Explanation of the formation dynamics of the bound state with ion implantation

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Abstract

Taking into account the structure and the size of localized electrons the density matrix of localized electrons is analytically derived. In the framework of Kohn's approximation the analytical expression is used for the density matrix, and the additional potential for the three-body Coulomb systems is determined. Our result shows that, the consideration of the structure and size of localized electrons leads to an additional potential. If the size parameter is small, then the additional potential is the oscillator one. This gives a possibility to explain experimental results.

1 Introduction

One of the main methods receiving new materials for the micro electronics is the implantation of ions on the surface of the solid state. In accordance with many forecasts the main research problem in XXI century is the creation of new materials with established behavior [1]. For realization of this idea it is first of all necessary to carry out the investigation of the formation dynamics of the bound state with an ion implantation at high energy. At the present time, the mechanism of interaction of ions on the surface of the solid states was considered in the framework of LShSh method [2]. In this method the interaction potential between ion and target-nucleus was determined in the framework of the Tomas-Fermi approximation(TFA) [3]. In [4], the modern status of TFA was discussed. In the case of high pressure is the TFA an formally exact but in the case of normal pressure the accuracy is poor [5]. On the other hand, the last experimental results [6, 7] show that the difference between theoretical results obtained in the framework of the LShSh method and experimental data increased with energy of incident ions. The Tomas-Fermi theory can be applicable for the system with weak changing of electron density; however, this is inconsistent with the real case of crystal. Most serious problems also arise in describing kinetic energy and polarization of crystals (for details see Ref. [8]). To get more clear and full details on the nature of many-body quantum systems it is necessary, to take into account the electronic structure of molecules and condensed matter. At the present time this problem is realized in the framework of the density functional theory formulated in [9, 10]. The main ideas of this method are represented in the Kohn’s lecture [11]. In this method the density distribution $n(\vec{r})$ is determined from the single-particle Kohn-Sham equations:

$$\left(-\frac{1}{2}\Delta + V_{\text{eff}}(\vec{r}) - \epsilon_j\right) \phi_j(\vec{r}) = 0,$$  

where $V_{\text{eff}}(\vec{r})$ is the effective potential, and $n(\vec{r})$ is the density distribution represented as

$$V_{\text{eff}}(\vec{r}) = V_{\text{ex}}(\vec{r}) + \int \frac{d\vec{r}' n(\vec{r}')}{|\vec{r} - \vec{r}'|} + V_{\text{xc}}(\vec{r}); \quad n(\vec{r}) = \sum_{j=0}^{N} |\phi_j(\vec{r})|^2.$$  

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Here $V_{xe}(\vec{r})$ is the local exchange-correlation potential. However, this approach has some drawbacks. First, it is necessary to carry out bulky calculations requiring powerful supercomputers; second, universality of this approach, that is the use of the block representation for wave functions of electrons in crystals of any type, in leads to some cases non physical results (for details see [5]). Thus, to get a more clear and full representation of the dynamics of multi-particle quantum systems, with the one needs to take account of the electronic structure of molecules and condensed matter.

2 The localization of electrons and density matrix

Let us consider the three-body Coulomb systems consisting of the ion, target-nucleus, and localized electrons. First of all, the localized electrons are identified with fictitious particles with mass $m_3$ and charge $-Z_3e$. Then the interaction hamiltonian for the three-body Coulomb systems with masses $m_1$, $m_2$, $m_3$ and charges $Z_1e$, $Z_2e$, $-Z_3e$ can be written as

$$H = \frac{1}{2} \sum_{j=1}^{3} \frac{1}{m_j} \vec{p}_j^2 + \frac{Z_1Z_2e^2}{|\vec{r}_1 - \vec{r}_2|} - \frac{Z_1Z_3e^2}{|\vec{r}_1 - \vec{r}_3|} - \frac{Z_3Z_2e^2}{|\vec{r}_2 - \vec{r}_3|}. \quad (2.1)$$

This Hamiltonian is considered as a boundary condition. Let us take into account the structure of localized electrons. We suppose that the electrons are in a bound state. First of all, a kind of the confinement potential chosen as a parabolic one. In this case, the Hamiltonian is represented as

$$H_g = \frac{1}{2m} \vec{P}_x^2 + \frac{1}{2}m\omega^2 x^2. \quad (2.2)$$

Then the density matrix of electrons is determined by the following equation:

$$i\hbar \frac{\partial \rho(x, x'; f)}{\partial f} = H_g \rho(x, x'; f), \quad (2.3)$$

where $f$ is the size parameter connected with the localized electrons. The solution of this equation (2.3) can be represented as

$$\rho(x, x'; f) = \sqrt{\frac{m\omega}{2\pi\sinh(2f)}} \exp\left(-\frac{m\omega}{2\sinh(2f)}[(x^2 + x'^2)\cosh(2f) - 2xx']\right). \quad (2.4)$$

The density matrix satisfies the requirements

$$\lim_{f \to 0} \rho(x, x'; f) = \delta(x - x'). \quad (2.5)$$

We analytically define the matrix density for the parabolic confinement potential. Now we give the details of determination the matrix density for any kind of potentials. Let the localized electrons be in the bound state and the interaction Hamiltonian be written as

$$H_{cg} = \frac{1}{2m} \vec{p}_x^2 + \frac{1}{2}m\omega^2 x^2 + \frac{Ze^2}{r}. \quad (2.6)$$

Then in the framework the oscillator representation method [12] the interaction Hamiltonian represented in (2.6) should be modified as a Hamiltonian of oscillator in the $d$-dimensional auxiliary space

$$\tilde{H}_{cg} = \frac{1}{2} \tilde{P}_q^2 + \frac{1}{2}\Omega^2 q^2, \quad (2.7)$$
where \( \Omega \) is the oscillator frequency determined by the following equation:

\[
\Omega^2 + \Omega^{3/2} \frac{Zm \alpha \Gamma(1 + \ell)}{\Gamma(5/2 + \ell)} - m^2 \omega^2 = 0 ,
\]

(2.8)

the variables \( P_j \) and \( q_j \) are the vectors in d-dimensional auxiliary space and the dimensions of auxiliary space equals \( d = 3 + 2\ell \) (for details see [12]). After some simplifications we obtain from (2.7) the following result for the modified Hamiltonian:

\[
\tilde{H}_{cg} = \sum_{j=1}^{d} \tilde{H}_{cg}^j , \quad \tilde{H}_{cg}^j = \frac{1}{2} P_{q_j}^2 + \frac{1}{2} \Omega^2 q_{j}^2 ,
\]

(2.9)

where \( \tilde{H}_{cg}^j \) is the Hamiltonian for the one-dimensional oscillator and the corresponding density matrix is represented in (2.4). According to (2.9), the density matrix of the total Hamiltonian looks like

\[
\rho(q, q'; f) = \sum_{j=1}^{d} \rho_j(q_j, q'_j; f) .
\]

(2.10)

Taking into account the structure and size of localized electrons we can rewrite the interaction Hamiltonian for the three-body bound state system in the following way:

\[
H_f = \frac{1}{2} \sum_{j=1}^{3} \frac{1}{m_j} \tilde{P}_j^2 + \frac{Z_1 Z_2 e^2}{|\tilde{r}_1 - \tilde{r}_2|} - Z_1 Z_3 e^2 \int dq \frac{\rho(q, |\tilde{r}_1 - \tilde{r}_3|; f)}{q} - \quad \nonumber
\]

\[
- Z_3 Z_2 e^2 \int dq \frac{\rho(q, |\tilde{r}_2 - \tilde{r}_3|; f)}{q} .
\]

(2.11)

Here we do not include the so-called exchange-correlation term. If the \( f \) size parameter is very small, then we can carry out expansion in the order of the small parameter. After some simplification from (2.11) we have

\[
H_f = H + (Z_1 + Z_2) Z_3 e^2 A \sqrt{f} + Z_3 e^2 f^{3/2} B (Z_1 |\tilde{r}_1 - \tilde{r}_3|^2 + Z_2 |\tilde{r}_2 - \tilde{r}_3|^2) , \quad (2.12)
\]

where \( H \) is shown in (2.1); \( A \) and \( B \) are the same constants. Our result shows that taking into account the structure and size of localized electrons leads to an additional potential. Also, when the size parameter is small, then the additional potential is the oscillator one.

3 Conclusions

- The main parameter of Kohn’s theory, i.e., the density matrix of localized electrons is analytically derived taking into account the structure and size of localized electrons and orbital excitation. Our result shows that taking into account the structure and size of localized electrons leads to an additional potential. The dynamics and properties of quantum-mechanical system are defined by the kind of interaction potentials, therefore, the analytically determined interaction potentials give a possibility to describe the formation dynamics bound state systems.
The results of experimental investigation [6] show that the spectrum of the bound state of systems produced due to proton implantation on the surface of silicon is the spectrum of the oscillator. The recent results of these author [7] prove that the spectrum in the case of implantation by the hydrogen isotopes on the other surface is also the spectrum of oscillator. Our result shows that taking into account the structure and size of localized electrons leads to an additional potential and that when the size parameter is small, the additional potential is the oscillator one.

Thus, with increasing energy of incident ion the interaction potential of Coulomb type becomes parabolic. The spectrum of the bound state of systems produced due to proton implantation on the surface of silicon can correspond to the spectrum of the oscillator potential. This gives a possibility to explain the experimental results.

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