True self-consistent solution of Kohn-Sham equations for infinite systems with inhomogeneous electron gas

A. Ya. Shul'man, D.V. Posvyanskii
V.A. Kotel'nikov Institute of Radio Engineering and Electronics of the RAS

The density functional approach in the Kohn-Sham approximation is widely used to study properties of many-electron systems. Due to the nonlinearity of the Kohn-Sham equations, the general self-consistence searching method involves iterations with alternate solving of the Poisson and Schrödinger equations. One of problems of such an approach is that the charge distribution renewed by means of the Schrödinger equation solution may be incompatible with boundary conditions on Poisson equation for Coulomb potential, as it has long been known since the articles of Bardeen [1] and Lang and Kohn [2]. The resulting instability or even divergence of iterations manifests itself most appreciably in the case of infinitely extended systems because the corresponding boundary-value problem becomes singular. The published attempts to deal with this problem were shown to be reduced in fact to abandoning the iterative method initially declared and replacing it with some approximate calculation scheme [3]. In general, these schemes are usually semi-empirical and do not permit to evaluate the extent of deviation from the exact solution. In [3] the iterative algorithm of solving the Kohn-Sham equations for unbounded systems with inhomogeneous electron gas has been formulated, which is based on eliminating the long-range character of Coulomb interaction as the cause of tight coupling between charge distribution and boundary conditions. This algorithm was implemented to the semi-infinite degenerate electron gas bounded by infinitely high potential wall or self-consistent potential barrier [4]. The work function and surface energy of simple metals in the jellium model have been calculated and successfully compared with the published experimental and computational results [5, 6].

Here we present the results of applying our algorithm to the calculation of the energy spectrum of quasi-two-dimensional (2D) electron gas in accumulation layer on the semiconductor surface. In such a structure, the states electrons are occupied belong both discrete and continuous parts of the energy spectrum. As a result, there are the high density of electrons bound close to the surface and the degenerate electron gas in the bulk of semiconductor. The stable convergence of iteration is obtained even in that case. To evaluate the adequacy of the method for the real structures, we calculated the energy spectrum of the quasi-2D electron gas in the case of the accumulation layer on the surface of n-InAs. This semiconductor has narrow band gap and appreciably non-parabolic conduction band that has to be taken into account. The computed energy levels correspond well to experimental data measured by the angle-resolved photoelectron spectroscopy method [7, 8]. Also, the difference between self-consistent solutions in the Hartree approximation and those with taking into account the exchange-correlation interaction is analyzed. This allows one to assess when the calculations can be restricted to the more simple case.

References

[1] J. Bardeen. Phys. Rev. **49**, 653 (1936)

[2] N.D. Lang and W. Kohn. Phys. Rev. B **1**, 4555 (1970)

[3] A.Ya. Shul'man. J. Phys.: Conf. Ser. **35**, 163 (2006)

[4] D.V. Posvyanskii and A.Ya. Shul'man. JETP **109**, 145 (2009) [Zh. Eksp. Teor. Fiz. **136**, 169 (2009)]

[5] N.D. Lang and W.Kohn. Phys. Rev. B **3**, 1251 (1971)

[6] J.P. Perdew and Y. Wang. Phys. Rev. B **38**, 12228 (1988)

[7] V.Yu. Aristov, G. Le Lay, V.M. Zhilin et al. Phys. Rev. B **60**, 7752 (1999)

[8] M.G. Betti, V. Corradini, G. Bertoni et al. Phys. Rev. B **63**, 155315 (2001)