at different donor positions with the calculations obtained by MacMillen and Landman. The authors of Ref. [2] ensured that their calculated energy values are accurate to four significant figures. However, in Ref. [1] it was claimed that the errors in the result of Ref. [2] may be even greater than 9%. The aim of this comment is to resolve this contradiction. We argue that the comparison in Ref. [1] is not adequate.

To calculate the electronic spectrum under consideration an eigenvalue problem for the following equation (written in dimensionless form) should be solved:

$$\left(-\nabla^2 - \frac{2}{r_D} - \frac{2Q^*}{r_D^2} + \frac{Q^*}{2z}\right)F(\vec{r}) = EF(\vec{r}).$$

All distances are scaled to units of effective Bohr radius ($a_B^* \approx 8387$) and the energy $E$ is given in effective Rydbergs (Ry*). The parameter $Q^*$ is given by:

$$Q^* = \frac{\epsilon_s - \epsilon_{ins}}{\epsilon_s + \epsilon_{ins}},$$

where $\epsilon_s$ and $\epsilon_{ins}$ are the dielectric constants of the semiconductor and the insulator respectively. The distance of the donor from the interface is $R$ and $r_D$ and $r_D$ are the distances of an impurity electron from the donor ($D$) and its image ($\bar{D}$), respectively.

HDAP compared their results calculated for $Q^* = 1$ in Eq. (1) (see Table I in Ref. [1]) to the values calculated in Ref. [2] for $Q^* \approx 0.8387$ ($\epsilon_s = 11.4$, $\epsilon_{ins} = 1$). The latter one corresponds to the interface between silicon and vacuum (see Table II in Ref. [2]). It seems that this incorrectness has been arisen due to the same mistake made in Ref. [3].

In order to test this assertion we have performed calculations for $Q^* \approx 0.8387$ using variational and finite-element approaches. For variational calculations a trial wave function was chosen as a sum $\Psi_{trial} = \sum c_{ik}\phi_{ik}$ with the basis wave functions:

$$\phi_{ik} = 2\alpha^{3/2}R\pi^{-1/2}\exp\left[-\alpha R(\xi - \eta)\right]L_i(\xi)P_k(\eta),$$

where $\xi = \frac{r_D + \bar{r}}{2R}$ and $\eta = \frac{r_D - \bar{r}}{2R}$ are prolate spheroidal coordinates, $\alpha$ is a variational parameter, and $L_i(\xi)$ and $P_k(\eta)$ are polynomials of $i$-th and $k$-th degrees, respectively. As $P_k(\eta)$ we choose the Legendre polynomials of odd degree which allow to satisfy the boundary condition $F(\vec{r}) = 0$ at the interface ($z = 0$). Choosing this basis we avoid the necessity of numerical integration. Another advantage of this basis set is a lower number of basis functions which is necessary to obtain the same accuracy for the ground state energy $E_0$ as in Ref. [2].

To carry out numerical computations using finite element method (FEM), the system is assumed to be rotationally symmetric around $z$-axis and the problem is reformulated in cylindrical coordinates $(r, z)$. The equation is posed in a bounded domain $\Omega = (0, \delta) \times (-\delta - R, 0)$ with $\delta = 10$ chosen for an approximation of the semi-infinite region $(0, +\infty) \times (-\infty, 0)$ with a donor position at $(0, -R)$. Using MATLAB we discretize this problem by linear finite elements on a triangular mesh with a number of unknowns $\approx 150000$. The generalized sparse eigenvalue problem is solved by the implicitly restarted Arnoldi method in MATLAB.

The comparison of our results for $Q^* \approx 0.8387$ with the theoretical results of MacMillen and Landman is presented in Table I which has the form similar to that one in Ref. [1]. We found that our values are practically coinciding to those obtained by MacMillen and Landman at the same distances from the interface. So our calculations confirm the evaluation of the significant figures for energy values presented by MacMillen and Landman.

To evaluate the quality of the trial function with two parameters suggested by HDAP we have also performed
imperative electron near the semiconductor-insulator interface for different values of $R/a_B^*$, calculated on the basis of the variational wave functions of Eq. (2) with $Q^* = 0.8387$, and $E_0$ found in Ref. [2] for the same value of $Q^*$.

### TABLE I. The values of the ground state energy $E_0$ of the impurity electron near the semiconductor-insulator interface for different values of $R/a_B^*$ calculated on the basis of the variational wave functions of Eq. (2) with $Q^* = 0.8387$, and $E_0$ found in Ref. [2] for the same value of $Q^*$.

| $R/a_B^*$ | $\alpha$ | $E_0$/Ry$^*$ | $E_0$/Ry$^*$ | $E_0$/Ry$^*$ | $E_0$/Ry$^*$ |
|-----------|----------|--------------|--------------|--------------|--------------|
|           | variational, present | variational, present | variational, present | Ref. [2] |
| 0.2       | 0.854    | -0.6064      | -0.6062      | -0.6064      |               |
| 0.4       | 0.908    | -0.6508      | -0.6507      | -0.6507      |               |
| 0.6       | 0.961    | -0.7223      | -0.7222      | -0.7221      |               |
| 0.8       | 0.988    | -0.8099      | -0.8098      | -0.8098      |               |
| 1.0       | 0.908    | -0.8946      | -0.8946      | -0.8945      |               |
| 1.2       | 0.827    | -0.9640      | -0.9643      | -0.9640      |               |
| 1.4       | 0.773    | -1.0158      | -1.0164      | -1.0158      |               |
| 1.6       | 0.639    | -1.0522      | -1.0530      | -1.0521      |               |
| 1.8       | 0.666    | -1.0767      | -1.0771      | -1.0767      |               |
| 2.0       | 0.666    | -1.0925      | -1.0932      | -1.0925      |               |
| 3.0       | 0.666    | -1.1085      | -1.1089      | -1.1086      |               |
| 4.0       | 0.666    | -1.0943      | -1.0952      | -1.0944      |               |
| 5.0       | 0.720    | -1.0794      | -1.0804      | -1.0794      |               |
| 6.0       | 0.720    | -1.0676      | -1.0679      | -1.0676      |               |

### TABLE II. The values of the ground state energy $E_0$ of the impurity electron near the semiconductor-insulator interface for different values of $R/a_B^*$ calculated on the basis of the variational wave functions of Eq. (2) with $Q^* = 1$, and $E_0$ found in Ref. [1] for the same value of $Q^*$.

| $R/a_B^*$ | $E_0$/Ry$^*$ | $E_0$/Ry$^*$ | $E_0$/Ry$^*$ | Relative error |
|-----------|--------------|--------------|--------------|----------------|
|           | variational, present | variational, present | Ref. [1] | in % |
| 0.4       | -0.7208      | -0.7208      | -0.716       | 0.6            |
| 1.0       | -0.9491      | -0.9491      | -0.927       | 2.3            |
| 1.6       | -1.0917      | -1.0925      | -1.077       | 1.4            |
| 2.0       | -1.1256      | -1.1264      | -1.116       | 0.9            |
| 3.0       | -1.1323      | -1.1327      | -1.128       | 0.4            |
| 4.0       | -1.1131      | -1.1139      | -1.111       | 0.3            |
| 6.0       | -1.0806      | -1.0810      | -1.080       | < 0.1          |

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