Effects of many-electron atom polarization in
electron-hole formalism

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Abstract
The method has been developed to calculate effects of polarization not only
for a atomic core in a field of valent electron, but also polarization of atom as a
whole in the electron-hole formalism. A secondary quantized density matrix for
many-electron system was used to find the Green function of a quasiparticle and
its effective mass due to many-particle effects.

1 Introduction
As is known \cite{1}, for odd number of electrons the Hartree - Fock method of self-consistent
field gives the equation, calculation with which help is connected to a problem of diagonalizing
a matrix Lagrange multiplier. It results to possible noncommutativity of a Fock
operator with the operator density matrix (a projector on subspace of orbitals for electron
in a atomic core) and, hence, to absence of an interpretation of the Fock operator as a
Hamiltonian for single-particle state \cite{2}, \cite{3}, \cite{4}. The method of pseudo-potential allows to interpret diagonal elements of the Lagrange multiplier in a Hartree - Fock equation as the
energy of single-particle state. However, a pseudo-valent orbital constructed by the method
appears so compressed one, that results to very underestimated lengths of chemical bonds in
comparison with experiments \cite{5}, \cite{6}. It, seemingly, is stipulated by the incorrect description
of polarization effects in an atom as in the method of pseudo-potential one uses approximation
of spherically symmetric unexcited atomic core ("frozen" core). Therefore, at the last
time in the "ab initio" calculations fulfilled the pseudo-potential is utilized only within the
limits of core, supplementing with the phenomenological potential describing polarization of
the core in the classical way \cite{7}, \cite{8}. Although, for example, for halogen dimers a relativistic
calculation taking into account the dipole polarizability of atomic cores gives lengths of
chemical bounds matching satisfactorily with experiment data, the found binding energy is
underestimated with respect to its real value \cite{9}, \cite{10}, \cite{11}. Obviously, it is due to the fact
that the correct quantum description of polarization of an atom is possible, if one assumes
the existence of quasiparticle exitations for the spherically symmetric core.

The goal of this paper is to develop a self-consistent method allowing to calculate effects
of core polarization in a field of valent electron within the framework of secondary quantized
electron-"hole" formalizm.

2 Wave function of many-electron system
Let an arbitrary function $\psi$ to depend on coordinates $\vec{r}_i$, $i, \ldots, n$ of $n$ electrons: $\psi =
\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n)$. To be of a wave function for a system from $n$ electrons the function
\[ \psi(\vec{r}_{\alpha_1}, \vec{r}_{\alpha_2}, \ldots, \vec{r}_{\alpha_n}) \] has to satisfy the Pauli principle, i.e., to be antisymmetric over space coordinates. Here the index \( \alpha_i, \ i = 1, \ldots, n \) runs \( \{1, 2, \ldots, n\} \) so that \( \alpha_i \neq \alpha_j \) for \( i \neq j \). It can be achieved if one represents this function as

\[ \psi(\vec{r}_{\alpha_1}, \vec{r}_{\alpha_2}, \ldots, \vec{r}_{\alpha_n}) = \epsilon(P_{\alpha_1 \alpha_2 \ldots \alpha_n}) \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n), \tag{1} \]

where \( P_{\alpha_1 \alpha_2 \ldots \alpha_n} \) is a permutation:

\[ P_{\alpha_1 \alpha_2 \ldots \alpha_n} = \left( \begin{array}{cccc} 1 & 2 & \ldots & n \\ \alpha_1 & \alpha_2 & \ldots & \alpha_n \end{array} \right) \tag{2} \]

which converts 1 into \( \alpha_1 \), 2 into \( \alpha_2 \) and so on. A symbol \( \epsilon(P) \) denotes a number equal to +1 if the permutation is even, and a number equal to −1 if the permutation is odd.

It is easy to prove that the functions (1) satisfy the following equality:

\[ \sum_{\{\alpha_i\}_{i=1}^n} \psi(\vec{r}_{\alpha_1}, \vec{r}_{\alpha_2}, \ldots, \vec{r}_{\alpha_n}) = 0. \tag{3} \]

To do it we divide up the left side of the expression (3) into functions so that one describes the spin configuration as \( \{\uparrow \uparrow \ldots \uparrow \uparrow \mid \downarrow \downarrow \ldots \downarrow\} \), and another one describes the spin configurations: \( \{\uparrow \uparrow \ldots \uparrow \uparrow \mid \uparrow \uparrow \ldots \downarrow\} \), \( \{\uparrow \uparrow \ldots \uparrow \uparrow \mid \downarrow \downarrow \ldots \downarrow\} \), \( \{\uparrow \uparrow \ldots \uparrow \uparrow \mid \downarrow \downarrow \ldots \downarrow\} \), \ldots, \( \{\uparrow \uparrow \ldots \uparrow \uparrow \mid \downarrow \downarrow \ldots \downarrow\} \), with the sign minus “−”. Graphically this partitioning is shown in fig. 1 and is written mathematically as

\[
\psi(\vec{r}_1, \ldots, \vec{r}_{k-1}, \vec{r}_k|\vec{r}_{k+1}, \vec{r}_{k+2}, \ldots, \vec{r}_n) = \psi(\vec{r}_1, \ldots, \vec{r}_{k-1}, \vec{r}_{k+1}|\vec{r}_k\vec{r}_{k+2}, \ldots, \vec{r}_n) + \ldots + \psi(\vec{r}_1, \ldots, \vec{r}_{k-1}, \vec{r}_{k+l}|\vec{r}_{k+1}, \ldots, \vec{r}_{k+l-1}, \vec{r}_k\vec{r}_{k+l+1}, \ldots, \vec{r}_n) + \ldots + \psi(\vec{r}_1, \ldots, \vec{r}_{k-1}, \vec{r}_n|\vec{r}_{k+1}, \ldots, \vec{r}_{k-n}, \vec{r}_k). \tag{4}
\]

Fig. 1. Graphics represents the property of cyclic symmetry for a wave function of electron.

But the wave function situated in the right side of symbolical expression in fig. 1, describes a configuration obtained by a cyclic permutation of electrons from the configuration at the left in fig. 1. Thus we have proved, that the electron function is symmetric with respect to the cyclic permutation and a mathematical notation of this property of cyclic symmetry is the expression (4).

The set of functions (1) is a basic set to construct the wave function of a many-electron system. Slater determinants possess the properties such as functions from the introduced basic set.

Further we use a method of secondary quantization to establish a Hartree - Fock equation describing a single-electron state in the self-consistent field, within the framework of electron-hole formalism.

### 3 Electron-hole formalism

Hamiltonian \( H \) for the many-electron system reads:

\[
H(\vec{r}_1, \ldots, \vec{r}_n) = \sum_{i=1}^{n} \left[-\frac{h^2}{2m} \nabla^2(\vec{r}_i) + V(\vec{r}_i)\right] + \sum_{i>j=1}^{n} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} = \sum_{i=1}^{n} H(\vec{r}_i) + \sum_{i>j=1}^{n} V(\vec{r}_i - \vec{r}_j), \tag{5}
\]
where $\nabla^2$ is the Laplacian, $V(\vec{r}_i)$ is the potential energy of $i$-th electron in a field of atomic nucleus or nuclei, $V(\vec{r}_i - \vec{r}_j)$ is the Coulomb interaction potential.

Let us go into representation of secondary quantization where a single-particle state is given by creation operators $\hat{\psi}^\dagger(x_i)$ and annihilation operators $\hat{\psi}(x_i)$ of $i$-th Fermi particle with generalized coordinates $x_i = \{\vec{r}_i, t_i, \sigma_i\}$ being its radius-vector $\vec{r}_i$, time $t_i$ and spin $\sigma_i$. These operators satisfy the commutation relations [12]:

$$\hat{\psi}(x')\hat{\psi}^\dagger(x) + \hat{\psi}^\dagger(x)\hat{\psi}(x') = \delta(x - x')$$  \hspace{0.5cm} (6)

$$\hat{\psi}(x')\hat{\psi}(x) + \hat{\psi}(x)\hat{\psi}(x') = 0.$$  \hspace{0.5cm} (7)

Now one can introduce an operator of "hole" creation in the following way. Since the wave function of the system can be written in the form

$$\hat{\psi}(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}^\dagger(x)\cdots = \hat{\psi}(x)\hat{\psi}^\dagger(x)= \hat{\psi}(x)\hat{\psi}^\dagger(x),$$

the operator $[\hat{\psi}_{n+1}^\dagger(\vec{r}_n) + \hat{\psi}_{(n+1)}^\dagger(\vec{r}_{n+1})]$ is a creation operator of a "hole" by $n$-th electron. Here $\hat{\psi}_{n+1}^\dagger(\vec{r}_n, \vec{r}_{k+2}, \vec{r}_{k+1})\hat{\psi}_{k+1}^\dagger(\vec{r}_k, \vec{r}_{k-1}, \ldots, \vec{r}_1)$ is a secondary quantized wave function of the system describing the configuration from $k$ electrons with spin "up" and $n - k$ electrons with spin "down", $n = 2k + 1$, i.e. there is one unpaired electron; $|0\rangle$ is a vacuum state. The wave function (8) describes systems with outer unpaired electron or with a "hole", having spin "up" $\uparrow$ by outer electron.

Let us assume that core polarization happens at the moment $t$. Then in this moment $t$ the secondary quantized wave function of system can be obtained as a result of cyclic permutation $P^{(cycl)}(t)$:

$$P^{(cycl)}(t)[\hat{\psi}_{n+1}^\dagger(\vec{r}_n) + \hat{\psi}_{(n+1)}^\dagger(\vec{r}_{n+1})]|\psi_1, \ldots, \psi_{n+1}\rangle.$$

(9)

Since the operators $P^{(cycl)}(t)$ and $[\hat{\psi}_{n+1}^\dagger(\vec{r}_n) + \hat{\psi}_{(n+1)}^\dagger(\vec{r}_{n+1})]$ commute with each other then according to the definition of permutation operator which is shown in fig. 1 the expression (10) can be rewritten as

$$P^{(cycl)}(t)[\hat{\psi}_{n+1}^\dagger(\vec{r}_n) + \hat{\psi}_{(n+1)}^\dagger(\vec{r}_{n+1})]|\psi_1, \ldots, \psi_{n+1}\rangle$$

(11)

$$= \sum_{m=1}^{k} c_{nm}(t)\hat{\psi}_{m+1}^\dagger(\vec{r}_m, t) + \sum_{m=k+1}^{n} c_{nm}(t)\hat{\psi}_{m+1}^\dagger(\vec{r}_{m+1}, t) P^{(cycl)}_m|\psi_1, \ldots, \psi_{n+1}\rangle$$

$$= \sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m) P^{(cycl)}_m|\psi_1, \ldots, \psi_{n+1}\rangle,$$

(10)

where $m$-th term of the sum describes a "hole" which is created at $m$-th core electron after the cyclic permutation $P^{(cycl)}_m$ in the sense of the expression (4), a matrix $|c_{nm}(t)|$ converts the creation operator of the "hole" by $n$-th electron into the creation operator of the "hole" by $m$-th electron.

According to the property of cyclic symmetry (4) one can formally write the expression

$$[\hat{\psi}_{n+1}^\dagger(\vec{r}_n) + \hat{\psi}_{(n+1)}^\dagger(\vec{r}_{n+1})] = \sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m) P^{(cycl)}_m.$$  \hspace{0.5cm} (11)
It follows from here that the sum $\sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m)$ has to satisfy the same quantum
equations of motion as for $[\hat{\psi}_{n\downarrow}(\vec{r}_n) + \hat{\psi}_{(n+1)\uparrow}(\vec{r}_{n+1})]$. Heisenberg equation of motion for the "hole"
creation operator $[\hat{\psi}_{n\downarrow}(\vec{r}_n) + \hat{\psi}_{(n+1)\uparrow}(\vec{r}_{n+1})]$ reads:

$$\frac{\hbar}{i} \frac{\partial}{\partial t} [\hat{\psi}_{n\downarrow}(\vec{r}_n) + \hat{\psi}_{(n+1)\uparrow}(\vec{r}_{n+1})] = \left[ [\hat{\psi}_{n\downarrow}(\vec{r}_n) + \hat{\psi}_{(n+1)\uparrow}(\vec{r}_{n+1})], \hat{H} \right]; \quad (12)$$

$$\hat{H} = \left( \sum_{i=1}^{n} \int \hat{H}(x_i) d\vec{r}_i + \sum_{i>j=1}^{n} \int \int \hat{V}(x_i, x_j) d\vec{r}_i d\vec{r}_j \right)$$

$$\hat{H}(x_i) = \hat{\psi}^\dagger(x_i) H(\vec{r}_i) \hat{\psi}(x_i); \quad (14)$$

$$\hat{V}(x_i, x_j) = \frac{1}{2} \hat{\psi}^\dagger(x_j) \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_j) \hat{\psi}(x_i) \hat{\psi}(x_j) \quad (15)$$

where $[\hat{A}, \hat{B}]$ is a commutator of operators $\hat{A}$ and $\hat{B}$, $\hat{H}$ is the Hamiltonian operator in the
secondary quantization formalism which is obtained by a secondary quantization procedure
[12] from the operator $\langle 5 \rangle$.

Substituting the expression (11) into the equation of motion (12) one gets

$$\frac{\hbar}{i} \frac{\partial}{\partial t} \sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m) P_m^{(cycl)} = \sum_{m,i=1}^{n} c_{nm}(t) \left\{ \int d\vec{r}_i \right.$$  

$$\times \hat{\psi}(x_m) \left[ \hat{\psi}^\dagger(x_i) H(\vec{r}_i) \hat{\psi}(x_i) + \sum_{j=1}^{n} \int \frac{d\vec{r}_j}{2} \hat{\psi}^\dagger(x_j) \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_j) \hat{\psi}(x_i) \hat{\psi}(x_j) \right]$$

$$\left. - \left[ \hat{\psi}^\dagger(x_i) H(\vec{r}_i) \hat{\psi}(x_i) + \sum_{j=1}^{n} \int \frac{d\vec{r}_j}{2} \hat{\psi}^\dagger(x_j) \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_j) \hat{\psi}(x_i) \hat{\psi}(x_j) \right] \hat{\psi}(x_m) \right\} P_m^{(cycl)} \quad (16)$$

for $j < i$

for the "hole" creation operator $\sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m)$ which depends on configuration. Using the commutation rules [3] [7] for quantized fermion fields one transforms eq. (16) to the form:

$$\frac{\hbar}{i} \frac{\partial}{\partial t} \sum_{m=1}^{n} c_{nm}(t)\hat{\psi}(x_m) P_m^{(cycl)} = \sum_{m,i=1}^{n} c_{nm}(t) \left\{ \int d\vec{r}_i \right.$$  

$$\times \hat{\psi}(x_m) \left[ \delta(x_i - x_m) H(\vec{r}_i) \hat{\psi}(x_i) + \sum_{j=1}^{n} \int \frac{d\vec{r}_j}{2} \delta(x_j - x_m) \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_j) \hat{\psi}(x_i) \hat{\psi}(x_j) \right]$$

$$\left. - \left[ \sum_{j=1}^{n} \int \frac{d\vec{r}_j}{2} \delta(x_i - x_m) \hat{\psi}^\dagger(x_j) V(\vec{r}_i - \vec{r}_j) \hat{\psi}(x_i) \hat{\psi}(x_j) \right] \hat{\psi}(x_m) \right\} P_m^{(cycl)} \quad (17)$$

for $j < i$

where $\delta(x_k - x_m)$ is the Dirac $\delta$-function. Differentiating over time at the left side and
integrating over the Dirac $\delta$-function at the right side of eq. (17) one gets finally

$$\left( \frac{\hbar}{i} \frac{\partial \ln c_{nm}(t)}{\partial t} - \hat{\varepsilon} \hat{1} \right) \hat{\psi}(x_m) P_m^{(cycl)} = \left( H(\vec{r}_m) \hat{\psi}(x_m) + \frac{1}{2} \sum_{i=1}^{n} \int d\vec{r}_i \right.$$  

$$\times \left( \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_m) \hat{\psi}(x_i) \hat{\psi}(x_m) - \hat{\psi}^\dagger(x_i) V(\vec{r}_m - \vec{r}_i) \hat{\psi}(x_m) \hat{\psi}(x_i) \right) \right) P_m^{(cycl)}$$

$$= \left( H(\vec{r}_m) \hat{\psi}(x_m) - \sum_{i=1}^{n} \int d\vec{r}_i \hat{\psi}^\dagger(x_i) V(\vec{r}_i - \vec{r}_m) \hat{\psi}(x_m) (\hat{\psi}(x_m) \delta_{mi}) \right) P_m^{(cycl)}, \quad (18)$$
where \( \hat{I} \) is the unity operator, \( \hat{c} \) is the operator of "hole" energy as

\[
\hat{\psi}(x_m) = \hat{\psi}(\vec{r}_m, \sigma_m)\exp(-i\hat{c}\hat{t}/\hbar);
\]

and the right side of eq. (18) is rewritten taking into account matrix multiplication rules.

Now we can find the equations, describing single-particle state neglecting correlations in movement of electrons relative to each other. To examine the configuration shown in fig. 1, we shall assume that electrons with spins "up" move independent on electrons with spins "down". In other words their movement are not correlated. Therefore the wave function of such configuration is factorized in the following way:

\[
\hat{\psi}_{(n-k)\uparrow}(\vec{r}_n, \ldots, \vec{r}_{k+2}, \vec{r}_{k+1})\hat{\psi}_{k\downarrow}^\dagger(\vec{r}_k, \vec{r}_{k-1}, \ldots, \vec{r}_1)|0\rangle = |\psi_1, \ldots, \psi_n\rangle
\]

\[
= |\psi_n, \ldots, \psi_{k+2}, \psi_{k+1}\rangle|\psi_k, \psi_{k-1}, \ldots, \psi_1\rangle
\]

\[
= \hat{\psi}_{(n-k)\downarrow}^\dagger(\vec{r}_n, \ldots, \vec{r}_{k+2}, \vec{r}_{k+1})|0 \downarrow\rangle\hat{\psi}_{k\uparrow}^\dagger(\vec{r}_k, \vec{r}_{k-1}, \ldots, \vec{r}_1)|0 \uparrow\rangle.
\]

From here it follows an expansion for the vacuum state \(|0\rangle\)

\[
|0\rangle = |0 \downarrow\rangle|0 \uparrow\rangle \equiv |0, \sigma_m\rangle|0, -\sigma_i\rangle,
\]

which means that \(|0\rangle\) consists of non-occupation states with spins "down" \(|0 \downarrow\rangle\) and with spins "up" \(|0 \uparrow\rangle\).

Hermitian conjugation of eq. (18) has the form:

\[
\left( i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} - \hat{c}^\dagger \hat{I} \right) P_{m}^{(\text{cycl})} \hat{\psi}_{m}^\dagger(x_m)
\]

\[
= P_{m}^{(\text{cycl})} \left( H(\vec{r}_m)\hat{\psi}_{m}^\dagger(x_m) - \sum_{i=1}^{n} \int d\vec{r}_i \hat{\psi}_{m}^\dagger(x_m)V(\vec{r}_i - \vec{r}_m)(\hat{\psi}_{m}^\dagger(x_m)\delta_{mi})\hat{\psi}(x_i) \right)
\]

\[
= P_{m}^{(\text{cycl})} \left( H(\vec{r}_m)\hat{\psi}_{m}^\dagger(x_m) - \sum_{i=1}^{n} \int d\vec{r}_i \hat{\psi}_{m}^\dagger(x_m)V(\vec{r}_i - \vec{r}_m)\hat{\psi}_{m}^\dagger(x_i)\hat{\psi}(x_i) \right).
\]

Acting with the hermitian conjugate equation (21) on the found non-occupied states \(|0\sigma_m\rangle\) in the vacuum state (20), one gets the following equation

\[
\left( i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} - \hat{c}^\dagger \hat{I} \right) P_{m}^{(\text{cycl})} \hat{\psi}_{\sigma_m}^\dagger(\vec{r}_m)|0\sigma_m\rangle|0, -\sigma_i\rangle
\]

\[
= P_{m}^{(\text{cycl})} \left( H(\vec{r}_m)\hat{\psi}_{\sigma_m}^\dagger(\vec{r}_m) - \sum_{i=1}^{n} \int d\vec{r}_i \hat{\psi}_{\sigma_m}^\dagger(\vec{r}_m)\hat{\psi}_{\sigma_{i}}(\vec{r}_i)V(\vec{r}_i - \vec{r}_m)\hat{\psi}_{\sigma_{i}}(\vec{r}_i) \right)|0\sigma_m\rangle|0, -\sigma_i\rangle.
\]

According to the expression (11) the operation of permutation \(P_{m}^{(\text{cycl})}\) entered into eq. (22) is written in the explicit form as

\[
P_{m}^{(\text{cycl})}\hat{\psi}_{\sigma_m}^\dagger(\vec{r}_m)\hat{\psi}_{\sigma_{i}}(\vec{r}_i)\hat{\psi}_{\sigma_{i}}(\vec{r}_i) - \hat{\psi}_{\sigma_m}^\dagger(\vec{r}_m)\hat{\psi}_{\sigma_{i}}(\vec{r}_i)\hat{\psi}_{\sigma_{i}}(\vec{r}_i).
\]

Substitution of the explicit expression for \(P_{m}^{(\text{cycl})}\) (23) into eq. (22) gives the following equa-
Multiplying on the left side of eq. (24) by the vector $\langle 0, -\sigma_i |$ one gets

$$i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} \psi^\dagger_{\sigma_m}(\vec{r}_m)|0\sigma_m\rangle = \left( H(\vec{r}_m)\psi^\dagger_{\sigma_m}(\vec{r}_m) - \sum_{i=1}^n \int d\vec{r}_i \right) \times \langle 0|0\sigma_m\rangle - \int d\vec{r}_i \psi^\dagger_{\sigma_m}(\vec{r}_m) V(\vec{r}_i - \vec{r}_m) \psi_{\sigma_m}(\vec{r}_i) - \psi^\dagger_{\sigma_m}(\vec{r}_m) V(\vec{r}_i - \vec{r}_m) \psi_{\sigma_m}(\vec{r}_i)) \times |0\sigma_m\rangle |0, -\sigma_i\rangle. \quad (24)$$

Multiplying on the left side of eq. (24) by the vector $\langle 0, -\sigma_i |$ one gets

$$i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} \psi^\dagger_{\sigma_m}(\vec{r}_m)|0\sigma_m\rangle = \langle 0, -\sigma_i | \hat{1} |0, -\sigma_i \rangle \psi^\dagger_{\sigma_m}(\vec{r}_m)|0\sigma_m\rangle = H(\vec{r}_m)\psi^\dagger_{\sigma_m}(\vec{r}_m)|0\sigma_m\rangle$$

$$- \sum_{i=1}^n \int d\vec{r}_i \psi^\dagger_{\sigma_i}(\vec{r}_m)|0\sigma_m\rangle V(\vec{r}_i - \vec{r}_m) \langle 0, -\sigma_i | \psi^\dagger_{\sigma_i}(\vec{r}_i) \psi_{\sigma_m}(\vec{r}_i)|0, -\sigma_i\rangle$$

$$+ \sum_{i=1}^n \int d\vec{r}_i \psi^\dagger_{\sigma_m}(\vec{r}_m)|0\sigma_m\rangle V(\vec{r}_i - \vec{r}_m) \langle 0, -\sigma_i | \psi^\dagger_{\sigma_i}(\vec{r}_i) \psi_{\sigma_i}(\vec{r}_i)|0, -\sigma_i\rangle, \quad (25)$$

as $\langle 0, -\sigma_i | 0, -\sigma_i \rangle = 1$. If one introduces the following designation: $\hat{\psi}^\dagger_{\sigma_j}(\vec{r}_j)|0\sigma_j\rangle \equiv \psi_j(x_k)$ and represents the unity operator in the explicit form:

$$\hat{1} = \sum_{j=1}^n \hat{\psi}^\dagger_{\sigma_j}(\vec{r}_j)|0\sigma_j\rangle \langle 0\sigma_j | \hat{\psi}_{\sigma_j}(\vec{r}_j) \equiv \sum_{j=1}^n P_j, \quad \text{then eq. (25) can be rewritten as}$$

$$i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} \psi_m(x_m) = H(\vec{r}_m)\psi_m(x_m) - \sum_{j=1}^n \epsilon^\dagger P_j \psi_m(x_m) + \sum_{i=1}^n \int d\vec{r}_i \psi_m(x_m) V(\vec{r}_i - \vec{r}_m) \psi_i(x_i) \psi_i(x_i) - \psi_i(x_m) V(\vec{r}_i - \vec{r}_m) \psi_i(x_i) \psi(m)(26)$$

Eq. (26) taking at initial time $t = 0$ is the equation describing single-particle state $\psi_m(x_m)$:

$$\left[ H(\vec{r}_m) + \hat{V}^{sc}(x_m) - \hat{\Sigma}^x(x_m) \right] \psi_m(x_m) = \left( \epsilon_m(0) + \sum_{j=1}^n \epsilon^\dagger P_j \right) \psi_m(x_m). \quad (27)$$

where the differentiation over time $t$ taking at initial time $t = 0$ is designated as $\epsilon_m(0)$:

$$\epsilon_m(0) = -i\hbar \frac{\partial \ln c_{nm}(t)}{\partial t} \bigg|_{t=0},$$

$\hat{V}^{sc}$ and $\hat{\Sigma}^x$ are the Coulomb and exchange interactions, respectively:

$$\hat{V}^{sc}(x_i) \psi_n(x_i) = \sum_{m=1}^n \int \psi^*_m(x_j)v(|\vec{r}_i - \vec{r}_j|)\psi_m(x_j) d\vec{r}_j \psi_n(x_i), \quad (28)$$

$$\hat{\Sigma}^x(x_i) \psi_n(x_i) = \sum_{m=1}^n \int \psi^*_m(x_j)v(|\vec{r}_i - \vec{r}_j|)\psi_n(x_j) d\vec{r}_j \psi_n(x_i). \quad (29)$$
Physical meaning of the operators [28, 29] becomes evident if one rewrites them in terms of spinless electronic density $\rho(\vec{r}, \vec{r}')$ and supposes that the interaction $v$ is the Coulomb one:

$$\rho(\vec{r}, \vec{r}') = \frac{1}{2} \sum_{m=1}^{n-1} (\psi_m^*(\vec{r}, \sigma)\psi_m(\vec{r}', -\sigma) + \psi_m^*(\vec{r}', -\sigma)\psi_m(\vec{r}, \sigma))$$

$$= \sum_{m=1}^{(n-1)/2} \psi_m^*(\vec{r})\psi_m(\vec{r}'), \quad v = e^2/|\vec{r} - \vec{r}'|. \quad (30)$$

From here it follows that the operator $\hat{V}^{sc}$ represents electrostatic interaction of one electron with the electron density produced by remaining $n-1$ electrons and electrostatic self-action (s.a.):

$$\hat{V}^{sc}(x_i)\psi_n(x_i) = \sum_{\sigma} \sum_{m=1}^{(n-1)/2} \int \psi_m^*(\vec{r}_j)\psi_n(\vec{r}_j) \, d\vec{r}_j \psi_n(x_i) + \text{s.a.}$$

$$= 2 \int d\vec{r}_j \frac{e^2\rho(\vec{r}_j, \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|} \psi_n(x_i) + \text{s.a.} \quad (31)$$

Analogously one obtains that the operator $\hat{\Sigma}^x$ gives quantum exchange with exchange self-action (s.a.):

$$\hat{\Sigma}^x(x_i)\psi_n(x_i) = \sum_{m=1}^{n-1} \int d\vec{r}_j \psi_m^*(\vec{r}_j, \sigma_j)\psi_n(\vec{r}_j, \sigma_j) \psi_m(\vec{r}_j, \sigma_j) + \text{s.a.}$$

$$= \frac{1}{2} \sum_{m=1}^{n-1} \int d\vec{r}_j d\sigma_j \left( \psi_m^*(\vec{r}_j, \sigma_j)\psi_m(\vec{r}_j, -\sigma_j)\delta(\sigma_j - \sigma_i) + \psi_m^*(\vec{r}_j, -\sigma_j)\psi_m(\vec{r}_j, \sigma_j)\delta(\sigma_j - \sigma_i) \right) \psi_n(\vec{r}_j, \sigma_j) + \text{s.a.}$$

$$= \int d\vec{r}_j \frac{e^2\rho(\vec{r}_j, \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|} \psi_n(x_j) + \text{s.a.} \quad (32)$$

Since the operators $\hat{V}^{sc}$ and $\hat{\Sigma}^x$ into the expression (27) are subtracted from each other then the self-acting terms (s.a.) entering into it are mutually cancelled.

Let us suppose that there exists a representation in which the energy operator of a "hole" $\hat{\epsilon}^\dagger$ entering into eq. (27) is diagonalized $\hat{\epsilon}^\dagger = \epsilon(k_i)I$, where $I$ is an unitary matrix. The replacing $\vec{r}_m \to \vec{r}_i$ and the taking into account of the diagonalization condition into eq. (27) allow to describe the core polarization as a quasiparticle exitation with the energy $\epsilon(k_i)$ which stationary state is determined as

$$\left[ H(\vec{r}_i) + \hat{V}^{sc}(k_i x_i) - \hat{\Sigma}^x(k_i x_i) \right] \psi_m(k_i x_i) = \left( \epsilon_m(0) + \sum_{j=1}^{n} \hat{\epsilon}^\dagger P_j \right) \psi_m(k_i x_i), \quad (33)$$

$$\hat{\epsilon}^\dagger = \epsilon(k_i)I. \quad (34)$$

**Approximation of a "frozen" atom**

Let us call by approximation of a "frozen" atom the calculations with assumption that almost all time a "hole" is near $m$-th electron which is located in a point with radius-vector $\vec{r}_i$. Since the energy operator of "hole" by $m$-th electron in the point $\vec{r}_i$ can be of a work only which has to be perfomed to shift an electron occupying the "hole" near $m$-th electron to $j$-th non-occupied orbital of atom "frozen" in the moment, then $\hat{\epsilon}$ is equal to:

$$\hat{\epsilon}_j^{(m)} = -\left( \epsilon_j - \epsilon_i^{(m)} \right). \quad (35)$$
Substituting the expression (35) into eq. (33) one gets

\[
[H(\vec{r}_i) + \hat{V}^{sc}(x_i) - \hat{\Sigma}^x(x_i)] \psi_m(x_i) = \left( \epsilon_m(0) - \sum_{j=1}^{n} (\epsilon_i^{(m)} - \epsilon_j) P_j \right) \psi_m(x_i).
\] (36)

The approximation of valent electron \( \psi_v \) or the approximation of a "frozen" atomic core appears if there exists an outer valent \( v \)-th electron located in a point with a radius - vector \( \vec{r}_v \) such that it always is outside limits of atomic core: \( \vec{r}_v > \vec{R}_c \), where \( |\vec{R}_c| \) is a radius of the "frozen" core. Existence of outer electron means that one of electrons can not be placed inside of the core. It is possible if the core has no "holes". Since in this approximation the core has no "holes" then eq. (36) can be rewritten as

\[
[H(\vec{r}_i) + \hat{V}^{sc}(x_i) - \hat{\Sigma}^x(x_i)] \psi_m(x_i) = \left( \epsilon_m(0) - (1 - \delta_{ic}) \sum_{j=1}^{n} (\epsilon_i - \epsilon_j) P_j \right) \psi_m(x_i),
\] (37)

the valent orbital is the orbital determined by the expression

\[
\psi_v = (1 - \sum_{c} P_c) \psi_m(x_i), \quad i \neq c.
\] (38)

Here index "c" labels core electrons. It is easy see that eq. (37) is the equation for Phillips - Kleinman pseudo-potential \( V^{PK} \) [2, 3, 4] in the case of wave function depending on both coordinates and spin variables of electron. Therefore eq. (33) and eq. (36) are generalization of eq. (37) and with their help one can describe many-electron systems beyond the framework where the method of pseudo-potential is valid.

### 4 Secondary quantized density matrix

We rewrite (33) in the representation of the Dirac ket (bra) - vectors:

\[
\hat{h}(k)|n; k\rangle + \sum_{m=1, m \neq n}^{N} \int \delta(k - k') \, dk' |n; k\rangle \langle m; k'|v(kk')|m; k'| + \langle n; k'\rangle \delta_{nm} \langle m; k'|v(kk')|m; k\rangle \delta_{mn})
\]

\[
- \sum_{m=1}^{N} \int |m; k\rangle \langle m; k'|v(kk')|n; k\rangle \delta(k - k') \, dk' = |n; k\rangle (\epsilon_n(0) + \epsilon_n(k))
\] (39)

where \( k_i \equiv \{\vec{k}_i, \sigma_i\} \), \( \hat{h}(k) \) is a momentum representation of the non-perturbed hamiltonian, \( v(kk') = \int d\vec{r} \overline{d\vec{r}} |\vec{r}\rangle \langle \vec{r}'| [\hat{\vec{k}} \cdot \vec{r}] v(|\vec{r} - \vec{r}'|) \hat{\vec{k}}' \cdot \vec{r}' \rangle \langle \vec{r}'| \) is a momentum representation of the Coulomb interaction operator, \( \delta(k - k') \) is the Dirac \( \delta \)-function manifesting the presence of the law of conservation of momentum.

Let us introduce projective operators \( \hat{\rho}_{kk}^{mn} \) [13]:

\[
\hat{\rho}_{kk}^{mn} \equiv |m; k\rangle \langle n; k|.
\] (40)

and express eq. (39) through these operators \( \hat{\rho}_{kk}^{mn} \). For this purpose, Eq. (39) is multiplied from the right by bra-vector \( \langle n; k| \). Then, additional summating over \( n \) and integrating over
We see that the first and second terms in the left side of the equation (41) are traces of a matrix representation of operators $\hat{\rho} \hat{h}$ and $\hat{\rho}^\ast \hat{\rho} v$, and the third and fourth terms in the left side of equation (41) are mutually canceled. Hence, it means that using normalization of the function $|n; k\rangle$: $\int dk \langle n; k | n; k \rangle = 1$, we obtain the following equation:

$$Sp\hat{\rho} \hat{h} + Sp\hat{\rho}^\ast \hat{\rho} v = \epsilon_n(0)N + \int dk \sum_{n=1}^{N} \langle n; k | n; k \rangle \epsilon_n(k).$$

(42)

Using properties of the projective operators $\hat{\rho}_{mn}^{kk'}$: $(\hat{\rho}_{mn}^{kk'})^\ast = \hat{\rho}_{mn}^{km'}$ and $(\hat{\rho}_{mn}^{kk'})^2 = \hat{\rho}_{mn}^{kk'}$, one can transform eq. (42) to the form:

$$Sp\hat{\rho} (\hat{h} + v) = \epsilon_n(0)N + \int dk \sum_{n=1}^{N} \langle n; k | n; k \rangle \epsilon_n(k) = \epsilon_n(0)N + \epsilon.$$  

(43)

Let us elucidate physical sense of introduced projective operators $\hat{\rho}_{mn}^{kk'}$. The energy of a quasiparticle $\epsilon$ is in the right side of Eq. (43) up to the constant $\epsilon_n(0)N$. From here it follows that the operator $\hat{\rho}_{mn}^{kk'}$ allows to calculate the energy $\epsilon$ of quasiparticle excitations. It means that the expression (43) is nothing else but a procedure of average over density matrix. Since the averaging with the help of the operator $\hat{\rho}_{mn}^{kk'}$ yields the energy $\epsilon$ of quasiparticle, this operator is a secondary quantized density matrix.

Thus, it is proved that eq. (33) can be considered as the equation describing the state of quasiparticle and determining its energy with accuracy up to the constant $\epsilon_n(0)N$. Since for description of single-electron state it is necessary to take into account the presence of "hole", then the quasiparticle state describes the electron-hole pair.

5 Green function for single-particle state

It follows also from Eq. (43) that the quantity $\epsilon_n(k_i)$ can be interpreted as an eigenvalue of the Hamiltonian for a quasiparticle excitation without taking into account interaction of quasiparticles. Therefore, the equation (13), written in the formalism of the density
matrix $\hat{\rho}_{nn';kk'}^{(0)} \equiv \hat{\rho}_{kk'}^{nn'}$ can be rewritten in the formalism of wave functions in coordinate representation and in the limit of large $N$, $N \to \infty$ in the following way:

$$
\left( i \frac{\partial}{\partial t} - (\hat{h} + \Sigma^x + V^{sc}) \right) \sum_n \hat{\rho}_{nn';rr'}^{(0)} = \lim_{N \to \infty} (-\epsilon_n(0))N \delta_{rr'},
$$

where property $\int dk \langle n; kr | n; kr' \rangle = \delta_{rr'}$ has been used; $\delta_{rr'}$ is a delta symbol. Since the energy $\epsilon_n(0)$ of the bound one-electron state is negative: $\epsilon_n(0) < 0$, the right side of Eq. (44) represents itself the Dirac $\delta$-function $\delta(r - r')$. It allows to write Eq. (44) as:

$$
\left( i \frac{\partial}{\partial t} - \hat{h}^{HF} \right) \sum_n \hat{\rho}_{nn';rr'}^{(0)} = \delta(r - r'),
$$

where $\hat{h}^{HF} = (\hat{h} + \Sigma^x + V^{sc})$, $\Sigma^x = -\Sigma^x$. Eq. (45) is the equation for the Green function. It means that in the secondary quantized representation the operator $\hat{G}_{1}^{(0)}(n'; r, r') = \sum_n \hat{\rho}_{nn';rr'}^{(0)}$ possesses properties of non-perturbed Green function.

So, the quasiparticle excitation determined by the Hamiltonian $\hat{h}^{HF}$ can be considered as a free particle whose equation of motion is the equation (45).

In many-body problem, in particular, in calculations of energy-band of crystal structure a contribution given by the interaction of an electromagnetic field with matter plays an essential role. To take into account many-particle effects due to correlated motion of an electron we should describe the system by self-consistent solutions of the non-stationary equation

$$
i \frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t)
$$

where $\hat{H}$ is the Schrödinger hamiltonian in a non-relativistic case or a Dirac hamiltonian in relativistic one.

We have proved that for the secondary quantized representation the operator $\hat{\rho}$ looks like $\hat{\rho} = |\hat{\psi} \rangle \langle \hat{\psi}|$ and possesses the properties of the Green function $G_{1}$. Therefore the sum $\hat{G}_{1}$ over $n$ from elements of the matrix $\hat{\rho}_{nn';rr'}^{(0)}$ for the secondary quantized density matrix $\hat{\rho}$ describing an interacting particle satisfies the Dyson equation in nonrelativistic case or to the Schwinger - Dyson equation in relativistic case:

$$
G_{1}(1; 2) = G_{1}^{(0)}(1; 2) + \int d3 d4 G_{1}^{(0)}(1; 3) \hat{\Sigma}(3, 4) G_{1}(4; 2)
$$

where $G_{1}^{(0)}(1; 2)$ is the free Green function, $\hat{\Sigma}(3, 4)$ is the self-energy operator: $\hat{\Sigma} = \Sigma^x + \hat{\Sigma}^c$; $\hat{\Sigma}^c$ is correlation interactions, representing itself a part of the self-energy which describes the many-particle effects. Here numerical labels for the arguments are used: $\{r_1, t_1\} = x_1 \equiv 1$, etc. Acting on Eq. (48) by the operator $i \frac{\partial}{\partial t} - \hat{h}^{HF}$ and using the equation of motion for the free particle (45) we get the equation for the perturbed Green function as

$$
\left[ i \frac{\partial}{\partial t} - \hat{h}^{HF}(r_1) \right] G_{1}(n'; 1, 2) = \int d3 \hat{\Sigma}^c(n'; 1, 3) G_{1}(n'; 3, 2) = (-\epsilon_n(0))N \delta_{r_1 r_2}.
$$
Rewriting Eq. (49) in the formalism of wave functions one gets
\[
\left[ \frac{i}{\hbar} \frac{\partial}{\partial t} - \hat{H}^{HF}(r_1) \right] \psi_n(k_1 r_1) - \int d\vec{r}_2 \hat{\Sigma}^c(n; 1, 2) \psi_n(k_1 r_2) = (-\epsilon_n(0)) \psi_n(k_1 r_1). \tag{50}
\]

Since the expression: \( i \frac{\partial}{\partial t} = \epsilon_n(k_1) \) takes place, then Eq. (50) yields the Hartree - Fock equation taking into account of interacting quasiparticles
\[
\hat{H}^{HF}(r_1) \psi_n(k_1 r_1) + \int d\vec{r}_2 \hat{\Sigma}^c(n; 1, 2) \psi_n(k_1 r_2) = (\epsilon_n(0) + \epsilon_n(k_1)) \psi_n(k_1 r_1). \tag{51}
\]

Let us define a mass operator \( \hat{\Delta}M \) as:
\[
\hat{\Delta}M \psi_n(k_1 r_1) = \int d\vec{r}_2 \hat{\Sigma}^c(n; 1, 2) \psi_n(k_1 r_2). \tag{52}
\]

Within the framework of the concept of quasiparticle excitations it is possible to represent the operator \( \hat{\Delta}M \) in the diagonal form:
\[
\hat{\Delta}M \psi_n(k_i r_i) = -(\Delta M_n(0) + \Delta M_n(k_i)) \psi_n(k_i r_i), \tag{53}
\]

the eigenvalue of mass operator possesses the property:
\( \Delta M_n(k_i) = \Delta M_n(-k_i) \). Here \( \Delta M_n(0) \) is an eigenvalue of mass operator \( \hat{\Delta}M \) in the limit \( \vec{k} \to 0 \).

From here it follows physical sense of \( \hat{\Delta}M \). It determines an effective mass of the quasiparticle and an efficient bottom of the energy band:
\[
\hat{H}^{HF}(r_1) \psi_n(k_1 r_1) = (\epsilon_n(0) + \epsilon_n(k_1)) \psi_n(k_1 r_1) \equiv
\quad \equiv \left[ (\epsilon_n(0)) + \Delta M_n(0) \right] + (\epsilon_n(k_1) + \Delta M_n(k_1)) \psi_n(k_1 r_1). \tag{54}
\]

Extremum of energy band \( \text{Extr} E_n(k_i) \) in the presence of interaction between quasiparticles is determined by the following expression:
\[
\text{Extr} E_n(k_i) = (\Delta M_n(0) + \epsilon_n(0)) N. \tag{55}
\]

Let us consider the Green function normalized per unit volume \( V = 1 \) so that average energy in \( V \) is equal to the energy of single-particle state and \( N = 1 \). If \( -\epsilon_n(0) \to \infty \) then Eq. (49) describes propagation of single particle and should be rewritten as
\[
\left[ \frac{i}{\hbar} \frac{\partial}{\partial t} - \hat{H}^{HF}(r_1) \right] G_1(n'; 1, 2) - \int d\vec{r} \hat{\Sigma}^c(n'; 1, 3) G_1(n'; 3, 2) = \left( -\epsilon_n(0) \right) \delta_{r_1 r_2}. \tag{56}
\]

Then according to the definition of the Green functions we have the following expression for the energy \( \epsilon_n(0) \):
\[
-\epsilon_n(0) = C - a_n, \quad C \to \infty; \tag{57}
\]

where \( a_n \) is a finite quantity. Hence, since the energy is counted off from an arbitrary value, Eq. (55) yields the following expression for the reference points \( \epsilon(0)^{\pm}_n \) of quasiparticle energy and antiquasiparticle energy
\[
\epsilon(0)^{\pm}_n = \pm a_n = \left( \text{Extr} E(k_1) \mp \Delta M_n(0) \right) / 2. \tag{58}
\]
Here one took into account that $N = 1$; an extremum of zone is redefined as $\text{Extr} \tilde{E}(k_1) = \text{Extr} E_n(k_1) - C$, the sign $\{\pm\}$ in the left-hand side denotes cases of quasiparticles and antiquasiparticles, respectively; and the energy of particles in the pair is counted off from zero level. From the expression (58) one gets that $a_n$ is the energy which is required to create a pair from quasiparticle and antiquasiparticle when $k_1 = 0$ because

$$a_n = \frac{(\epsilon(0)_n^+ - \epsilon(0)_n^-)}{2}. \quad (59)$$

Because of an additional term $\tilde{\epsilon}_n(0)$ in the right-hand side of Eq. (54) we, generally speaking, cannot examine the left-hand side as a Hamiltonian operator of quasiparticles system acting on a corresponding wave function and as a consequence, can not construct a basis set of single-particle states of the problem. However, further we show, that $\hat{h}^{HF}$ is a Hamiltonian of an electron - hole pair.

**Non-relativistic case**

In non-relativistic limit one can examine quantum systems which are characterized by a small value of $\Delta M_n(0)$:

$$\Delta M_n(0) \to 0. \quad (60)$$

It means that weak many-particle effects occur and, accordingly, we can speak about a "light" electron. The equality (58) occurs under condition of (60) only in the case if $a_n = 0$. From here it follows, that the energy $a_n$ of a pair is equal to zero. In other words, the energy is not expended to create an electron - hole pair.

Substituting Eqs. (57), (60) into (54) and taking into account the condition $a_n = 0$ one gets the Schrödinger equation in the form

$$\hat{h}^{HF}(r_1)\psi_n(k_1r_1) = \tilde{\epsilon}_n \psi_n(k_1r_1), \quad n \to \infty. \quad (61)$$

which describes the quasiparticle - antiquasiparticle pair (a non-relativistic electron - hole pair). Here $\tilde{\epsilon}_n = \tilde{\epsilon}_n - C$.

Since the energy $a_n$, expended on creation of a pair, equals to zero we have proved that the variable $\tilde{\epsilon}_n$ can be understood as the energy of an electron - hole pair. Therefore, Eq. (61) has a group of dynamic symmetry, which algebra is $\text{so}(3) \times \text{so}(3) \sim \text{so}(4)$ if to neglect exchange interaction. As is known, a nonrelativistic hydrogen-like atom possesses such a symmetry. Hence, we have proved that to calculate quasiparticle states in non-relativistic case it is possible to use a basis set of states of a nonrelativistic hydrogen-like atom.

However, for a heavy electron $\Delta M_n(0) \geq 1$ according to the formula (59) we always have

$$a_n = -\Delta M_n(0)/2 \quad (62)$$

and, hence, there is no an equation such as the Schrödinger one for its description. From here we conclude that the heavy electron can not be examined in nonrelativistic limit.

**Relativistic case**

Let us generalize the proposed approach to relativistic case. To do it we substitute Eqs. (57) and (62) into (54) and let $n$ tends to $n \to \infty$:

$$\hat{h}^{HF}(r_1)\psi_n(k_1r_1) = \left(\frac{\Delta M_n(0)}{2} + \tilde{\epsilon}_n(k_1)\right)\psi_n(k_1r_1), \quad n \to \infty. \quad (63)$$

Then, one can assume that the operator $\frac{\partial}{\partial t} - \hat{h}^{HF}$ in Eq. (63) is a quasirelativistic hamiltonian written in the implicit form in the Hartee - Fock approximation.

From consideration carried out above it follows that the desired relativistic equation of motion should describe a charged composite system from a pair of particles and have
the dynamic symmetry $SO(4)$. A spin of a given quantum system should be equal 1 as motion of a hole is a motion of an electron in many-particle positively charged matrix. In [14] the equation of motion of a relativistic charged vector boson has been found and it was shown, that it describes a relativistic hydrogen-like atom. The relativistic charged vector-boson appears as a composite system with a corresponding spectrum of masses and in quasirelativistic limit $n \to \infty$ its energy $E_1$ is determined by the expression:

$$E_1 \approx \frac{m}{2} - \frac{m\gamma^2}{2n^2} - \frac{m\gamma^4}{8n^3} \left( \frac{4}{|k|} - \frac{3}{n} \right) - \frac{m\gamma^6}{8n^4} \left( \frac{3}{n^2} - \frac{8}{n|k|} + \frac{4}{k^2} \right) + O(\gamma^8).$$

(64)

Here $k$ is a quantum number of relativistic angular momentum: $k = -l, l+1, l$ is a quantum number of orbital moment. Comparison of right-hand sides of formulas (63) and (64) yields that $\Delta M_{\infty} \equiv \lim_{n \to \infty} \Delta M_n(0) = m$ is a rest mass $m$ of an electron. Hence, Eq. (63) is an equation of motion for a relativistic electron - hole pair with a reduced mass $\Delta M_{\infty}/2 = m/2$ which, apparently, is a relativistic charged vector-boson considered in quasirelativistic limit $n \to \infty$.

6 Conclusion

The method of Hartree - Fock self-consistent field in non-relativistic case or of Dirac - Fock self-consistent field in relativistic case is applicable for description of valent electron and polarization of atomic core only within the framework of the perturbation theory with the pseudopotential method as a zero-order approximation. To describe effects of polarization of electron density distribution in the case of intensive electromagnetic interactions with a atomic core it is necessary to take into account correlation interaction which is neglected in the above mentioned method. The method offered in this paper allows to describe effects of polarization not only for a atomic core in a field of valent electron, but also polarization of atom as the whole in the electron-hole formalism.

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