GENERAL QUESTIONS OF THERMODYNAMICS, STATISTICAL PHYSICS, AND QUANTUM MECHANICS

DYNAMICS OF BOUND STATES OF PARTICLES IN THE SECONDARY QUANTIZATION METHOD

S.V. PELETMINSKII, YU.V. SLYUSARENKO

National Science Center "Kharkiv Institute of Physics and Technology"
(1, Akademichna Str., Kharkiv 61108, Ukraine; e-mail: slusarenko@kipt.kharkov.ua)

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This paper is dedicated to Victor G. Bar'yakhtar on the occasion of his 75 birthday

We develop an approximate secondary quantization method for describing the many-particle systems in the presence of bound states of particles at low energies [1] (the kinetic energy of particles is small in comparison to the binding energy of compound particles). In this approximation, the compound particles are considered on an equal basis with elementary particles that means that the creation and annihilation operators of compound particles can be introduced. The Hamiltonians, which specify the interactions between compound and elementary particles and between compound particles themselves, are found in terms of the interaction amplitudes for elementary particles.

1. Introduction

The goal of this paper was to develop a microscopic approach for describing the physical processes in many-particle systems in the presence of bound states of particles. To achieve this goal, we developed a secondary quantization method for systems containing the bound states of particles.

The basic results obtained in this paper are the following:

1. The Fock space is introduced in the secondary quantization formalism. In this space, the creation and annihilation operators of elementary particles $\hat{\chi}^+$, $\hat{\chi}$ and their bound states $\hat{\eta}^+$, $\hat{\eta}$ are introduced on an equal basis.
2. The operators of the basic physical quantities acting in this space including the Hamiltonians of interactions of elementary particles and their bound states are constructed.
3. It is shown that, in the approximation of a "small radius of interaction", the above-mentioned Hamiltonians transform into the well-known Hamiltonians for the Coulomb and dipole interactions between particles of various kinds.
4. The theory of the van der Waals forces that act between atoms is considered as the approbation of the developed formalism. The description of such effects within the usual formalism requires more considerable efforts associated with the introduction of interactions for the neutral currents of bound states with electromagnetic fields.

Especially, we would like to note a role of the obtained Hamiltonians which describe the interaction between quasineutral particles (the bound states of charged fermions) and an electromagnetic field, elementary particles and bound states, and bound states with one another. On the basis of these Hamiltonians, one can study such phenomena as the Bose-Einstein condensation in a gas of excited atoms, the interaction of condensates with an electromagnetic field in Bose and Fermi systems. These Hamiltonians can be also a foundation for developing the kinetic theory for the systems with bound states of particles.

Finally, we would like to stress that the developed method can be easily generalized to the case of bound states containing more than two particles. The

generalization of the offered method for describing the systems with bound states of bosons and also bosons with fermions taking into account spins of particles can be also performed without principal difficulties.

2. Fock Space $\tilde{H}$ for Systems with Bound States of Particles

Consider a system consisting of two kinds of fermions with masses m_1 and m_2. As was mentioned in the introduction, it is more visual in this case to show the recipe for the construction of the operators of physical quantities in the presence of bound states of particles within the secondary quantization method. For simplicity we do not take into account a spin variable, because its accounting is evident.

Let $\hat{\psi}_1(\mathbf{x})$, $\hat{\psi}_2(\mathbf{x})$ be the annihilation operators of two kinds of fermions at a point $\mathbf{x}$,

$$\hat{\psi}_1(\mathbf{x})|0\rangle = \hat{\psi}_2(\mathbf{x})|0\rangle = 0,$$

where $|0\rangle$ is the vacuum state vector. Then the state vectors

$$|\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{y}_1, \dots, \mathbf{y}_m\rangle =$$

$$= \hat{\psi}_1^+(\mathbf{x}_1) \dots \hat{\psi}_1^+(\mathbf{x}_n)\hat{\psi}_2^+(\mathbf{y}_1) \dots \hat{\psi}_2^+(\mathbf{y}_m)|0\rangle, \qquad (1)$$

$(n, m = 0, 1, 2, \dots)$ form a basis in the space of states H. In these states, the particles are at certain points $\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{y}_1, \dots, \mathbf{y}_m \in R$ of the coordinate space. The state vectors (1) satisfy the orthogonality and normalization relations and form the complete set of state vectors.

We assume that a particle of the first kind and a particle of the second kind can form a bound state specified by the wave function

$$\varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\delta(\mathbf{x} - \mathbf{X}), \quad \mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}, \qquad (2)$$

where $\mathbf{x}$ is the space coordinate and α are the quantum numbers of a bound state (atom) (we suppose that the particles of the same kind do not form the bound states). The corresponding state vector has the form

$$|\alpha, \mathbf{x}\rangle = \int d\mathbf{x}_1 \int d\mathbf{x}_2 \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\times$$

$$\times\delta(\mathbf{x} - \mathbf{X})\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2)|0\rangle.$$

For this reason, the operators

$$\hat{\varphi}_\alpha^+(\mathbf{x}) = \int d\mathbf{x}_1 \int d\mathbf{x}_2 \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\times$$

$$\times\delta(\mathbf{x} - \mathbf{X})\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2) \qquad (3)$$

are called as the creation operators of bound states (atoms), so that

$$\hat{\varphi}_\alpha^+(\mathbf{x})|0\rangle = |\alpha, \mathbf{x}\rangle, \qquad \hat{\varphi}_\alpha(\mathbf{x})|0\rangle = 0.$$

If the atom has a certain momentum, then its state vector is given by

$$|\alpha, \mathbf{p}\rangle = \frac{1}{\sqrt{\mathcal{V}}} \int d\mathbf{x}_1 \int d\mathbf{x}_2 \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\times$$

$$\times e^{i\mathbf{p}\mathbf{X}}\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2)|0\rangle,$$

where $\mathcal{V}$ is the system volume. The corresponding creation operator $\hat{\varphi}_\alpha^+(\mathbf{p})$ of an atom in a state with momentum $\mathbf{p}$ is defined by

$$|\alpha, \mathbf{p}\rangle = \hat{\varphi}_\alpha^+(\mathbf{p})|0\rangle,$$

$$\hat{\varphi}_\alpha^+(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{p}} \hat{\varphi}_\alpha^+(\mathbf{p})e^{-i\mathbf{p}\mathbf{x}}.$$

Taking into account that

$$\int d\mathbf{y}_1 \varphi_\alpha^*(\mathbf{y}_1 - \mathbf{y}_2)\varphi_\beta(\mathbf{y}_1 - \mathbf{y}_2) = \delta_{\alpha\beta}, \qquad (4)$$

it is easy to get the commutation relations

$$[\hat{\varphi}_\alpha(\mathbf{x}), \hat{\varphi}_{\alpha'}^+(\mathbf{x}')] = \delta_{\alpha\alpha'}\delta(\mathbf{x} - \mathbf{x}') + \hat{\chi}_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}'),$$

$$[\hat{\varphi}_\alpha(\mathbf{x}), \hat{\varphi}_{\alpha'}(\mathbf{x}')] = 0, \qquad (5)$$

where

$$\hat{\chi}_{\alpha\alpha'}(\mathbf{x}, \mathbf{x}') = \int d\mathbf{y} \int d\mathbf{y}' \varphi_\alpha^*(\mathbf{y})\varphi_{\alpha'}(\mathbf{y}')\times$$

$$\times\Big\{\hat{\psi}_1^+(\mathbf{x} + \frac{m_2}{M}\mathbf{y})\hat{\psi}_1(\mathbf{x}' + \frac{m_2}{M}\mathbf{y}')\times$$

$$\times\delta(\mathbf{y} - \mathbf{y}' - \frac{m_1}{M}(\mathbf{x} - \mathbf{x}')) +$$

$$+\hat{\psi}_2^+(\mathbf{x}' - \frac{m_1}{M}\mathbf{y}')\hat{\psi}_2(\mathbf{x} - \frac{m_1}{M}\mathbf{y})\times$$

$$\times\delta(\mathbf{y} - \mathbf{y}' + \frac{m_2}{M}(\mathbf{x} - \mathbf{x}'))\Big\}, \quad M = m_1 + m_2.$$

Moreover,

$$\hat{\chi}_{\alpha\alpha'}(\mathbf{x},\mathbf{x}')|0\rangle = 0.$$

The vectors

$$|\underbrace{\mathbf{x}_1,\ldots}_{n},\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l}\rangle \equiv$$

$$\equiv \prod_{i=1}^{n}\hat{\psi}_1^+(\mathbf{x}_i)\prod_{k=1}^{m}\hat{\psi}_2^+(\mathbf{y}_k)\prod_{j=1}^{l}\hat{\varphi}_{\alpha_j}^+(\mathbf{z}_j)|0\rangle \qquad (6)$$

have obvious physical meaning under the following conditions:

$$|\mathbf{x}_i-\mathbf{x}_j|\gtrsim a,\quad |\mathbf{y}_i-\mathbf{y}_j|\gtrsim a,\quad |\mathbf{z}_i-\mathbf{z}_j|\gtrsim a,$$

$$|\mathbf{x}_i-\mathbf{y}_j|\gtrsim a,\quad |\mathbf{x}_i-\mathbf{z}_j|\gtrsim a,\quad |\mathbf{y}_i-\mathbf{z}_j|\gtrsim a \qquad (7)$$

($\mathbf{x},\mathbf{y},\mathbf{z}\in R_a$, $a\gg r_0$, r_0 is the radius of the bound state; see the definition of a below). In this case, the elementary particles and their bound states are at certain space points.

Notice that the state vectors (6) do not form a basis in the Hilbert space H if conditions (7) are valid. However, their linear span, which is a totality of the following vectors

$$\sum_{n,m,l}\underbrace{\int d\mathbf{x}_1\ldots\int d\mathbf{y}_1\ldots\int d\mathbf{z}_1\ldots}_{R_a}C(\underbrace{\mathbf{x}_1,\ldots}_{n},$$

$$\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l})|\underbrace{\mathbf{x}_1,\ldots}_{n},\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l}\rangle, \qquad (8)$$

forms a subspace H_a of the space H. Let us show that the state vectors (6) (with conditions (7)) form an orthonormalized basis in the subspace H_a. To this end, we need to take into account that, while calculating the vacuum averages of the kind

$$\langle 0|\hat{\psi}_1(\mathbf{x}_1)\ldots\hat{\psi}_2(\mathbf{x}_2)\ldots\hat{\varphi}_\alpha(\mathbf{x})\times$$

$$\times\hat{\varphi}_{\alpha'}^+(\mathbf{x}')\ldots\hat{\psi}_2^+(\mathbf{x}_2')\ldots\hat{\psi}_1^+(\mathbf{x}_1')\ldots|0\rangle, \qquad (9)$$

we can use the Wick theorem with the contractions

$$\underset{a}{\hat{\psi}_i}(\mathbf{x})\underset{a}{\hat{\psi}_{i'}^+}(\mathbf{x}') = \langle 0|\hat{\psi}_i(\mathbf{x})\hat{\psi}_{i'}^+(\mathbf{x}')|0\rangle = \delta_{ii'}\delta(\mathbf{x}-\mathbf{x}'),$$

$$\underset{a}{\hat{\psi}_i}(\mathbf{x})\underset{a}{\hat{\psi}_{i'}}(\mathbf{x}') = 0 \qquad (10)$$

if we consider the operators $\hat{\psi}_1$, $\hat{\psi}_2$, and $\hat{\varphi}$ to be referred to the time moment $+0$ and the operators $\hat{\varphi}^+$, $\hat{\psi}_2^+$, $\hat{\psi}_1^+$ to the time moment -0. In addition, we should remember that the creation and annihilation operators $\hat{\varphi}_\alpha$, $\hat{\varphi}_{\alpha'}^+$ depend on $\hat{\psi}_i,\hat{\psi}_{i'}$ (see (3)). We also assume that the wave function of atom (2) differs from zero for $|\mathbf{x}_1-\mathbf{x}_2|<r_0$. Taking into account (3) and noting that, for $|\mathbf{x}_1'-\mathbf{x}_2'|>a$,

$$\underset{ab}{\hat{\varphi}_\alpha}(\mathbf{z})\underset{b}{\hat{\psi}_2^+}(\mathbf{x}_2')\underset{a}{\hat{\psi}_1^+}(\mathbf{x}_1') = \int d\mathbf{z}_1\int d\mathbf{z}_2\varphi_\alpha^*(\mathbf{z}_1-\mathbf{z_2})\times$$

$$\times\delta(\mathbf{z}-\mathbf{Z})\underset{a}{\hat{\psi}_1}(\mathbf{z}_1)\underset{b}{\hat{\psi}_2}(\mathbf{z}_2)\underset{b}{\hat{\psi}_2^+}(\mathbf{x}_2')\underset{a}{\hat{\psi}_1^+}(\mathbf{x}_1') =$$

$$= \varphi_\alpha^*(\mathbf{x}_1'-\mathbf{x_2}')\delta(\mathbf{z}-\mathbf{X}') = 0,$$

$$\mathbf{X}' = \frac{m_1\mathbf{x}_1'+m_2\mathbf{x}_2'}{m_1+m_2}$$

and

$$\underset{ab}{\hat{\varphi}_\alpha}(\mathbf{z})\underset{ba}{\hat{\varphi}_{\alpha'}^+}(\mathbf{z}') = \int d\mathbf{z}_1\int d\mathbf{z}_2\int d\mathbf{z}_1'\int d\mathbf{z}_2'\varphi_\alpha^*(\mathbf{z}_1-\mathbf{z_2})\times$$

$$\times\delta(\mathbf{z}-\mathbf{Z})\varphi_{\alpha'}(\mathbf{z}_1'-\mathbf{z_2}')\delta(\mathbf{z}'-\mathbf{Z}')\times$$

$$\times\underset{a}{\hat{\psi}_1}(\mathbf{z}_1)\underset{b}{\hat{\psi}_2}(\mathbf{z}_2)\underset{b}{\hat{\psi}_2^+}(\mathbf{z}_2')\underset{a}{\hat{\psi}_1^+}(\mathbf{z}_1') =$$

$$= \int d\mathbf{z}_1\int d\mathbf{z}_2\varphi_\alpha^*(\mathbf{z}_1-\mathbf{z_2})\delta(\mathbf{z}-\mathbf{Z})\times$$

$$\times\varphi_{\alpha'}(\mathbf{z}_1-\mathbf{z}_2)\delta(\mathbf{z}'-\mathbf{Z}) = \delta_{\alpha\alpha'}\delta(\mathbf{z}-\mathbf{z}')$$

(double contractions correspond to the operators $\hat{\varphi}_\alpha$, $\hat{\varphi}_\alpha^+$), we get

$$\langle 0|\underbrace{\hat{\psi}_1(\mathbf{x}_1)\ldots}_{n}\underbrace{\hat{\psi}_2(\mathbf{y}_1)\ldots}_{m}\underbrace{\hat{\varphi}_{\alpha_1}(\mathbf{z}_1)\ldots}_{l}$$

$$\underbrace{\hat{\varphi}_{\alpha_1'}^+(\mathbf{z}_1')\ldots}_{l'}\underbrace{\hat{\psi}_2^+(\mathbf{y}_1')\ldots}_{m'}\underbrace{\hat{\psi}_1(\mathbf{x}_1')\ldots}_{n'}|0\rangle =$$

$$= \delta_{nn'}\delta_{mm'}\delta_{ll'}\sum\mathcal{P}_{x'}\mathcal{P}_{y'}\underbrace{\delta(\mathbf{x}_1-\mathbf{x}_1')\ldots}_{n}\times$$

$$\times\underbrace{\delta(\mathbf{y}-\mathbf{y}_1')\ldots}_{m}\underbrace{\delta(\mathbf{z}_1-\mathbf{z}_1')\delta_{\alpha_1\alpha_1'}\ldots}_{l}. \qquad (11)$$

This relation shows that vectors (8) form the orthonormalized basis in the subspace H_a if we consider the creation and annihilation operators $\hat{\varphi}_\alpha^+(\mathbf{z})$ and $\hat{\varphi}_\alpha(\mathbf{z})$ as Bose operators which commute with $\hat{\psi}_i(\mathbf{x})$, $\hat{\psi}_i^+(\mathbf{x})$. The quantity $\mathcal{P}_{x'}$ in (11) is equal to $+1$ if the number

of permutations of the arguments $\mathbf{x}'_1 \dots \mathbf{x}'_n$ is even and it is equal to -1 if the number of these permutations is odd. The quantity $\mathcal{P}_{y'}$ is defined similarly.

With the use of (11), it is easy to find the projection operator $\mathcal{P}_{H_a}$ onto the subspace H_a:

$$\mathcal{P}_{H_a} = \sum_{k+m+l\le n} \frac{1}{k!}\frac{1}{m!}\frac{1}{l!} \underbrace{\int d\mathbf{x}_1 \dots \int d\mathbf{y}_1 \dots \int d\mathbf{z}_1 \dots}_{R_a} \times$$

$$\times |\underbrace{\mathbf{x}_1 \dots}_{k}\underbrace{\mathbf{y}_1 \dots}_{m}\underbrace{\mathbf{z}_1 \dots}_{l}\rangle\langle\underbrace{\mathbf{x}_1 \dots}_{k}\underbrace{\mathbf{y}_1 \dots}_{m}\underbrace{\mathbf{z}_1 \dots}_{l}|.$$

This operator is such that the operators $\underline{A}$ acting in the subspace $H_a \in H$ correspond to the operators of physical quantities A acting in H (hereinafter, the sums of $1, 2, \dots n$-particle subspaces over the bound states are considered; $n \approx a/r_0 \gg 1$), and

$$\underline{A} = \mathcal{P}_{H_a} A \mathcal{P}_{H_a}. \tag{12}$$

Let us introduce now an auxiliary space $\tilde{H}$ with Fermi creation and annihilation operators $\hat{\chi}_1^+(\mathbf{x}), \hat{\chi}_2^+(\mathbf{x})$, $\hat{\chi}_1(\mathbf{x}), \hat{\chi}_2(\mathbf{x})$ and Bose creation and annihilation operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ and let us take the vectors

$$|\mathbf{x}_1, \dots, \mathbf{y}_1, \dots, \mathbf{z}_1, \dots) =$$

$$= \hat{\chi}_1^+(\mathbf{x}_1) \dots \hat{\chi}_2^+(\mathbf{y}_1) \dots \hat{\eta}_\alpha^+(\mathbf{z}_1) \dots |0)$$

as a basis of this space, where $|0)$ is the vacuum vector in $\tilde{H}$. Then the linear span of the vectors

$$|\mathbf{x}_1, \dots, \mathbf{y}_1, \dots, \mathbf{z}_1, \dots) \in \tilde{H}_a, \quad \mathbf{x}, \mathbf{y}, \mathbf{z} \in R_a \tag{13}$$

determines the subspace $\tilde{H}_a$ of the space $\tilde{H}$.

Now we can easily establish the isomorphic correspondence between H_a and $\tilde{H}_a$,

$$|\mathbf{x}_1, \dots, \mathbf{y}_1, \dots, \mathbf{z}_1, \dots\rangle \iff$$

$$\iff |\mathbf{x}_1, \dots, \mathbf{y}_1, \dots, \mathbf{z}_1, \dots), \tag{14}$$

which preserves the scalar product

$$\langle \mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots \rangle =$$

$$= (\mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots),$$

$$\mathbf{x}, \mathbf{y}, \mathbf{z} \in R_a, \quad \mathbf{x}', \mathbf{y}', \mathbf{z}' \in R_a. \tag{15}$$

We can also establish the isomorphism between the operators $\underline{A} \iff \tilde{A}$ acting in the spaces H_a and $\tilde{H}_a$ according to the formula:

$$\langle \mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | \underline{A} | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots \rangle =$$

$$= (\mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | \tilde{A} | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots),$$

$$\mathbf{x}, \mathbf{y}, \mathbf{z} \in R_a, \quad \mathbf{x}', \mathbf{y}', \mathbf{z}' \in R_a. \tag{16}$$

This isomorphic correspondence is remained after the multiplication of an operator by a number, after the addition of operators, and after the multiplication of operators:

$$\lambda \underline{A} \iff \lambda \tilde{A}, \quad \underline{A} + \underline{B} \iff \tilde{A} + \tilde{B},$$

$$\underline{A}\,\underline{B} \iff \tilde{A}\tilde{B}. \tag{17}$$

Formulas (12),(16) lead to

$$(\mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | \tilde{A} | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots) =$$

$$= \langle \mathbf{x}', \dots, \mathbf{y}', \dots, \mathbf{z}', \dots | A | \mathbf{x}, \dots, \mathbf{y}, \dots, \mathbf{z} \dots \rangle,$$

$$\mathbf{x}, \mathbf{y}, \mathbf{z} \in R_a, \quad \mathbf{x}', \mathbf{y}', \mathbf{z}' \in R_a. \tag{18}$$

This relation determines the operators of various physical quantities $\tilde{A}$ acting in $\tilde{H}_a$ and, hence, transfers the quantum theory, in which the compound particles (bound states) and elementary particles exist on an equal basis from the space of states H into the space of states $\tilde{H}_a$. We would like to recall here that $\hat{\varphi}_\alpha^+$ entering (6) is determined by (3).

Relation (18) determines the operator $\tilde{A}$ uniquely in $\tilde{H}_a$, but it does not determine it uniquely in $\tilde{H}$. It is evident that the operator $\tilde{A}$ acting in $\tilde{H}$ (continued from $\tilde{H}_a$ to the whole space $\tilde{H}$) is determined up to the term $\tilde{A}'$, the matrix elements of which are zero in the space $\tilde{H}_a$ ($\tilde{A} = \tilde{A}' + \tilde{A}''$). If we introduce the projection operator $\mathcal{P}_{\tilde{H}_a}$ onto the subspace $\tilde{H}_a$ and require that the operator $\tilde{A}$ have no nonzero matrix elements in the orthogonal subspace, then the operator $\tilde{A}$ will be determined uniquely in $\tilde{H}$, and $\tilde{A} = \mathcal{P}_{\tilde{H}_a} \tilde{A}'' \mathcal{P}_{\tilde{H}_a}$. When constructing the operator $\tilde{A}$ acting in $\tilde{H}$, we will omit the projection operator $\mathcal{P}_{\tilde{H}_a}$. The reason for this is the assumption that the matrix elements of operators (in the position space), corresponding to a quite large external parameter $R \sim |\mathbf{x}_i - \mathbf{x}_j|$, give a dominant contribution to quantum-mechanical processes. Further, we consider that $R \gg r_0$ (usually in the case of collisions between particles, $R^{-1} \sim \sqrt{m\mathcal{E}}$, where $\mathcal{E}$ is the particle

kinetic energy). The above inequality makes it possible to choose the parameter a (see (7)) as follows [1]:

$$R \gg a \gg r_0. \tag{19}$$

The operators' matrix elements shouldn't depend on the parameter a chosen in such a way. We will conceptually lower the bound state's radius, $r_0 \to 0$. Then the whole scheme will not depend on the parameter a, as we have already remarked, up to the values of $a = r_0$. Therefore, owing to the inequality $R \gg a$, the subspace $\tilde{H}_a$ can be identified with the space $\tilde{H}$ $(a \to 0, a \gg r_0)$, i.e. $\mathcal{P}_{\tilde{H}_a} \to 1$ while $a \to 0$. At the same time, we haven't violated the quantum-mechanical description of the bound states due to the inequality $a \gg r_0$.

The matrix elements of operators should not depend on the parameter a chosen in this way. Let us mentally decrease the radius of a bound state, $r_0 \to 0$. Then the whole scheme, as we have already noted, will not depend on a up to the values $a = r_0$ and, hence, the subspace $\tilde{H}_a$ can be identified with $\tilde{H}$ due to the inequality $R \gg a$. In other words one can considers that $\mathcal{P}_{\tilde{H}_a} \to 1$ for $a \to 0$. At the same time, we do not break the quantum-mechanical description of bound states by virtue of the inequality $a \gg r_0$. From the physical point of view, the inequality $r_0 \ll R$ gives a stability domain for bound states considered as elementary particles. The calculation of the following approximation is to be associated with regard for a difference of the subspace H_a from the space H.

Finally, we note that, for an arbitrary vector $|\ ) \in \tilde{H}_a$, the following evident relations are true:

$$\hat{\zeta}(\mathbf{x})\hat{\xi}(\mathbf{x}')|\ ) = 0, \quad (\ |\hat{\zeta}^+(\mathbf{x})\hat{\xi}^+(\mathbf{x}') = 0,$$

$$|\mathbf{x} - \mathbf{x}'| < a, \tag{20}$$

or

$$\hat{\zeta}(\mathbf{x})\hat{\xi}(\mathbf{x}')\tilde{H}_a = 0, \quad \tilde{H}_a\hat{\zeta}^+(\mathbf{x})\hat{\xi}^+(\mathbf{x}') = 0,$$

$$|\mathbf{x} - \mathbf{x}'| < a,$$

where $\hat{\zeta}$ and $\hat{\xi}$ are any of the annihilation operators $\hat{\chi}_1, \hat{\chi}_2, and \hat{\eta}$.

3. Operators of Physical Quantities in Space $\tilde{H}$

Here, we consider a method for obtaining the operators $\tilde{\hat{A}}$. Let operator $\hat{A}$ represent the normal-ordered product of the operators $\hat{\psi}_i(\mathbf{v})$, $\hat{\psi}_i^+(\mathbf{u})$, $(i = 1, 2)$:

$$\hat{A}(\mathbf{u}, \mathbf{v}) = \hat{\psi}_1^+(\mathbf{u}_1)\ldots\hat{\psi}_2^+(\mathbf{u}_2)\hat{\psi}_1(\mathbf{v}_1)\ldots\hat{\psi}_2(\mathbf{v}_2)\ldots \tag{21}$$

The operators of such a type are the particle density operator $\hat{\rho}_i(\mathbf{x})$,

$$\hat{\rho}_i(\mathbf{x}) = \hat{\psi}_i^+(\mathbf{x})\hat{\psi}_i(\mathbf{x})$$

the momentum density operator $\hat{\pi}_i(\mathbf{x})$,

$$\pi_i(\mathbf{x}) = -\frac{i}{2}\left(\hat{\psi}_i^+(\mathbf{x})\frac{\partial}{\partial\mathbf{x}}\hat{\psi}_i(\mathbf{x}) - \frac{\partial}{\partial\mathbf{x}}\hat{\psi}_i^+(\mathbf{x})\hat{\psi}_i(\mathbf{x})\right),$$

the Hamiltonian of a system, etc.

The matrix element on the right-hand side of (18) may be written as the following vacuum average:

$$\langle 0|\hat{\psi}_1(\mathbf{x}_1)\ldots\hat{\psi}_2(\mathbf{x}_2)\ldots\hat{\varphi}_\alpha(\mathbf{x})\ldots\hat{A}(\mathbf{u}, \mathbf{v})\times$$

$$\times\hat{\varphi}_{\alpha'}^+(\mathbf{x})\ldots\hat{\psi}_2(\mathbf{x}_2')\ldots\hat{\psi}_1(\mathbf{x}_1')\ldots|0\rangle. \tag{22}$$

Let us note that, while calculating this average by using the Wick theorem, the quantity which is averaged over the vacuum state has the meaning of a mixed T-product if one considers the operators $\hat{\psi}_1, \ldots, \hat{\psi}_2, \ldots, \hat{\varphi}\ldots$ to be referred to the time moment $+0$, operators $\hat{\psi}_1^+, \ldots, \hat{\psi}_2^+, \ldots, \hat{\varphi}^+\ldots$ to -0, and the normal-ordered operator $\hat{A}(\mathbf{u}, \mathbf{v})$ to the time moment 0. Thus, there is no need to place the contractions inside the expression for $\hat{A}(\mathbf{u}, \mathbf{v})$. Let

$$A_b(\mathbf{y}_1, \ldots, \mathbf{y}_2, \ldots, \mathbf{y}, \ldots;$$

$$\mathbf{y}_1', \ldots, \mathbf{y}_2', \ldots, \mathbf{y}', \ldots; \mathbf{u}, \mathbf{v}) \equiv A_b(\mathbf{y}; \mathbf{y}'; \mathbf{u}, \mathbf{v}) \tag{23}$$

be the analytic expression that corresponds to the diagram "b", for which the operators with arguments $\mathbf{u}$ are related to the operators with arguments $\mathbf{y}_1, \ldots, \mathbf{y}_2, \ldots, \mathbf{y}, \ldots$. The latter arguments are spaced apart by the distances greater than a and coincide with some of arguments $\mathbf{x}_1, \ldots, \mathbf{x}_2, \ldots, \mathbf{x}, \ldots,$. The similar statement should be also made concerning the arguments $\mathbf{y}_1', \ldots, \mathbf{y}_2', \ldots, \mathbf{y}', \ldots$. Therefore, the operator $\tilde{\hat{A}}(\mathbf{u}, \mathbf{v})$ acting in $\tilde{H}$ is given, in according to (7), by

$$\tilde{\hat{A}}(\mathbf{u}, \mathbf{v}) = \sum_b \int \hat{R}_1\hat{R}_2\hat{R}A_b(\mathbf{y}; \mathbf{y}'; \mathbf{u}, \mathbf{v})\hat{R}_1'\hat{R}_2'\hat{R}', \tag{24}$$

[1] For the Coulomb interaction, the inequality $R \gg r_0$ is equivalent to $\mathcal{E} \ll \varepsilon_0$, because $r_0 = \frac{n^2\hbar^2}{me^2}$, $\varepsilon_0 = \frac{me^4}{2n^2\hbar^2}$, $n \sim 1$.

where

$$\hat{R}_1 = \prod \hat{\chi}^+(\mathbf{y}_1)d\mathbf{y}_1, \quad \hat{R}_2 = \prod \hat{\chi}^+(\mathbf{y}_2)d\mathbf{y}_2,$$

$$\hat{R} = \prod \hat{\eta}^+(\mathbf{y})d\mathbf{y}, \quad \hat{R}'_1 = \prod \hat{\chi}(\mathbf{y}'_1)d\mathbf{y}'_1,$$

$$\hat{R}'_2 = \prod \hat{\chi}(\mathbf{y}'_2)d\mathbf{y}'_2, \quad \hat{R}' = \prod \hat{\eta}(\mathbf{y}')d\mathbf{y}'$$

and the summation is taken over all diagrams of the described type.

If $\hat{A}(\mathbf{v}) = 1$ (see proof of (11)), then $\tilde{\hat{A}}(\mathbf{v}) = 1$ on the subspace $\tilde{H}_a$. Let now $\hat{A}(\mathbf{u}, \mathbf{v}) = \hat{\psi}_1(\mathbf{v})$. Then the only diagrams of the described type for the vacuum average $\langle 0|\dots\hat{\psi}_1(\mathbf{v})\dots|0\rangle$ will be the diagrams

$$A_{b_1} = \underset{a}{\hat{\psi}}(\mathbf{v})\dots\underset{a}{\hat{\psi}^+_1}(\mathbf{y}'),$$

$$A_{b_2} = \underset{a}{\hat{\psi}_2}(\mathbf{y}_2)\dots\underset{b}{\hat{\psi}_1}(\mathbf{v})\dots\underset{ba}{\hat{\varphi}^+_\alpha}(\mathbf{y}'). \tag{25}$$

The expressions

$$A_{b_1}(\mathbf{y}'_1; \mathbf{v}) = \delta(\mathbf{v} - \mathbf{y}'_1),$$

$$A_{b_2}(\mathbf{y}_2; \mathbf{y}', \mathbf{v}) = \int d\mathbf{x}_1 \int d\mathbf{x}_2 \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)$$

$$\times\delta(\mathbf{X} - \mathbf{y}')\delta(\mathbf{v} - \mathbf{x}_1)\delta(\mathbf{x}_2 - \mathbf{y}_2) = \varphi_\alpha(\mathbf{v}, \mathbf{y}_2, \mathbf{y}')$$

correspond to these diagrams. Here, $\varphi_\alpha(\mathbf{v}, \mathbf{y}_2, \mathbf{y}')$ is defined in accordance with (2). Therefore, according to (24), we have

$$\tilde{\hat{\psi}}_1(\mathbf{v}) = \int d\mathbf{y}'_1 A_{b_1}(\mathbf{y}'_1, \mathbf{v})\hat{\chi}_1(\mathbf{y}'_1) +$$

$$+ \int d\mathbf{y}_2 \int d\mathbf{y}' A_{b_2}(\mathbf{y}_2; \mathbf{y}', \mathbf{v})\hat{\chi}^+_2(\mathbf{y}_2)\hat{\eta}(\mathbf{y}')$$

or

$$\tilde{\hat{\psi}}_1(\mathbf{v}) = \hat{\chi}_1(\mathbf{v}) + \hat{O}_1(\mathbf{v}), \tag{26}$$

where

$$\hat{O}_1(\mathbf{v}) = \int d\mathbf{y}\hat{\varphi}(\mathbf{v}, \mathbf{y})\hat{\chi}^+_2(\mathbf{y}),$$

$$\hat{\varphi}(\mathbf{x}_1, \mathbf{x}_2) = \varphi_\alpha(\mathbf{x})\hat{\eta}_\alpha(\mathbf{X}), \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2,$$

$$\mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}. \tag{27}$$

Similarly, we obtain

$$\tilde{\hat{\psi}}_2(\mathbf{v}) = \hat{\chi}_2(\mathbf{v}) + \hat{O}_2(\mathbf{v}), \tag{28}$$

where

$$\hat{O}_2(\mathbf{v}) = -\int d\mathbf{y}\hat{\chi}^+_1(\mathbf{y})\hat{\varphi}(\mathbf{y}, \mathbf{v}).$$

Deriving (27) and (28), we essentially used inequalities (7).

Now let us consider $\hat{A}(\mathbf{u}, \mathbf{v}) = \hat{\psi}^+_1(\mathbf{u})\hat{\psi}_1(\mathbf{v})$. In this case, the following five diagrams

$$A_1 = \underset{a}{\hat{\psi}}\dots\underset{a}{\mathbf{u}_1}\underset{b}{\mathbf{v}_1}\dots\underset{b}{\hat{\psi}^+},$$

$$A_2 = \underset{a}{\hat{\psi}}\dots\underset{b}{\hat{\psi}}\dots\underset{b}{\mathbf{u}_1}\underset{c}{\mathbf{v}_1}\dots\underset{ca}{\hat{\varphi}^+},$$

$$A_3 = \underset{ab}{\hat{\varphi}}\dots\underset{b}{\mathbf{u}_1}\underset{c}{\mathbf{v}_1}\dots\underset{c}{\hat{\psi}^+}\dots\underset{a}{\hat{\psi}^+},$$

$$A_4 = \underset{ab}{\hat{\varphi}}\dots\underset{b}{\mathbf{u}_1}\underset{c}{\mathbf{v}_1}\dots\underset{ca}{\hat{\varphi}^+},$$

$$A_5 = \underset{a}{\hat{\psi}}\dots\underset{bd}{\hat{\varphi}}\dots\underset{d}{\mathbf{u}_1}\underset{c}{\mathbf{v}_1}\dots\underset{ca}{\hat{\varphi}^+}\dots\underset{b}{\hat{\psi}^+}$$

correspond to this operator (indices 1 and 2 for $\hat{\psi}$ and $\hat{\psi}^+$ can be easy restored if we take into account (3) and the definition of contractions). The analytic expressions corresponding to these diagrams have the form

$$\tilde{\hat{A}}_1 = \hat{\chi}^+_1(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1),$$

$$\tilde{\hat{A}}_2 = \int d\mathbf{z}_1 \int d\mathbf{z}_2\hat{\varphi}(\mathbf{z}_1, \mathbf{z}_2)\delta(\mathbf{z}_1 - v_1)\hat{\chi}^+_1(\mathbf{u}_1)\hat{\chi}^+_2(\mathbf{z}_2) =$$

$$= \int d\mathbf{z}_2\hat{\varphi}(\mathbf{v}_1, \mathbf{z}_2)\hat{\chi}^+_1(\mathbf{u}_1)\hat{\chi}^+_2(\mathbf{z}_2),$$

$$\tilde{\hat{A}}_3 = \int d\mathbf{z}_1 \int d\mathbf{z}_2\hat{\varphi}^+(\mathbf{z}_1, \mathbf{z}_2)\delta(\mathbf{z}_1 - \mathbf{u}_1)\times$$

$$\times\hat{\chi}_2(\mathbf{z}_2)\hat{\chi}_1(\mathbf{v}_1) = \int d\mathbf{z}_2\hat{\varphi}^+(\mathbf{u}_1, \mathbf{z}_2)\hat{\chi}_2(\mathbf{z}_2)\hat{\chi}_1(\mathbf{v}_1),$$

$$\tilde{\hat{A}}_4 = \int d\mathbf{z}_1 \int d\mathbf{z}_2 \int d\mathbf{z}'_1 \int d\mathbf{z}'_2\hat{\varphi}^+(\mathbf{z}_1, \mathbf{z}_2)\times$$

$$\times\hat{\varphi}(\mathbf{z}'_1, \mathbf{z}'_2)\delta(\mathbf{z}_1 - \mathbf{u}_1)\delta(\mathbf{v}_1 - \mathbf{z}'_1)\delta(\mathbf{z}_2 - \mathbf{z}'_2) =$$

$$= \int d\mathbf{z}_2\hat{\varphi}^+(\mathbf{u}_1, \mathbf{z}_2)\hat{\varphi}(\mathbf{v}_1, \mathbf{z}_2),$$

$$\tilde{\hat{A}}_5 = \int d\mathbf{z}_1 \int d\mathbf{z}_2 \int d\mathbf{z}'_1 \int d\mathbf{z}'_2\hat{\varphi}^+(\mathbf{z}_1, \mathbf{z}_2)\times$$

$$\times\hat{\varphi}(\mathbf{z}'_1,\mathbf{z}'_2)\delta(\mathbf{z}_1-\mathbf{u}_1)\delta(\mathbf{v}_1-\mathbf{z}'_1)\hat{\chi}_2^+(\mathbf{z}'_2)\hat{\chi}_2(\mathbf{z}_2)=$$

$$=\int d\mathbf{z}_2\int d\mathbf{z}'_2\hat{\varphi}^+(\mathbf{u}_1,\mathbf{z}_2)\hat{\varphi}(\mathbf{v}_1,\mathbf{z}'_2)\hat{\chi}_2^+(\mathbf{z}'_2)\hat{\chi}_2(\mathbf{z}_2).$$

Whence, we find operators (24) corresponding to diagrams (23) as

$$\widetilde{\hat{A}}_1=\hat{\chi}_1^+(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1),\quad \widetilde{\hat{A}}_2=\hat{\chi}_1^+(\mathbf{u}_1)\hat{O}_1(\mathbf{v}_1),$$

$$\widetilde{\hat{A}}_3=\hat{O}_1^+(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1),\ \widetilde{\hat{A}}_4+\widetilde{\hat{A}}_5=\hat{O}_1^+(\mathbf{u}_1)\hat{O}_1(\mathbf{v}_1).$$

Deriving the latter expression we have taken into account the anticommutation relations for $\hat{\chi}$, $\hat{\chi}^+$. Hence, bearing in mind (27) and (28), we obtain the final expression for the operator $\tilde{\hat{A}}(\mathbf{u},\mathbf{v})=\hat{\psi}_1^+(\widetilde{\mathbf{u}_1)\hat{\psi}_1}(\mathbf{v}_1)$ that corresponds to $\hat{A}(\mathbf{u},\mathbf{v})=\hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1)$:

$$\hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1)\to\hat{\psi}_1^+(\widetilde{\mathbf{u}_1)\hat{\psi}_1}(\mathbf{v}_1)=$$

$$=\widetilde{\hat{\psi}}_1^+(\mathbf{u}_1)\widetilde{\hat{\psi}}_1(\mathbf{v}_1).\qquad(29)$$

Similarly, we get

$$\hat{\psi}_1(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1)\to\hat{\psi}_1(\widetilde{\mathbf{u}_1)\hat{\psi}_1}(\mathbf{v}_1)=\widetilde{\hat{\psi}}_1(\mathbf{u}_1)\widetilde{\hat{\psi}}_1(\mathbf{v}_1),$$

$$\hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_2(\mathbf{v}_1)\to\hat{\psi}_1^+(\widetilde{\mathbf{u}_1)\hat{\psi}_2}(\mathbf{v}_1)=$$

$$\widetilde{\hat{\psi}}_1^+(\mathbf{u}_1)\widetilde{\hat{\psi}}_2(\mathbf{v}_1),\quad\ldots\qquad(30)$$

In a general case, the following formula is true:

$$\hat{\psi}_{i_1}^+(\mathbf{u}_{i_1})\ldots\hat{\psi}_{i_n}^+(\mathbf{u}_{i_n})\hat{\psi}_{j_1}(\mathbf{v}_{j_1})\ldots\hat{\psi}_{j_m}(\mathbf{v}_{j_m})\to$$

$$\hat{\psi}_{i_1}^+(\mathbf{u}_{i_1})\widetilde{\ldots\hat{\psi}_{j_m}}(\mathbf{v}_{j_m})=\widetilde{\hat{\psi}}_{i_1}^+(\mathbf{u}_1)\widetilde{\hat{\psi}}_{j_m}(\mathbf{v}_{j_m}).\qquad(31)$$

To explain this formula, we note that each of the operators $\hat{\psi}_j(\mathbf{v}_j)$ (or $\hat{\psi}_i^+(\mathbf{u}_i)$) entering $\hat{A}(\mathbf{u},\mathbf{v})$ (see (21)) is related to other operators $\hat{\psi}^+$ (or $\hat{\psi}$) which do not enter $\hat{A}(\mathbf{u},\mathbf{v})$ only by a unique way, which leads to binary relations (29), (30). Therefore, we come to (31) by sorting out all the operators $\hat{\psi}_i$, $\hat{\psi}_{i'}$ contained in $\hat{A}(\mathbf{u},\mathbf{v})$.

The operators $\hat{\psi}_i(\mathbf{x})$, $\hat{\psi}_j(\mathbf{x}')$ are anticommutative. For this reason, there is a question concerning the consistency of (30), (31). The anticommutativity of $\tilde{\hat{\psi}}_i(\mathbf{x})$, $\tilde{\hat{\psi}}_j(\mathbf{x}')$ (and also $\tilde{\hat{\psi}}_i^+(\mathbf{x})$, $\tilde{\hat{\psi}}_j^+(\mathbf{x}')$) represents the consistency condition,

$$\{\tilde{\hat{\psi}}_i(\mathbf{x}),\tilde{\hat{\psi}}_j(\mathbf{x}')\}=\{\tilde{\hat{\psi}}_i^+(\mathbf{x}),\tilde{\hat{\psi}}_j^+(\mathbf{x}')\}=0.$$

The validity of these formulas can be easily proved if we use definitions (27)—(28) for $\tilde{\hat{\psi}}$, $\tilde{\hat{\psi}}^+$ and the commutation relations for $\hat{\chi}$, $\hat{\chi}^+$ and $\hat{\eta}_\alpha$, $\hat{\eta}_\alpha^+$.

4. Operators of Particle Density and Momentum Density in Space $\tilde{H}$

In this section, we consider the operators of basic physical quantities. These operators act in the Hilbert space $\tilde{H}$. Let us start from the density operator for particles of the first kind. The corresponding operator acting in the original Hilbert space H is of the form

$$\hat{\rho}_1(\mathbf{x})=\hat{\psi}_1^+(\mathbf{x})\hat{\psi}_1(\mathbf{x}).\qquad(32)$$

Hence, in accordance with (30), we obtain

$$\widetilde{\hat{\rho}}_1(\mathbf{x})=\widetilde{\hat{\psi}}_1^+(\mathbf{x})\widetilde{\hat{\psi}}_1(\mathbf{x})=\hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x})+$$

$$+\hat{O}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x})+\hat{\chi}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x})+\hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x}).\qquad(33)$$

Note that the operators with zero matrix elements in the subspace $\tilde{H}_a$ occur on the right-hand side of (29), because the points $\mathbf{u}_1$ and $\mathbf{v}_1$ are close to each other. Since

$$\hat{O}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x})=\int d\mathbf{y}\hat{\phi}^+(\mathbf{x},\mathbf{y})\hat{\chi}_2(\mathbf{y})\hat{\chi}_1(\mathbf{x}),$$

$$\hat{\chi}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x})=\int d\mathbf{y}\hat{\chi}_1^+(\mathbf{x})\hat{\chi}_2^+(\mathbf{y})\hat{\phi}(\mathbf{x},\mathbf{y}),$$

and the operator $\hat{\varphi}(\mathbf{x},\mathbf{y})$ differs from zero only for $|\mathbf{x}-\mathbf{y}|\lesssim a$, these operators do not have the matrix elements in the subspace $\tilde{H}_a$ according to (20) and, therefore, can be omitted. Using the permutation relation $\{\hat{\chi}_2^+(\mathbf{z}_1),\hat{\chi}_2(\mathbf{z}_2)\}=\delta(\mathbf{z}_1-\mathbf{z}_2)$, we write the operator $\hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x})$ as

$$\hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x})=\int d\mathbf{z}_1\int d\mathbf{z}_2\hat{\varphi}^+(\mathbf{x},\mathbf{z}_2)\hat{\varphi}(\mathbf{x},\mathbf{z}_1)\times$$

$$\times\hat{\chi}_2^+(\mathbf{z}_1)\hat{\chi}_2(\mathbf{z}_2)+\int d\mathbf{z}\hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}).$$

The matrix element of the second term is zero in the subspace $\tilde{H}_a$, because $\mathbf{z}_1\approx\mathbf{z}_2\approx\mathbf{x}$ (see (20)). For this reason, this term can be omitted. Thus, with the use of the method that was described in the previous section, we have

$$\widetilde{\hat{\rho}}_1(\mathbf{x})=\hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x})+\int d\mathbf{z}\hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}).\qquad(34)$$

Similarly, if $\hat{\rho}_2(\mathbf{x}) = \hat{\psi}_2^+(\mathbf{x})\hat{\psi}_2(\mathbf{x})$ represents the density operator for particles of the second kind, then

$$\hat{\rho}_2(\mathbf{x}) \to \widetilde{\hat{\rho}}_2(\mathbf{x}),$$

where

$$\widetilde{\hat{\rho}}_2(\mathbf{x}) = \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) + \int d\mathbf{z}\hat{\varphi}^+(\mathbf{z},\mathbf{x})\hat{\varphi}(\mathbf{z},\mathbf{x}). \tag{35}$$

Bearing in mind (27) and the assumption about the "small radius" of a bound state, we get the formulas

$$\int d\mathbf{z}\hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}) \approx \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}),$$

$$\int d\mathbf{z}\hat{\varphi}^+(\mathbf{z},\mathbf{x})\hat{\varphi}(\mathbf{z},\mathbf{x}) \approx \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}),$$

which allow us to obtain the density operators for particles of the first and second kinds

$$\widetilde{\hat{\rho}}_1(\mathbf{x}) = \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}),$$

$$\widetilde{\hat{\rho}}_2(\mathbf{x}) = \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) + \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}). \tag{36}$$

Thus, the operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ can be interpreted as the creation and annihilation operators of bound states with quantum numbers α at the point $\mathbf{x}$, and $\hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x})$ as the density operator of bound states. Formula (36) has a simple physical meaning: the density of particles of the first kind is equal to the sum of densities of free particles of the same kind and bound states (each bound state contains one particle of the first kind).

Consider the state vector $\Phi(\mathbf{X}) = \hat{\eta}_\alpha^+(\mathbf{X})|0\rangle$, which specifies a compound particle at the point $\mathbf{X}$ (this state vector corresponds to the continuous spectrum). Then, in accordance with (36), we have

$$(\Phi(\mathbf{X}), \hat{\rho}_1(\mathbf{x}_1)\Phi(\mathbf{X}')) =$$

$$= \delta(\mathbf{X}-\mathbf{X}')\left(\frac{M}{m_2}\right)^3\left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X})\right)\right|^2.$$

For a wave packet

$$\Psi_{\mathbf{X_0}} = \int d\mathbf{X} f_{\mathbf{X_0}}(\mathbf{X})\Phi(\mathbf{X}),$$

$$\int d\mathbf{X}\left|f_{\mathbf{X_0}}(\mathbf{X})\right|^2 = 1,$$

the quantity

$$(\Psi_{\mathbf{X_0}}, \hat{\rho}_1(\mathbf{x}_1)\Psi_{\mathbf{X_0}}) =$$

$$= \int d\mathbf{X}\left|f_{\mathbf{X_0}}(\mathbf{X})\right|^2\left(\frac{M}{m_2}\right)^3\left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X})\right)\right|^2$$

should be treated as the probability density to find the first particle at the point $\mathbf{x}_1$ if the atom is in a state $\Psi_{\mathbf{X}_0}$. If the bound state is localized near a point $\mathbf{X}_0$ (i.e., $|f_{\mathbf{X}_0}(\mathbf{X})|^2 \to \delta(\mathbf{X}-\mathbf{X}_0)$), then

$$(\Psi_{\mathbf{X_0}}, \hat{\rho}_1(\mathbf{x}_1)\Psi_{\mathbf{X_0}}) \to \left(\frac{M}{m_2}\right)^3\left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X}_0)\right)\right|^2.$$

Since $\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X}_0) = \mathbf{x} = \mathbf{x}_1-\mathbf{x}_2$, we come, as it should be, to the probability distribution for the space coordinate of the first particle in an atom, which is at the point $\mathbf{X}_0$.

Let us find now the momentum density operator in the space $\tilde{H}$. The momentum density operator $\hat{\boldsymbol{\pi}}_1(\mathbf{x})$ for particles of the first kind is defined in the original Hilbert space as

$$\hat{\boldsymbol{\pi}}_1(\mathbf{x}) = -\frac{i}{2}\left(\hat{\psi}_1^+(\mathbf{x})\frac{\partial\hat{\psi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\psi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\psi}_1(\mathbf{x})\right). \tag{37}$$

Then, according to (30),

$$\hat{\boldsymbol{\pi}}_1(\mathbf{x}) \to \widetilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) =$$

$$= -\frac{i}{2}\left(\widetilde{\hat{\psi}}_1^+(\mathbf{x})\frac{\partial\widetilde{\hat{\psi}}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\widetilde{\hat{\psi}}_1^+(\mathbf{x})}{\partial\mathbf{x}}\widetilde{\hat{\psi}}_1(\mathbf{x})\right). \tag{38}$$

Following the derivation of (34) and (35) for $\tilde{\hat{\rho}}_1(\mathbf{x})$ and $\tilde{\hat{\rho}}_2(\mathbf{x})$, we obtain

$$\widetilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) = -\frac{i}{2}\left(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\right) -$$

$$-\frac{i}{2}\int d\mathbf{y}\left(\hat{\varphi}^+(\mathbf{x},\mathbf{y})\frac{\partial\hat{\varphi}(\mathbf{x},\mathbf{y})}{\partial\mathbf{x}} - \frac{\partial\hat{\varphi}^+(\mathbf{x},\mathbf{y})}{\partial\mathbf{x}}\hat{\varphi}(\mathbf{x},\mathbf{y})\right). \tag{39}$$

Analogously,

$$\widetilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}) = -\frac{i}{2}\left(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\right) -$$

$$-\frac{i}{2}\int d\mathbf{y}\left(\hat{\varphi}^+(\mathbf{y},\mathbf{x})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{x})}{\partial\mathbf{x}}\hat{\varphi}(\mathbf{y},\mathbf{x})\right). \tag{40}$$

It is convenient for our further consideration to rewrite (39), (40) in terms of the center-of-mass variables $\mathbf{y} = \mathbf{y}_1 - \mathbf{y}_2$ and $\mathbf{Y} = \frac{m_1\mathbf{y}_1 + m_2\mathbf{y}_2}{m_1+m_2}$:

$$\widetilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) = -i2\Big(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\Big) -$$

$$-\frac{i}{2}\int d\mathbf{y}\int d\mathbf{Y}\delta(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y})\times$$

$$\times\Big\{\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\hat{\varphi}(\mathbf{y},\mathbf{Y}) +$$

$$+\frac{m_1}{M}\Big(\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}}\hat{\varphi}(\mathbf{y},\mathbf{Y})\Big)\Big\},$$

$$\widetilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}) = -i2\Big(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\Big) -$$

$$-\frac{i}{2}\int d\mathbf{y}\int d\mathbf{Y}\delta(\mathbf{x}-\mathbf{Y}+\frac{m_1}{M}\mathbf{y})\times$$

$$\times\Big\{-\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}} + \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\hat{\varphi}(\mathbf{y},\mathbf{Y}) +$$

$$+\frac{m_2}{M}\Big(\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}} - -\frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}}\hat{\varphi}(\mathbf{y},\mathbf{Y})\Big)\Big\}, \tag{41}$$

where $\hat{\varphi}(\mathbf{y}_1,\mathbf{y}_2) \equiv \hat{\varphi}(\mathbf{y},\mathbf{Y})$. Note that, in terms of the same variables, the operators $\tilde{\hat{\rho}}_1(\mathbf{x})$ and $\tilde{\hat{\rho}}_2(\mathbf{x})$ have the form

$$\widetilde{\hat{\rho}}_1(\mathbf{x}) = \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) +$$

$$+\int d\mathbf{y}\int d\mathbf{Y}\delta(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y})\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\hat{\varphi}(\mathbf{y},\mathbf{Y}),$$

$$\widetilde{\hat{\rho}}_2(\mathbf{x}) = \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) +$$

$$+\int d\mathbf{y}\int d\mathbf{Y}\delta(\mathbf{x}-\mathbf{Y}+\frac{m_1}{M}\mathbf{y})\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\hat{\varphi}(\mathbf{y},\mathbf{Y}). \tag{42}$$

Formulas (41) and (42) can be explicitly expressed through the creation and annihilation operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ of atoms if we employ (26). Taking into account (41), it is easy to find the operator $\tilde{\hat{\boldsymbol{\pi}}} = \tilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) + \tilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x})$ of the total momentum density of the system in the approximation, in which the radius of a bound state is small,

$$\widetilde{\hat{\boldsymbol{\pi}}} = \widetilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) + \widetilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}) =$$

$$= -\frac{i}{2}\Big(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\Big) -$$

$$-\frac{i}{2}\Big(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\Big) -$$

$$-\frac{i}{2}\Big(\hat{\eta}_\alpha^+(\mathbf{x})\frac{\partial\hat{\eta}_\alpha(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\eta}_\alpha^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\eta}_\alpha(\mathbf{x})\Big). \tag{43}$$

The third term in this formula is in accordance with the interpretation of $\hat{\eta}_\alpha^+(\mathbf{x}), \hat{\eta}_\alpha(\mathbf{x})$ as the creation and annihilation operators of a bound state with quantum numbers α at the point $\mathbf{x}$.

5. Construction of Hamiltonians

Finally, let us consider a Hamiltonian in the space $\tilde{H}$. We suppose that this Hamiltonian has the standard form in the Hilbert space H and can be written as

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V}, \tag{44}$$

where $\hat{\mathcal{H}}_0$ and $\hat{V}$ are the operators of kinetic energy and potential energy given by

$$\hat{\mathcal{H}}_0 = \sum_{i=1}^{2}\frac{1}{2m_i}\int d\mathbf{x}\frac{\partial\hat{\psi}_i^+(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\hat{\psi}_i(\mathbf{x})}{\partial\mathbf{x}},$$

$$\hat{V} = \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\int d\mathbf{x}\int d\mathbf{x}'\nu_{ij}(\mathbf{x}-\mathbf{x}')\times$$

$$\times\hat{\psi}_i^+(\mathbf{x})\hat{\psi}_j^+(\mathbf{x}')\hat{\psi}_j(\mathbf{x}')\hat{\psi}_i(\mathbf{x}) \tag{45}$$

and $\nu_{ij}(\mathbf{x}-\mathbf{x}')$ is the potential energy of the interaction of particles of kinds i and j. After the similar calculations that lead us to the expressions for $\tilde{\hat{\rho}}$, $\tilde{\hat{\boldsymbol{\pi}}}$, we obtain

$$\hat{\mathcal{H}}_0 \to \widetilde{\hat{\mathcal{H}}}_0 = \sum_{i=1}^{2}\frac{1}{2m_i}\int d\mathbf{x}\frac{\partial\hat{\chi}_i^+(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\hat{\chi}_i(\mathbf{x})}{\partial\mathbf{x}} +$$

$$+\int d\mathbf{x}_1\int d\mathbf{x}_2\Big\{\frac{1}{2m_1}\frac{\partial\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)}{\partial\mathbf{x}_1}\frac{\partial\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)}{\partial\mathbf{x}_1} +$$

$$+\frac{1}{2m_2}\frac{\partial\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)}{\partial\mathbf{x}_2}\frac{\partial\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)}{\partial\mathbf{x}_2}\Big\}. \tag{46}$$

Next, by changing to the center-of-mass variables (see (2)) and noting that

$$\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2) = \varphi_\alpha(\mathbf{x})\hat{\eta}_\alpha(\mathbf{X}), \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2,$$

$$\mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1+m_2},$$

we get

$$\frac{\partial}{\partial \mathbf{x}_1}=\frac{\partial}{\partial \mathbf{x}}+\frac{m_1}{M}\frac{\partial}{\partial \mathbf{X}},\quad \frac{\partial}{\partial \mathbf{x}_2}=-\frac{\partial}{\partial \mathbf{x}}+\frac{m_2}{M}\frac{\partial}{\partial \mathbf{X}}.$$

We will bring the last term in (46) to the form

$$\frac{1}{2M}\int d\mathbf{X}\frac{\partial\hat{\eta}^+_\alpha(\mathbf{X})}{\partial \mathbf{X}}\frac{\partial\hat{\eta}_\alpha(\mathbf{X})}{\partial \mathbf{X}}-$$
$$-\frac{1}{2\mu}\int d\mathbf{x}\int d\mathbf{X}\hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\beta(\mathbf{X})\frac{\partial\varphi^*_\alpha(\mathbf{x})}{\partial \mathbf{x}}\frac{\partial\varphi_\beta(\mathbf{x})}{\partial \mathbf{x}},$$

where $\mu=m_1m_2/(m_1+m_2)$ is the reduced mass. Thus,

$$\widetilde{\hat{\mathcal{H}}}_0=\frac{1}{2m_1}\int d\mathbf{x}\frac{\partial\hat{\chi}^+_1(\mathbf{x})}{\partial \mathbf{x}}\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial \mathbf{x}}+$$
$$+\frac{1}{2m_2}\int d\mathbf{x}\frac{\partial\hat{\chi}^+_2(\mathbf{x})}{\partial \mathbf{x}}\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial \mathbf{x}}+$$
$$+\frac{1}{2M}\int d\mathbf{X}\frac{\partial\hat{\eta}^+_\alpha(\mathbf{X})}{\partial \mathbf{X}}\frac{\partial\hat{\eta}_\alpha(\mathbf{X})}{\partial \mathbf{X}}-$$
$$-\frac{1}{2\mu}\int d\mathbf{x}\int d\mathbf{X}\hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\beta(\mathbf{X})\frac{\partial\varphi^*_\alpha(\mathbf{x})}{\partial \mathbf{x}}\frac{\partial\varphi_\beta(\mathbf{x})}{\partial \mathbf{x}}. \qquad (47)$$

Let us now find $\tilde{\hat{V}}$ ($\hat{V}\to\tilde{\hat{V}}$). According to (30), we have

$$\widetilde{\hat{V}}=\frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\int d\mathbf{x}\int d\mathbf{x}'\nu_{ij}(\mathbf{x}-\mathbf{x}')\times$$
$$\times\widetilde{\hat{\psi}}^+_i(\mathbf{x})\widetilde{\hat{\psi}}^+_j(\mathbf{x}')\widetilde{\hat{\psi}}_j(\mathbf{x}')\widetilde{\hat{\psi}}_i(\mathbf{x}),$$

where $\tilde{\hat{\psi}}_i(\mathbf{x})=\hat{\chi}_i(\mathbf{x})+\hat{O}_i(\mathbf{x})$ (see (30)). Thus, $\tilde{\hat{V}}$ can be represented in the form

$$\widetilde{\hat{V}}=\widetilde{\hat{V}}_0+\widetilde{\hat{V}}_1+\widetilde{\hat{V}}_2+\widetilde{\hat{V}}_3+\widetilde{\hat{V}}_4,$$

where $\tilde{\hat{V}}_k$ ($k=0,\dots 4$) contains k multipliers of type $\hat{\chi}$ and $4-k$ multipliers of type $\hat{O}$. The operators $\hat{O}_i(\mathbf{x})$ have, according to (27) and (28), the form

$$\hat{O}_i(\mathbf{x})=\int d\mathbf{y}\hat{\varphi}_i(\mathbf{x},\mathbf{y})\hat{\chi}^+_{i'}(\mathbf{y}), \qquad (48)$$

where

$$\hat{\varphi}_1(\mathbf{x},\mathbf{y})=\hat{\varphi}(\mathbf{x},\mathbf{y}),\quad \hat{\varphi}_2(\mathbf{x},\mathbf{y})=\hat{\varphi}(\mathbf{y},\mathbf{x})$$

and the index i' is determined as follows: $1'=2, 2'=1$. Then the operator $\widetilde{\hat{V}}_0$ can be presented in the form

$$\widetilde{\hat{V}}_0=\frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\times$$
$$\times\int d\mathbf{y}_1\int d\mathbf{y}_2\int d\mathbf{y}_3\int d\mathbf{y}_4\hat{\varphi}^+_i(\mathbf{x}_1,\mathbf{y}_1)\times$$
$$\times\hat{\varphi}^+_j(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\times$$
$$\times\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}^+_{j'}(\mathbf{y}_3)\hat{\chi}^+_{i'}(\mathbf{y}_4). \qquad (49)$$

Note that the operators $\hat{\varphi}$ and $\hat{\varphi}^+$ in (49) are normally ordered, whereas $\hat{\chi}$ and $\hat{\chi}^+$ are not. Therefore, we order them by using the Wick theorem:

$$\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}^+_{j'}(\mathbf{y}_3)\hat{\chi}^+_{i'}(\mathbf{y}_4)=$$
$$=:\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}^+_{j'}(\mathbf{y}_3)\hat{\chi}^+_{i'}(\mathbf{y}_4):+$$
$$+:\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}^+_{j'}}}(\mathbf{y}_3)\hat{\chi}^+_{i'}(\mathbf{y}_4):+$$
$$+:\hat{\chi}_{i'}(\mathbf{y}_1)\overset{}{\underset{a}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\hat{\chi}^+_{j'}(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}^+_{i'}}}(\mathbf{y}_4):+$$
$$+:\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\overset{}{\underset{a}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}^+_{j'}}}(\mathbf{y}_3)\hat{\chi}^+_{i'}(\mathbf{y}_4):+$$
$$+:\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}^+_{j'}}}(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}^+_{i'}}}(\mathbf{y}_4):+$$
$$+:\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\overset{}{\underset{b}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}^+_{j'}}}(\mathbf{y}_3)\overset{}{\underset{b}{\hat{\chi}^+_{i'}}}(\mathbf{y}_4):+$$
$$+:\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\overset{}{\underset{b}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{b}{\hat{\chi}^+_{j'}}}(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}^+_{i'}}}(\mathbf{y}_4):. \qquad (50)$$

The operator $\hat{\varphi}(\mathbf{x},\mathbf{y})\equiv\varphi_\alpha(\mathbf{x}-\mathbf{y})\hat{\eta}_\alpha(\frac{m_1\mathbf{x}+m_2\mathbf{y}}{m_1+m_2})$ differs from zero only for $\mathbf{x}\approx\mathbf{y}$ ($|\mathbf{x}-\mathbf{y}|<a$). Thus, only those of φ_i, for which $|\mathbf{y}_1-\mathbf{y}_4|<a$ contribute to the integral over $\mathbf{y}$ in (49). This means that, by virtue of (20), the first term in (50) does not contribute to the matrix element of $\tilde{\hat{V}}_0$ taken between the states belonging to $\tilde{H}_a$, because $\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\hat{\chi}_i(\mathbf{y}_1)\Phi=0$. Similarly, one can prove that the terms which contain single contractions in (50) give no contribution to the matrix element of $\tilde{\hat{V}}_0$ taken between the states in $\tilde{H}_a$. The penultimate term in (50) containing the double contractions does not also contribute to the above-mentioned matrix element. Indeed, the penultimate term in (50) equals $\delta(\mathbf{y}_1-\mathbf{y}_3)\delta(\mathbf{y}_2-\mathbf{y}_4)$. In this case, the nonzero matrix element exists for $\mathbf{x}_1\approx\mathbf{x}_2$ and, in virtue of (20), $\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\Phi=0$. Thus, only the latter term in (50) equal to $\delta(\mathbf{y}_2-\mathbf{y}_3)\delta(\mathbf{y}_1-\mathbf{y}_4)$ can give a contribution

to the matrix element of $\tilde{\hat{V}}_0$. Therefore, not changing the matrix elements in $\tilde{H}_a$, the operator $\tilde{\hat{V}}_0$ can be represented in the form

$$\widetilde{\hat{V}}_0 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\int d\mathbf{y}_1\int d\mathbf{y}_2\times$$

$$\times\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\times$$

$$\times\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_1)$$

or, according to (48),

$$\widetilde{\hat{V}}_0 = \frac{1}{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\int d\mathbf{y}_1\int d\mathbf{y}_2\times$$

$$\times\hat{\varphi}^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{y}_1)\times$$

$$\times\Big\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+\nu_{22}(\mathbf{y}_1-\mathbf{y}_2)+$$

$$+\nu_{12}(\mathbf{x}_1-\mathbf{y}_2)+\nu_{21}(\mathbf{y}_1-\mathbf{x}_2)\Big\}. \qquad (51)$$

Similarly, noting that

$$\widetilde{\hat{V}}_1 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\times$$

$$\times\int d\mathbf{y}\Big\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y})\hat{\chi}_{i'}(\mathbf{y})\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+$$

$$+\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y})\hat{\chi}_i(\mathbf{x}_1)\hat{\chi}_{j'}^+(\mathbf{y})\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+h.c.\Big\},$$

$$\widetilde{\hat{V}}_3 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\times$$

$$\times\int d\mathbf{y}_1\int d\mathbf{y}_2\int d\mathbf{y}_3\Big\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\times$$

$$\times\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\hat{\chi}_i(\mathbf{x}_1)+$$

$$+\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_3)\times$$

$$\times\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_{i'}^+(\mathbf{y}_3)+h.c.\Big\}$$

and performing the same derivation as for obtaining $\tilde{\hat{V}}_0$, it is easy to verify (using the anticommutation relations for $\hat{\chi}$, $\hat{\chi}^+$ and (50)) that we can consider

$$\widetilde{\hat{V}}_1 = \widetilde{\hat{V}}_3 = 0 \qquad (52)$$

not changing the matrix elements of $\tilde{\hat{V}}_1$ and $\tilde{\hat{V}}_3$ in the subspace $\tilde{H}_a$. Next, it is evident that the following formula is valid:

$$\widetilde{\hat{V}}_4 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\times$$

$$\times\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1). \qquad (53)$$

Finally, we get

$$\widetilde{\hat{V}}_2 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\times$$

$$\times\Big\{\hat{O}_i^+(\mathbf{x}_1)\hat{O}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+$$

$$+\hat{O}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{O}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+h.c.+$$

$$+\hat{O}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{O}_i(\mathbf{x}_1)+$$

$$+\hat{\chi}_i^+(\mathbf{x}_1)\hat{O}_j^+(\mathbf{x}_2)\hat{O}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)\Big\}.$$

It can be easily seen that the first two terms and the corresponding Hermitian conjugate terms do not give a contribution to the matrix element of $\tilde{\hat{V}}_2$ in the subspace $\tilde{H}_a$. Therefore, we can consider

$$\widetilde{\hat{V}}_2 = \frac{1}{2}\sum_{i,j=1}^{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\int d\mathbf{y}_1\int d\mathbf{y}_2\times$$

$$\times\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\Big\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_2)\times$$

$$\times\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_{i'}^+(\mathbf{y}_2)+$$

$$+\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_1)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_2)\times$$

$$\times\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_{j'}(\mathbf{y}_1)\hat{\chi}_{j'}^+(\mathbf{y}_2)\hat{\chi}_i(\mathbf{x}_1)\Big\}.$$

The first and second terms in this expression give a contribution to the matrix element of $\tilde{\hat{V}}_2$ in $\tilde{H}_a$ under the arrangement of contractions

$$:\hat{\chi}_{\underset{a}{i'}}(\mathbf{y}_1)\hat{\chi}_{\underset{a}{j}}^+(\mathbf{x}_2)\hat{\chi}_{\underset{b}{j}}(\mathbf{x}_2)\hat{\chi}_{\underset{b}{i'}}^+(\mathbf{y}_2):+$$

$$+ : \underset{a}{\hat{\chi}_{i'}}(\mathbf{y}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\underset{a}{\hat{\chi}_{i'}^+}(\mathbf{y}_2) :=$$

$$= \delta_{ji'}\delta(\mathbf{y}_1-\mathbf{x}_2)\delta(\mathbf{y}_2-\mathbf{x}_2)+$$

$$+\delta(\mathbf{y}_1-\mathbf{y}_2)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2),$$

and the second term contributes under the following arrangement:

$$: \hat{\chi}_i^+(\mathbf{x}_1)\underset{a}{\hat{\chi}_{j'}}(\mathbf{y}_1)\underset{a}{\hat{\chi}_{j'}^+}(\mathbf{y}_2)\hat{\chi}_i(\mathbf{x}_1) :=$$

$$= \delta(\mathbf{y}_1-\mathbf{y}_2)\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_i(\mathbf{x}_1).$$

Thus, we have

$$\widetilde{\hat{V}}_2 = \int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)+$$

$$+\int d\mathbf{x}_1\int d\mathbf{x}_2\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\times$$

$$\times\Big\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)+$$

$$+\nu_{21}(\mathbf{x}_1-\mathbf{y}_2)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)+$$

$$+\nu_{22}(\mathbf{x}_1-\mathbf{y}_2)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)+$$

$$+\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)\Big\}. \tag{54}$$

The first term in this formula, being quadratic in the field operators, can be combined with the latter term in (47). As a result, we obtain

$$\int d\mathbf{x}_1\int d\mathbf{x}_2\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)-$$

$$-\frac{1}{2\mu}\int d\mathbf{x}\int d\mathbf{X}\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X})\frac{\partial\varphi_\alpha^*(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\varphi_\alpha(\mathbf{x})}{\partial\mathbf{x}} =$$

$$= \int d\mathbf{x}\int d\mathbf{X}\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\beta(\mathbf{X})\varphi_\alpha^*(\mathbf{x})\times$$

$$\times\Big\{-\frac{1}{2\mu}\Delta_{\mathbf{x}}+\nu_{12}(\mathbf{x})\Big\}\varphi_\beta(\mathbf{x}).$$

Since $\varphi_\beta(\mathbf{x})$ satisfies the Schrödinger equation

$$\Big\{-\frac{1}{2\mu}\Delta_{\mathbf{x}}+\nu_{12}(\mathbf{x})\Big\}\varphi_\beta(\mathbf{x}) = \varepsilon_\beta\varphi_\beta(\mathbf{x}),$$

where ε_β are atomic energy levels, the latter formula takes the form

$$\int d\mathbf{X}\sum_\alpha\varepsilon_\alpha\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X}).$$

Hence, in view of (46), (47), and (54), the Hamiltonian of the system $\tilde{\hat{\mathcal{H}}}$ takes the form

$$\widetilde{\hat{\mathcal{H}}} = \widetilde{\hat{\mathcal{H}}}_0+\widetilde{\mathcal{H}}_{int}^1+\widetilde{\mathcal{H}}_{int}^2+\widetilde{\mathcal{H}}_{int}^3,$$

where

$$\widetilde{\hat{\mathcal{H}}}_0 = \sum_{j=1}^2\frac{1}{2m_j}\int d\mathbf{x}\frac{\partial\hat{\chi}_j^+(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\hat{\chi}_j(\mathbf{x})}{\partial\mathbf{x}}+$$

$$+\sum_\alpha\int d\mathbf{X}\Big\{\frac{1}{2M}\frac{\partial\hat{\eta}_\alpha^+(\mathbf{X})}{\partial\mathbf{X}}\frac{\partial\hat{\eta}_\alpha(\mathbf{X})}{\partial\mathbf{X}}+E_\alpha\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X})\Big\} \tag{55}$$

is the Hamiltonian of free particles and bound states, and

$$\widetilde{\mathcal{H}}_{\rm int}^1 = \int d\mathbf{x}_1\int d\mathbf{x}_2\int d\mathbf{y}_2\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\times$$

$$\times\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\Big\{\Big(\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+$$

$$+\nu_{21}(\mathbf{x}_1-\mathbf{y}_2)\Big)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)\Big(\nu_{22}(\mathbf{x}_1-\mathbf{y}_2)+$$

$$+\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\Big)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)\Big\}, \tag{56}$$

$$\widetilde{\mathcal{H}}_{\rm int}^2 = \frac{1}{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\int d\mathbf{y}_1\int d\mathbf{y}_2\hat{\varphi}^+(\mathbf{x}_1,\mathbf{y}_1)\times$$

$$\times\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{y}_1)\times$$

$$\times\Big\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+\nu_{22}(\mathbf{y}_1-\mathbf{y}_2)+$$

$$+\nu_{12}(\mathbf{x}_1-\mathbf{y}_2)+\nu_{21}(\mathbf{y}_1-\mathbf{x}_2)\Big\}, \tag{57}$$

$$\widetilde{\mathcal{H}}_{\rm int}^3 = \frac{1}{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\Big\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)\times$$

$$\times\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1^+(\mathbf{x}_2)\hat{\chi}_1(\mathbf{x}_2)\hat{\chi}_1(\mathbf{x}_1)+$$

$$+\nu_{22}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2^+(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_1)+$$

$$+2\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)\hat{\chi}_2^+(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_2)\Big\} \quad (58)$$

are the interaction Hamiltonians. The Hamiltonian $\widetilde{\mathcal{H}}_{int}^1$ corresponds to scattering of particles of the first and second kinds by bound states; the Hamiltonian $\widetilde{\mathcal{H}}_{int}^2$ corresponds to the scattering of bound states by bound states; finally, the Hamiltonian $\widetilde{\mathcal{H}}_{int}^3$ corresponds to scattering of particles of the first and second kinds by particles of the same kinds. The interaction Hamiltonians (56) and (57) may be written through the creation $\hat{\eta}_\alpha^+(\mathbf{x})$ and annihilation $\hat{\eta}_\alpha(\mathbf{x})$ operators of atoms by using (26). We want to emphasize that the obtained interaction Hamiltonians do not lead to the decay and formation of compound particles, as it should be in the low-energy approximation. This reflects the fact that atoms are absolutely stable in the main approximation.

6. Van der Waals Forces

In this section, on the basis of the developed formalism, we investigate the forces acting between neutral atoms being in the ground state (van der Waals forces). To solve this problem, let us turn to the Schrödinger equation that determines the energy spectrum of the system,

$$\hat{\mathcal{H}}\Phi = E\Phi, \qquad \hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{V}}, \quad (59)$$

where the operators $\tilde{\hat{\mathcal{H}}}_0$ and $\tilde{\hat{V}} = \tilde{\hat{\mathcal{H}}}_{int}^1 + \tilde{\hat{\mathcal{H}}}_{int}^2 + \tilde{\hat{\mathcal{H}}}_{int}^3$ are defined by (55), (56)-(58). Since the studied system consists of two atoms, we should seek for a solution of (59) in the form

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}') = \sum_{\lambda\rho}\int d\mathbf{Y}\int d\mathbf{Y}' K_{\alpha\beta;\lambda\rho}(\mathbf{X},\mathbf{X}';\mathbf{Y},\mathbf{Y}')\times$$

$$\times\hat{\eta}_\lambda^+(\mathbf{Y})\hat{\eta}_\rho^+(\mathbf{Y}')\Phi_0. \quad (60)$$

The interaction Hamiltonian $\tilde{\hat{V}}$ is equal, in accordance with (56)—(58), to

$$\hat{V} = \frac{1}{2}\int d\mathbf{X}\int d\mathbf{Y}\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\beta^+(\mathbf{Y})\hat{\eta}_\gamma(\mathbf{Y})\hat{\eta}_\delta(\mathbf{X})\times$$

$$\times G_{\delta\gamma;\alpha\beta}(\mathbf{X}-\mathbf{Y}), \quad (61)$$

where

$$G_{\delta\gamma;\alpha\beta}(\mathbf{X}-\mathbf{Y}) = \int d\mathbf{x}\int d\mathbf{y}\varphi_\alpha^*(\mathbf{x})\varphi_\beta^*(\mathbf{y})\varphi_\gamma(\mathbf{y})\varphi_\delta(\mathbf{x})\times$$

$$\times\Big\{\nu_{12}(\mathbf{X}-\mathbf{Y}-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M})+$$

$$+\nu_{21}(\mathbf{X}-\mathbf{Y}+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M})+$$

$$+\nu_{11}(\mathbf{X}-\mathbf{Y}+\frac{m_2}{M}(\mathbf{x}-\mathbf{y}))+$$

$$+\nu_{22}(\mathbf{X}-\mathbf{Y}-\frac{m_1}{M}(\mathbf{x}-\mathbf{y}))\Big\}.$$

We suppose that the kinetic energy of atoms is small in comparison to the energy of levels $|\varepsilon_\alpha|$ ($\varepsilon_\alpha < 0$). In this case, according to (55), the operator $\tilde{\hat{\mathcal{H}}}_0$ can be represented in the form

$$\hat{\mathcal{H}}_0 = \sum_\alpha\int d\mathbf{X}\varepsilon_\alpha\hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X}). \quad (62)$$

It can be easily seen that

$$\hat{\mathcal{H}}_0\hat{\eta}_\lambda^+(\mathbf{Z})\hat{\eta}_\rho^+(\mathbf{Z}')\Phi_0 = (\varepsilon_\lambda+\varepsilon_\rho)\hat{\eta}_\lambda^+(\mathbf{Z})\hat{\eta}_\rho^+(\mathbf{Z}')\Phi_0,$$

$$\hat{V}\hat{\eta}_\lambda^+(\mathbf{Z})\hat{\eta}_\rho^+(\mathbf{Z}')\Phi_0 = \sum_{\alpha\beta}G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}')\hat{\eta}_\alpha^+(\mathbf{Z})\hat{\eta}_\beta^+(\mathbf{Z}')\Phi_0. \quad (63)$$

These formulas show that we can seek for a solution of (59) in the simpler, as compared to (60), form

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}') = \sum_{\lambda\rho}K_{\alpha\beta;\lambda\rho}(\mathbf{X},\mathbf{X}')\hat{\eta}_\lambda^+(\mathbf{X})\hat{\eta}_\rho^+(\mathbf{X}')\Phi_0,$$

so that the coordinates of atoms have definite values in the state $\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}')$. Upon substituting this expression into (59) and using (63), we obtain

$$K_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)+$$

$$+\sum_{\lambda\rho}K_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}') = E_{\alpha\beta}K_{\alpha\beta;\gamma\delta}. \quad (64)$$

A perturbative approach in conformity to this equation can be easily developed in the domain of great $|\mathbf{Z}-\mathbf{Z}'|$ when the quantity $G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')$ becomes small according to (61). Expanding $K_{\alpha\beta;\gamma\delta}$ in G,

$$K_{\alpha\beta;\gamma\delta} = K_{\alpha\beta;\gamma\delta}^1 + K_{\alpha\beta;\gamma\delta}^1 + K_{\alpha\beta;\gamma\delta}^2 + \dots,$$

$$E_{\alpha\beta} = E_{\alpha\beta}^0 + E_{\alpha\beta}^1 + E_{\alpha\beta}^2 + \dots,$$

we get, in the zeroth order,

$$K^0_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)=E^0_{\alpha\beta}K^0_{\alpha\beta;\gamma\delta},$$

whence

$$K^0_{\alpha\beta;\gamma\delta}=K^0_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\beta\delta},\qquad E^0_{\alpha\beta}=\varepsilon_\alpha+\varepsilon_\beta. \tag{65}$$

Taking into account this result, we have, in the first approximation,

$$K^1_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)+K^0_{\alpha\beta}G_{\alpha\beta;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')=$$

$$=(\varepsilon_\alpha+\varepsilon_\beta)K^1_{\alpha\beta;\gamma\delta}+E^1_{\alpha\beta}K^0_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\beta\delta}.$$

By setting here $\alpha=\gamma$, $\beta=\delta$, we get

$$E^1_{\alpha\beta}=G_{\alpha\beta;\alpha\beta}(\mathbf{Z}-\mathbf{Z}'), \tag{66}$$

and, for $\alpha,\beta\neq\gamma,\delta$,

$$K^1_{\alpha\beta;\gamma\delta}=K^0_{\alpha\beta}\frac{G_{\alpha\beta;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')}{(\varepsilon_\alpha+\varepsilon_\beta-\varepsilon_\gamma-\varepsilon_\delta)},\quad \alpha,\beta\neq\gamma,\delta \tag{67}$$

The second order of the perturbative approach gives

$$K^2_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)+\sum_{\lambda\rho}K^1_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')=$$

$$=(\varepsilon_\alpha+\varepsilon_\beta)K^2_{\alpha\beta;\gamma\delta}+E^1_{\alpha\beta}K^1_{\alpha\beta;\gamma\delta}+E^2_{\alpha\beta}K^0_{\alpha\beta;\gamma\delta}.$$

Taking here $\alpha=\gamma$, $\beta=\delta$, we obtain

$$\sum_{\lambda\rho}K^1_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}')=E^1_{\alpha\beta}K_{\alpha\beta;\alpha\beta}+K^0_{\alpha\beta}E^2_{\alpha\beta},$$

whence, according to (66), (67) we have

$$E^2_{\alpha\beta}=\sum_{\lambda\rho}{}'\frac{G_{\alpha\beta;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}')}{(\varepsilon_\alpha+\varepsilon_\beta-\varepsilon_\lambda-\varepsilon_\rho)}. \tag{68}$$

The prime above the sum means that the terms with $\lambda=\alpha$, $\rho=\beta$ are omitted. The state vector $\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}')$ in the main approximation of the perturbative approach is determined by

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}')=K^0_{\alpha\beta}\hat\eta^+_\alpha(\mathbf{X})\hat\eta^+_\beta(\mathbf{X}')\Phi_0+\ldots \tag{69}$$

(the constant $K^0_{\alpha\beta}$ may be found from the normalization relation $(\Phi_{\alpha\beta},\Phi_{\alpha\beta})=1$). Formulas (66) and (68) for $E^1_{\alpha\beta}$ and $E^2_{\alpha\beta}$ give us the corrections to the energy of levels $E^0_{\alpha\beta}=\varepsilon_\alpha+\varepsilon_\beta$. It follows from the obtained formulas that the energy of two atoms, being in the ground state α and spaced apart at sufficiently long distances, is defined by

$$E_{\alpha\alpha}=2\varepsilon_\alpha+G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')+$$

$$+\sum_{\lambda\rho}{}'\frac{G_{\alpha\alpha;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')G_{\lambda\rho;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')}{(2\varepsilon_\alpha-\varepsilon_\lambda-\varepsilon_\rho)}+\ldots \tag{70}$$

Let us prove now that $G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')\equiv 0$. In doing so, we use the formula [4]

$$\frac{1}{\sqrt{R^2-2R\rho x+\rho^2}}=\frac{1}{|\mathbf{R}-\boldsymbol{\rho}|}=$$
$$=\frac{1}{R}+\sum_{n=1}^{\infty}\left(\frac{\rho}{R}\right)^n\mathcal{P}_n(x),\quad x=\cos\vartheta,$$

where $x=\cos\vartheta$, ϑ is the angle between the vectors $\mathbf{R}$ and $\boldsymbol{\rho}$, and $\mathcal{P}_n(x)$ are the Legendre polynomials. Noting that (see (61))

$$G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')=\int d\mathbf{x}\int d\mathbf{y}\left|\varphi_\alpha(\mathbf{x})\right|^2\left|\varphi_\alpha(\mathbf{y})\right|^2\times$$
$$\times\Big\{\nu_{12}(\mathbf{Z}-\mathbf{z}'-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M})+$$
$$+\nu_{21}(\mathbf{Z}-\mathbf{z}'+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M})+$$
$$+\nu_{11}(\mathbf{Z}-\mathbf{z}'+\frac{m_2}{M}(\mathbf{x}-\mathbf{y}))+$$
$$+\nu_{22}(\mathbf{Z}-\mathbf{z}'-\frac{m_1}{M}(\mathbf{x}-\mathbf{y}))\Big\},$$

we come, taking into account the spherical symmetry of $|\varphi_\alpha(\mathbf{x})|^2$, to

$$G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')=0. \tag{71}$$

We have also used here that

$$\nu_{ab}(\mathbf{Z}-\mathbf{Z}')=\frac{e_ae_b}{|\mathbf{Z}-\mathbf{Z}'|},\qquad e_1=-e_2=e.$$

We also get

$$G_{\alpha\alpha;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')=\int d\mathbf{x}\int d\mathbf{y}\varphi^*_\rho(\mathbf{x})\varphi^*_\lambda(\mathbf{y})\times$$
$$\times\varphi_\alpha(\mathbf{y})\varphi_\alpha(\mathbf{x})\Big\{\nu_{12}(\mathbf{Z}-\mathbf{z}'-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M})+$$
$$+\nu_{21}(\mathbf{Z}-\mathbf{z}'+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M})+$$
$$+\nu_{11}(\mathbf{Z}-\mathbf{z}'+\frac{m_2}{M}(\mathbf{x}-\mathbf{y}))+$$

$$+\nu_{22}(\mathbf{Z}-\mathbf{z}'-\frac{m_1}{M}(\mathbf{x}-\mathbf{y}))\Big\}.$$

The presence of the multipliers $\varphi_\alpha(\mathbf{y})$ and $\varphi_\alpha(\mathbf{x})$ makes it possible to expand the expression in braces in powers of $\mathbf{x}$, $\mathbf{y}$. As a result, we have

$$G_{\alpha\alpha;\beta\lambda}(\mathbf{Z}-\mathbf{Z}') =$$

$$= \frac{1}{|\mathbf{Z}-\mathbf{Z}'|^3}\Big(-3(\mathbf{n}\mathbf{d}_{\beta\alpha})(\mathbf{n}\mathbf{d}_{\lambda\alpha})+(\mathbf{d}_{\beta\alpha}\mathbf{d}_{\lambda\alpha})\Big),$$

where

$$\mathbf{n}=\frac{\mathbf{Z}-\mathbf{Z}'}{|\mathbf{Z}-\mathbf{Z}'|}, \qquad \mathbf{d}_{\beta\alpha}=e\int d^3x\mathbf{x}\varphi^*_\beta(\mathbf{x})\varphi_\alpha(\mathbf{x}).$$

($\mathbf{d}_{\beta\alpha}$ are the matrix elements of the dipole moment of an atom). Thus, the potential energy of the interaction between atoms, $V(\mathbf{Z}-\mathbf{Z}')$, is defined by [2], [3]

$$V(\mathbf{Z}-\mathbf{Z}')\equiv E^2_{\alpha\alpha}-2\varepsilon_\alpha=\frac{1}{|\mathbf{Z}-\mathbf{Z}'|^6}\times$$

$$\times{\sum_{\beta\lambda}}'\frac{|-3(\mathbf{n}\mathbf{d}_{\beta\alpha})(\mathbf{n}\mathbf{d}_{\lambda\alpha})+(\mathbf{d}_{\beta\alpha}\mathbf{d}_{\lambda\alpha})|^2}{2\varepsilon_\alpha-\varepsilon_\beta-\varepsilon_\lambda}<0. \qquad (72)$$

Since $\varepsilon_\beta,\varepsilon_\lambda > \varepsilon_\alpha$, $V(\mathbf{Z}-\mathbf{Z}') < 0$. Therefore, the attractive forces (van der Waals forces) act between neutral atoms at long distances.

In conclusion, we note that, for the Coulomb interaction,

$$\nu_{11}=\nu_{22}=\frac{e^2}{|\mathbf{x}|}, \quad \nu_{12}=\nu_{21}=-\frac{e^2}{|\mathbf{x}|}.$$

As a result, formulas (56) and (57) take the form

$$\widetilde{\mathcal{H}}^1_{\rm int}=\int d\mathbf{x}_1d\mathbf{x}_2\hat\chi^+(\mathbf{x}_1)\hat\chi(\mathbf{x}_1)\times$$

$$\times v_{\alpha'\alpha}(\mathbf{x}_1-\mathbf{x}_2)\hat\eta^+_{\alpha'}(\mathbf{x}_2)\hat\eta_\alpha(\mathbf{x}_2),$$

$$\widetilde{\mathcal{H}}^2_{\rm int}=\int d\mathbf{x}_1d\mathbf{x}_2v_{\alpha\beta;\gamma\delta}(\mathbf{x}_1-\mathbf{x}_2)\hat\eta^+_\alpha(\mathbf{x}_1)\times$$

$$\times\hat\eta^+_\beta(\mathbf{x}_2)\hat\eta_\gamma(\mathbf{x}_2)\hat\eta_\delta(\mathbf{x}_1).$$

Moreover, for $|\mathbf{x}|\gg r_0$, we have

$$v_{\alpha'\alpha}(\mathbf{x}_1-\mathbf{x}_2)\to\frac{e}{x^3}\mathbf{x}\mathbf{d}_{\alpha'\alpha},$$

$$v_{\alpha\beta;\gamma\delta}(\mathbf{x})=\frac{1}{x^5}\left(x^2(\mathbf{d}_{\alpha\delta}\mathbf{d}_{\beta\gamma})-3(\mathbf{x}\mathbf{d}_{\alpha\delta})(\mathbf{x}\mathbf{d}_{\delta\gamma})\right).$$

Thus, the obtained Hamiltonians $\widetilde{\mathcal{H}}^1_{\rm int}$, $\widetilde{\mathcal{H}}^2_{\rm int}$ describe the dipole—particle and dipole–dipole interactions.

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ДИНАМІКА ЗВ'ЯЗАНИХ СТАНІВ ЧАСТИНОК У МЕТОДІ ВТОРИННОГО КВАНТУВАННЯ

С.В. Пелетминський, Ю.В. Слюсаренко

Р е з ю м е

Побудовано наближений метод вторинного квантування для опису систем багатьох частинок за наявності зв'язаних станів частинок з низькою енергією (кінетична енергія мала порівняно з енергією зв'язку складених частинок). У цьому наближенні складені частинки розглядаються на рівні з елементарними, що означає можливість введення операторів народження і знищення. Гамільтоніани, які визначають взаємодію між елементарними і складеними частинками, а також між самими складеними частинками, записані через амплітуди взаємодії елементарних частинок.