Self-consistent solution of the Kohn-Sham equations for systems with inhomogeneous electron gas

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1 INTRODUCTION

The gas of the interacted electrons is usually described within Kohn-Sham approximation by the set of Poisson and Schrödinger equations with an effective potential for the single-particle wave functions. The solution can be obtained using many-step iteration procedure. The well known difficulty in this task is that the wave functions obtained after every iteration step give the distribution of electron density which is not correspond to the boundary conditions for the Coulomb potential. As a result, either it is impossible to obtain the solution for the next iteration step or some parameters of the system are to be changed, for example, the density of the positive charge. The proposed new iterative scheme for solving Kohn-Sham equations is freed up of necessity to modify parameters of the system while iteration process.

2 SELF-CONSISTENCY PROCEDURE

The self-consistent electron density is constructed as the solution of the Kohn-Sham equations.

\[ \frac{1}{2} \nabla^2 \psi_{E}(z) + (E - u_{\text{eff}}(z))\psi_{E}(z) = 0 \]  \hspace{1cm} (1)

\[ u_{\text{eff}} = u(z) + u_{\text{xc}}(z) \]

\[ \nabla^2 u = (N_D - n(z)) \]  \hspace{1cm} (2)

Here \( N_D \) is the density of the positive background, \( u \) is the Coulomb potential energy of electron and \( u_{\text{xc}} \) is the exchange-correlation potential energy, which we assume in the local-density approximation.

We represent the total electron density as a sum

\[ n(z) = n_{\text{ind}}(z) + n_{\text{qu}}(z), \]  \hspace{1cm} (3)

where induced electron density depends on the potential as follows

\[ n_{\text{ind}}(z) = (\mu - u(z))^{3/2} \]
This expression is the usual quasi-classical solution of Eq. (1) averaged over Fermi wavelength scale and

\[ n_{qu}(z) = 2 \sum_{E \leq E_F} |\psi_E|^2(z) - n_{ind}(z) \]

will be named as the quantum electron density.

Using Eq. (3) Poisson equation can be rewritten in a new form

\[ \nabla^2 u + n_{ind}[u] = N_D - n_{qu}(z) \] (4)

The total iteration scheme can be described as following

\begin{align*}
  i &= 0, 1, \ldots, \quad n_{qu}^0 = 0 \\
  \nabla^2 u^i + n_{ind}(u^i) &= N_D - n_{qu}^i(z) \\
  \frac{1}{2} \nabla^2 \psi_E^i(z) + (E - u_{eff}^i(z))\psi_E^i(z) &= 0 \\
  n_{qu}^{i+1} &= \sum_{E \leq E_F} |\psi_E^i(z)|^2 - n_{ind}[u_{eff}^i] 
\end{align*} (5)

This procedure was tested in solving the self-consistent set of the equations for two tasks within the jellium model:
1. Semi-infinite electron gas which is bounded by self-consistent potential
2. Semi-infinite electron gas which is bounded by infinite potential barrier.

3 SEMI-INFINITE ELECTRON GAS BOUNDED BY SELF-CONSISTENT POTENTIAL

Using the local-density approximation for exchange and correlation potentials we calculated the self-consistent distribution of the electrons and the work function in the wide range of the bulk electron densities. All computations were done in the framework of the jellium model, where the positive ions are replaced by the uniform background of positive-charge density. This background fills the half-space \( z \geq 0 \) and is neutralized by the electron density. Figure 4 shows the distributions of electron density and effective potential calculated self-consistently for \( R_s = 4 \). These curves are compared with the corresponding results from [1], where the straight iteration scheme was claimed not converging (see [1], Appendix B) and authors did have to use, in fact, variational method for solving Eqs. (1-2). Our iteration scheme (3) allows to obtain the self-consistent answer through the straight solution of Kohn-Sham equation set. According to the well-known Budd-Vannimenus theorem [2], the self-consistent potential must satisfy to the follow sum rule

\[ \Delta_B = u(0) - u(\infty) = \bar{n} \frac{d\epsilon(\bar{n})}{dn}. \] (6)

Here \( \epsilon \) is an energy per one electron for the homogeneous electron gas. Substituting the explicit expression for \( \epsilon \), it is easy to calculate \( \Delta_B \) as the function of the electron density. The same parameter obtained from our self-consistent solution we denote as \( \Delta_{SC} \). As it can be seen in Table I, parameters \( \Delta_B \) and \( \Delta_{SC} \) are in a good agreement. This fact is the independent evidence that our solution is fully self-consistent [2]. The work function is defined as

\[ W = u_{eff}(-\infty) - \mu. \]
Comparative plot of distributions of electron density and effective potential near the surface of simple metal, $r_s = 4$

Figure 1:

The dependence of the self-consistently calculated $W_{SC}$ on Wigner-Seitz parameter $R_s$ is shown in Figure 2 in companion with results of not fully self-consistent calculations in [3]-[4]. This figure provides comparative analysis of work function calculations obtained by different technique.
2.4
2.8
3.2
3.6
4.0

Comparative plot of density dependence of work function within jellium model

Figure 2:

| $R_s$ | $W_{SC}(eV)$ | $\Delta_B$ | $\Delta_{SC}$ |
|-------|---------------|-------------|----------------|
| 0.5   | 3.21          | 0.358       | 0.358          |
| 1.0   | 3.40          | 0.317       | 0.317          |
| 1.3   | 3.51          | 0.291       | 0.291          |
| 1.5   | 3.60          | 0.274       | 0.274          |
| 1.65  | 3.63          | 0.261       | 0.261          |
| 1.8   | 3.64          | 0.248       | 0.248          |
| 2.07  | 3.60          | 0.224       | 0.224          |
| 2.3   | 3.53          | 0.204       | 0.204          |
| 3.28  | 3.12          | 0.115       | 0.115          |
| 3.99  | 2.87          | 0.051       | 0.063          |
| 4.96  | 2.51          | -0.048      | -0.041         |
| 5.23  | 2.46          | -0.075      | -0.074         |

4 SEMI-INFINITE ELECTRON GAS BOUNDED BY INFINITE POTENTIAL BARRIER

In this section we apply our iteration scheme for calculating self-consistent electron density in the case of electron gas bounded by infinite potential barrier. The positive charge and the electrons fill the half-space $z \geq 0$. The task was considered with accounting for the external electric field perpendicular to the surface plane. The presence of the electric field modifies the
boundary condition for Coulomb potential at the surface. Using the results of this task, the capacitance of a tunnel structure can be estimated. Figure 3 demonstrates the distributions of electron density, effective and Coulomb potentials for $R_s = 2.07$ calculated by our technique. The solution of this task can be used for an estimation of the capacitance of a real finite-height barrier structure. The structure consists of two $n$-doped semiconductor half-spaces, separated by a potential barrier of width $d$. The total capacitance is $C = dQ/dV$, where $Q$ is a total charge in the semiconductor lead and $V = u(\infty) - u(-\infty)$ is the voltage drop over the structure. Our calculations corresponds to the non-transparent infinitely high barrier with $d = 0$ and give us the maximum achievable specific capacitance in barrier structures. In Figure 4 we plot the dependences of the capacitance on $R_s$ calculated within the different approximations. The partial support from the Russian Foundation for Basic Researches is gratefully acknowledged.
Density dependences of the capacitance calculated within different approximations

Figure 4:

References

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