resonance. A peculiar feature of this phenomenon is that the stronger the two-particle resonance, the larger the number of three-particle resonances produced by it. Experiments show [1, 14, 15] that such resonant states in many-particle systems lead to anomalously high rates of chemical reactions, dynamic coupling of noninteracting particles, etc. [14-16]. The importance of studying such states is directly associated with determining the binding energy of a system of N bodies using information on subsystems of this many-particle system, i.e., the construction of dependences $E_N = f(E_{N-1}, E_{N-2}, ...)$ and the determination of the conditions for the formation of a coupled many-particle system provided that some subsystems are not coupled [16].

The physical foundation of the effect considered here is presented in [1], where the following aspects are revealed.

1. The effect of two-particle resonances on the spectrum of a three-particle system is clearly manifested; i.e., a two-particle resonance can radically reconstruct the discrete spectrum of three particles. However, not every two-particle resonant state can reconstruct the spectrum of three particles, but only the state whose size $r_{res} \sim (2m_{ij}|e_0|)^{1/2}$ is much larger than the range r_0 of its action (e_0 is the binding energy and m_{ij} is the reduced mass of a pair of particles. Such a resonance can only be an s resonance ($l = 0$) since such resonant states strongly differ in size from other types of resonant states. For $e_0 \to 0$, size $r_{res} \to \infty$. The size of a resonant state is manifested in the scattering of particles in the form of a large scattering length a, which is equal to the size of this resonant state for small e_0. Analyzing resonant states from the standpoint of their size, we can observe that all these states sharply differ from the resonance considered above. For example, the state occupied by the system in a partial wave with $l \neq 0$ has a size on the order of the range of forces due to the centrifugal barrier; a compound resonance is not large either. Thus, a two-particle s level with a small binding energy occupies an exceptional position among resonant states as regards its size.

2. Three-particle levels are stable and their number is proportional to $\ln(a/r)$. It can be proved [1, 13-15] that the interaction responsible for the emergence of these levels has the form $U \sim A/R^2$, where $R^2 = 2/3(r_1^2 + r_2^2 + r_3^2)$, r_i is the distance between a pair of particle, and is operative in the interval (r_0, a) (Fig. 1). In the general case, the constant A of this interaction is a function of quantum numbers of the three-particle state, angular momentum, parity, and symmetry relative to the transposition of the particles. The value of A is estimated in [1,14, 15]. The strongest attraction should be observed for the orbital angular momentum $L = 0$ for three particles since centrifugal forces are absent in this case. The symmetry of this state must be maximal; otherwise, the wave function has nodes and the coupling becomes weaker.

3. Centrifugal forces suppress the effect.

4. Such states possess the maximal symmetry.

5. Triple and many particles forces do not influence the effect.

6. The addition of a particle to the three-particle system suppresses the effect.

7. The particle charge has no influence on the effect which is manifested less clearly in this case.

8. For particles with spins, the effect is also pronounced less clearly.

It should be noted that such peculiar states of three particles are independent of the specific form of the potential (i.e., independent of the forces of interaction between particles) and are universal in the sense that these states reflect only the fact of existence of a resonance. Thus, irrespective of the form of pair forces between the particles, if it leads to a low-energy two-particle s resonance, this automatically leads to the formation of a family of three-particle resonances. Consequently, the reason for the emergence of three-particle level lies in the production of long-range interaction between three particles by a two-particle resonance with a large spatial size. Thus, the number of resonant states in a three-particle system is determined only by specific properties of paired subsystems. The masses of the particles have the strongest influence on the effect. The following three characteristic regimes can be singled out: the mode of identical particles, the mode of a heavy center, and the molecular mode [1, 13-15]. The heavy-center mode takes place when the masses of two particles are of the same order ml, while the mass mh of the third particle is much larger. The pair of light particle has no energy level and these particles do not interact with each other, but interact with the heavy particle through the attracting potential. In this case, if the mass of the third particle is infinitely large, we are dealing with the case of a pair of particles in a force center; naturally, three-particle levels do not emerge in such a system. In this case, the heavy particle does not respond to the motion of the noninteracting particles moving independently from each other in the field of the stationary heavy particle. Consequently, in this limit, the binding energy of the three particles is the additive sum of the binding energies of two-particle systems. However, for a finite mass of the heavy particle, the motion of all the three particles is correlated, so that the center of mass of the system remains at rest. In this case, the heavy particle responds to a change in the position of other particles whose motion becomes correlated in spite of the absence of a direct interaction between them. Thus, dynamic correlation in the motion of coupled particles can be treated as a sort of attraction. It should be noted that such a dynamic attraction also appears in the case when repulsive force act between the particles coupled in this way. In this case, dynamic attraction compensates mutual repulsion and leads to stabilization of the system. This can be clearly seen, for example, for the ion of positronium $e^+e^-e^-$ [14-16]. In this case, for any finite mass of a heavy center, the number of levels is

$$N \sim \frac{m_l}{m_h} \ln \frac{1}{e_0 m_l r_0^2}$$

A special feature of this mode is that extremely shallow levels in paired subsystem are required for the existence of three-particle levels in contrast to the molecular mode, where the requirements imposed on paired levels are much less stringent and more realistic.

In the molecular mode, when a light particle has shallow levels in the interaction with the heavy particles, the number of levels is

$$N \sim \sqrt{\frac{m_l}{m_h}} \ln \frac{1}{|e_0| m_l r_0^2}$$

and the potential of the interaction produced by the light particle has the form

$$V \sim \frac{-0.32}{m_l r_{hh}^2},$$

which is precisely the energy of the molecular energy level. The simple example of this mode is a system consisting of an electron and two neutral atoms. The molecule formed in this way differs from a conventional molecule in that its nuclei vibrate in region R whose size is determined by the energy e0 of the shallow paired level; in addition to vibrational levels, this system also has a rotational spectrum. Thus, two-particle levels in this mode lead to the formation of a series of not only vibrational, but also rotational levels [1, 13-15]. It should be noted that such peculiar resonance states are manifested in a wide range of conditions and form a stable phenomenon which can be reliably identified and confirmed experimentally.

2 Basic Equations and Main Approximation

We will analyze these peculiar resonant states quantitatively in the case of the molecular mode using the Faddeev integral equations [13]. In the given approximation (three particles, viz., two atoms and an electron), these equations are formulated for three parts into which the total wave function of the three-body system splits,

$$\Psi = \sum_{i=1}^{3} \Psi_i,$$

Each part corresponds to possible divisions of the system of three particles into noninterecting subgroups. In the momentum space, in the case of scattering of particle 1 from the coupled pair (2,3) the equations have the form [13,14]

$$\Psi_i = \Phi_i \delta_{i1} - G_0(Z) T_i (\Psi_j + \Psi_k), \quad i, j, k = 1, 2, 3; 3, 1, 2; 2, 1, 3; \qquad (1)$$

Here, Φ_1 describes the initial state of the three body systems: free motion particle 1 and the bound state of pair (2,3); $G_0(Z) = (H_0 - Z)^{-1}$, $Z = E + i0$, where H_0 is the operator of free motion of three particles; E is the total energy of three-body system, which is equal to the sum of kinetic energy of projectile 1 and the binding energy of pair (2,3); T_i is a paired T-matrix that can be unambigously defined in terms of the paired interaction potential V_i with the help of the Lippmann-Schwinger equations

$$T_i = V_i + V_i G_i T_i, \quad G_i = (h_i - Z_i)^{-1}, \quad h_i = \Delta_i + V_i \quad (2)$$

To describe the motion of three particles in center-of-mass system we use the generally accepted Jacobi coordinates. It should be borne in mind that we must use as integration variables in Eq. (1) a certain system of variables which is found to be most convenient. For example, in the integral corresponding to the expression $G_0T_1\Psi_2$, it is more convenient to take $\boldsymbol{k}_2$ and $\boldsymbol{p}_2$ as integration variables. In this case, variables $\boldsymbol{k}_1$ and $\boldsymbol{p}_1$ determining the kernel of operator T_1 should be expressed in terms of variables $\boldsymbol{k}_2$ and $\boldsymbol{p}_2$. Sometimes, it is more convenient to use variables $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ in the same situation.

Paired T matrices $t_i(\boldsymbol{k}_i, k_i'; Z)$ appearing in the kernels of the equations have singularities in variable Z: the poles corresponding to the discrete spectrum of paired subsystems and a cut along the positive part of the real axis generated by the spectrum of the two-body problem. The explicit form of these singularities gives the spectral representation of matrix T. The poles of the T matrix corresponding to the discrete spectrum generate singularities in the wave function components Ψ_i; separating these components, we obtain the representation

$$\Psi_i(\boldsymbol{k}_i, \boldsymbol{p}_i; \boldsymbol{p}_i^o) = \varphi(\boldsymbol{k}_i)\delta(\boldsymbol{p}_i - \boldsymbol{p}_i^o) - B_i(\boldsymbol{k}_i, \boldsymbol{p}_i; \boldsymbol{p}_i^o; Z)/(p_i^2/2n_i + k_i^2/2m_{jk} - Z), \quad (3)$$

where

$$B_i(\boldsymbol{k}_i, \boldsymbol{p}_i; \boldsymbol{p}_i^o; Z) = -\sum_{j=1}^{3}[Q_j(\boldsymbol{k}_i, \boldsymbol{p}_i; \boldsymbol{p}_i^o; Z) - \varphi_j(\boldsymbol{p}_j)R_{ji}(\boldsymbol{k}_j; \boldsymbol{p}_i^o; Z)/(p_j^2/2n_j - \kappa_j - Z)],$$

and Q_j, R_{ji} are smooth function of their variables. Such a division of singularities appears automatically in the numerical solution of integral equations. To define functions Q_j and R_{ij} unambiguously, we can proceed as follows. We substitute Ψ_i in form (3) into initial equations (1) and equate the coefficients of identical singularities. This gives the equations for these functions which can be used for expressing explicitly all main characteristics of the three-body problem: wave function, elements of the S matrix, as well as the amplitudes and cross sections of all processes occurring in the three-body system. Thus, the cross section of the elastic scattering process has the form

$$d\sigma_{11}/d\Theta = (2\pi)^4 n_1 |R_{11}|^2,$$

the cross section of rearrangement processes is given by

$$d\sigma_{1i}/d\Theta = (2\pi)^4 n_i p_f |R_{1i}|^2/p_1^0$$

and the cross section of the process of decay into three free particles has the form

$$d\sigma_{1\to 3}/d\Theta dp = (2\pi)^4 n_i p_f |B_{0i}|^2/p_1^0,$$

where

$$p_f^2 = 2n_i(p_i^{02}/2n_i - \kappa_1^2 - \kappa_i^2)$$

.

The main advantage of the Faddeev equations (1) is that

(i) the solution of this equation gives simultaneously the amplitudes and cross sections of all processes occurring in the three-particle system;

(ii) the accuracy in determining the bound state from the solution of the Faddeev equations is much higher than the accuracy obtained by solving the Schrodinger equations (this peculiarity is associated with the fact that Eqs. (1) were formulated for the wave function components and, hence, take into account possible asymptotic forms of the three-particle system);

(iii) these equations make it possible to carry out a correct (from the standpoint of mathematics) analysis of scattering processes, in which all three free particles are in the initial state [12, 13]; this is impossible in all approaches proposed earlier [5-11]:

$$1+2+3 \rightarrow \begin{cases} 1+(2,3) & \text{-elastic scattering processes} \\ 1+(2,3)^* & \text{-excitation processes} \\ 3+(1,2)^* & \text{-rearrangment processes} \\ 2+(1,3)^* & \text{-with excitation} \\ 1+2+3 & \text{-ionization processes} \end{cases}$$

In this case, we have the following representation for the wave function [13-15]:

$$\Psi_0(\boldsymbol{k},\boldsymbol{p};\boldsymbol{k}^0,\boldsymbol{p}^0)=\delta(\boldsymbol{k}-\boldsymbol{k}^0)\delta(\boldsymbol{p}-\boldsymbol{p}^0)-\frac{\sum_{i,j}M_{ij}(\boldsymbol{k},\boldsymbol{p};\boldsymbol{k}^0,\boldsymbol{p}^0;\frac{k^{02}}{2m}+\frac{p^{02}}{2n}+i0)}{\frac{p^2}{2n}+\frac{k^2}{2m}-\frac{k^{02}}{2m}+\frac{p^{02}}{2n}+i0},$$

where functions Mi, j satisfy the following system of equations:

$$M_{ij}(Z)=\delta_{i,j}T_i(Z)+T_i(Z)G_0(Z)\sum_{k\neq i}M_{kj}(Z)$$

For cross sections of these processes, we obtain the following expression [13,15]

$$S_{00}(\boldsymbol{k},\boldsymbol{p};\boldsymbol{k}',\boldsymbol{p}')=\delta(\boldsymbol{k}-\boldsymbol{k}')\delta(\boldsymbol{p}-\boldsymbol{p}')-2\pi i\delta(\frac{p^2}{2n}+\frac{k^2}{2m}-\frac{p^{'2}}{2n}-\frac{k^{'2}}{2m})$$

$$\sum_{i,j}M_{ij}(\boldsymbol{k},\boldsymbol{p};\boldsymbol{k}',\boldsymbol{p}';\frac{k^{'2}}{2m}+\frac{p^{'2}}{2n}+i0);$$

corresponds to processes in which three free particles are in the initial and final states,

$$S_{0s_i}(\boldsymbol{k},\boldsymbol{p};,\boldsymbol{p}_i')=2\pi i\delta(\frac{p^2}{2n}+\frac{k^2}{2m}+\kappa_{s_i}^2-\frac{p_i^{'2}}{2n_i})\sum_k Q_{ki}^{s_i}(\boldsymbol{k},\boldsymbol{p};\boldsymbol{p}_i';-\kappa_{s_i}^2+\frac{p_i^{'2}}{2n_i}-i0)+$$

$$\sum_{s_k}\psi_{s_k}(\boldsymbol{k}_k)R_{ki}^{s_k s_i}(\boldsymbol{p};\boldsymbol{p}_i';-\kappa_{s_i}^2+\frac{p_i^{'2}}{2n_i}+i0),$$

$$S_{s_i0}(\boldsymbol{p}_i;\boldsymbol{k}',\boldsymbol{p}')=2\pi i\delta(-\kappa_{s_i}^2+\frac{p_i^{'2}}{2n_i}-\frac{p^{'2}}{2n}-\frac{k^{'2}}{2m})\sum_j\tilde{Q}_{ji}^{s_i}(\boldsymbol{p}_i;\boldsymbol{k}',\boldsymbol{p}';\frac{k^{'2}}{2m}+\frac{p^{'2}}{2n}+i0)+$$

$$\sum_{s_j}\psi_{s_j}(\boldsymbol{k}_j')R_{ij}^{s_i s_j}(\boldsymbol{p}_i;\boldsymbol{p}_i';\frac{k^{'2}}{2m}+\frac{p^{'2}}{2n}+i0),$$

correspond to processes in which a coupled pair of particles s_j is present in the initial or the final state. The equations for functions Q_j, Q_j, and R_{ij} are analogous to the equations for M_{ij} and are given in [13-15]. It should be noted that potentials do not appear explicitly in integral equations (1); these equations contain a more general characteristic, viz., T matrices, which are connected with the potentials of the Lippmann-Schwinger equations (2). Consequently, although potentials are formally used in the given method, we essentially model T matrices, which are constructed on the basis of the Bateman method [13, 14] suitable for any local potential. This method considerably simplifies numerical solution of the system of integral equations (1) and sometimes even leads an analytic solution [13-17].

Integral equations (1) possess good properties (from the mathematical point of view) such as the Fredholm property and unambiguous solvability only under certain conditions imposed on two-particle data [13]:

(i) paired potentials $V_i(\boldsymbol{k},\boldsymbol{k}')$, which are nonlocal in the general case, are smooth functions of $\boldsymbol{k}$,$\boldsymbol{k}'$ and satisfy the condition

$$\mid V_i(\boldsymbol{k},\boldsymbol{k}^{'})\mid\leq(1-\mid\boldsymbol{k}-\boldsymbol{k}^{'}\mid)^{1-\epsilon},\quad\epsilon>0;$$

(ii) point $Z = 0$ is not a singular point for Eqs. (2); i.e., all three scattering lengths in pair channels are finite;

(iii) the positive two-particle spectrum is continu- ous. This condition is essential for nonlocal potentials since positive eigenvalues may appear only in this case, and this condition is satisfied virtually for all physical processes.

Coulomb potentials and hard-core potentials do not satisfy the first condition:

Coulomb potentials lead to a singularity of the type $|\boldsymbol{k}-\boldsymbol{k}'|^{-2}$ in T matrices, while hard-core potentials result in a slow decrease in the T matrix for large momenta. When the second condition is violated, the Fredholm property of Eqs. (1) is lost for $Z = 0$, which leads to the above-mentioned effect of emergence of an infinitely large discrete spectrum in a three-body system under certain conditions. A similar situation emerges in the case of scattering of electrons from diatomic molecules, for which the Efimov levels were experimentally observed for the first time. The approximation considered here reproduces these experimental results in a quite natural way.

It should be emphasized once again that the given approximation appears quite reasonable for values of the impinging electron energy lower than the electron excitation energy of the molecule.

As the initial data in such a formulation of the problem, we use pair interaction potentials, masses, and energies of colliding particles. For potentials of pair interaction of electrons with atoms of the molecule, we used potentials of the form

$$V(r) = \lambda \exp(-\beta r)/r, \qquad (4)$$

whose parameters were determined on the basis of the electron binding energy at a negative ion, scattering lengths, and effective radius. Allowance for spin (in the case of homonuclear molecules) was made as follows. For the scattering length, we used the quantity [5, 6, 14-17]

$$\frac{1}{a} = \frac{1}{a_1} = \frac{1}{a_2} = \frac{1}{4}(\frac{3}{a_t} + \frac{1}{a_s}),$$

where a_t and a_s are the triplet and singlet scattering lengths, respectively. Pair potentials of interaction between atoms in molecules were simulated by the Morse potentials

$$V(r) = D(1 - \exp(-\alpha(r - r_0))), \quad (5)$$

whose parameters were determined on the basis of spectroscopic data [18].

Numerical solution of integral equations (1) involves considerable difficulties because the kernels of integral equations (1) contain the same singularities [13-15] but here, we propose a quite universal method for solving system of equations (1) for calculating bound states as well as scattering states in systems with arbitrary masses, which interact via arbitrary pair short-lived potentials that can also be defined numerically. In the method proposed here, the domain of an unknown function is divided into a number of intervals on each of which the function is approximated with the help of corresponding interpolation polynomials. The method for solving system of equations (1) is a modification of the standard method for solving integral equations, in which the integral on the right-hand side is replaced with the help of a quadratures formula for solving Eq. (1). As a result, we arrive at a system of algebraic equations for values of the sought function at the nodes of the quadratures formula. In the proposed method, the domaine of the sought function is divided into a number of segments, on each of which the function is determined with the help of interpolation polynomials reproducing the correct behavior of the function in the vicinity of the above singularities, after which integration is carried out using quadratures formulas. A package of applied programs were used for realization of the proposed numerical method for solving system of integral equations (1)[13,15].

Computational difficulties encountered in calculation of cross sections in the given approximation are mainly associated with the long-range Coulomb interaction potentials. It was mentioned above that in this case the integral Faddeev equations cannot be applied directly; either these equations should be modified, or the differential formulation of the Faddeev equations in the coordinate state should be used [13-15]. In case for three charged particles Faddeev equation in the coordinate space, which have the form [13-15]

$$(-\Delta_{x_i} - \Delta_{y_i} + V_i(x_i) - E)\Psi_i = -V_i \sum_{j \neq i} \Psi_j, \quad (6)$$

where

$$V_i = n_i/x_i + V_{st}(x_i), \quad n_i = \frac{q_k q_j}{\sqrt{2m_{kj}}},$$

$$\boldsymbol{x}_i = \sqrt{\frac{2m_j m_k}{m_j + m_k}}(\boldsymbol{r}_j - \boldsymbol{r}_k), \quad \boldsymbol{y}_i = \sqrt{\frac{2m_i(m_j + m_k)}{m_i + m_j + m_k}}\boldsymbol{r}_i - \frac{m_j\boldsymbol{r}_j + m_k\boldsymbol{r}_k}{m_j + m_k},$$

and the coordinates are connected via the relations

$$\boldsymbol{x}_i = c_{ij}\boldsymbol{x}_j + s_{ij}\boldsymbol{y}_j, \qquad \boldsymbol{y}_i = -s_{ij}\boldsymbol{x}_j + c_{ij}\boldsymbol{y}_j,$$

$$s_{ij}^2 = \frac{m_k \sum_k m_k}{(m_i + m_j)(m_j + m_k)}, \qquad s_{ij}^2 + c_{ij}^2 = 1$$

V_{st} being pair short-range interaction potentials defines by (4) and (5).

The relation between the momentum and coordinate representations is defined by the Fourier transformation,

$$\Psi(\boldsymbol{k}_i, \boldsymbol{p}_i) = (2\pi)^{-3} \int \exp -i(\boldsymbol{k}_i\boldsymbol{x}_i + \boldsymbol{p}_i\boldsymbol{y}_i)\Psi(\boldsymbol{x}_i, \boldsymbol{y}_i)d\boldsymbol{x}_i d\boldsymbol{y}_i$$

To obtain a unique solution of integrodifferential equations in the coordinate space, we must add the boundary conditions, which have the form [13-15]

$$\Psi_i(\boldsymbol{x}_i, \boldsymbol{y}_i)_{x_i, y_i \to 0} \to 0, \qquad (7)$$

$$\Psi_i(\boldsymbol{x}_i, \boldsymbol{y}_i)_{\rho=\sqrt{x^2+y^2}\to\infty} \to \phi_i(x_i)\exp(i\boldsymbol{k}_i\boldsymbol{y}_i - iw_i^0)+$$

$$\sum_j A_{ij}(\hat{y}_j, \hat{k}_i)\phi_i(x_j)\frac{\exp(i\sqrt{E_j}|\boldsymbol{y}_j| + iw_{ij})}{|y_j|} + A_{0i}(\hat{X}, \hat{k}_i)\frac{\exp(i\sqrt{E}|X| + iw_0)}{|X|^{5/2}}, \quad (8)$$

where

$$w_i^0 = \frac{n_i}{2|\boldsymbol{k}_i|}\ln[|\hat{k}_i||\hat{x}_i| - (\boldsymbol{k}_i, \boldsymbol{x}_i)], \quad w_{ij} = \sum_{k\neq j}\frac{n_k}{2|s_{jk}\sqrt{E_k}}\ln 2\sqrt{E_k}|\boldsymbol{y}_k|,$$

$$w_0 = -\frac{|\boldsymbol{X}|}{2\sqrt{E}}\sum_i \frac{n_i}{|\boldsymbol{x}_i|}\ln 2\sqrt{E}|\boldsymbol{X}|, \quad n_i = \frac{kq_iq_j}{\sqrt{2m_{ij}}}, \quad E_k = E - \kappa_j,$$

A large number of various numerical methods have been developed on the basis of approximation of components Ψ by bicubic Hermite splines, quintet basis splines, etc. However, an effective, reliable, and universal algorithm of numerical solution of Eqs. (6) with boundary conditions (7) and (8) in the coordinate space has not been developed for the following reasons.

First, an algorithm of numerical solution for processes with three free particles in the initial and final states does not exist in view of rather complex boundary conditions.

Second, point-by-point convergence of the obtained result to the exact solution upon a decrease in the mesh size cannot be proved analytically in any of the known numerical methods based on finite different approximation.

Consequently, the application of the mesh method in the polar coordinate system [14] for solving numerically the system of coupled integrodifferential equations (6) in partial derivatives with boundary conditions (7) and (8) appears as most justified since analytic solutions also exist in this case for some potentials determining the resonant states under investigation [13,14,22]. This makes it possible to monitor the accuracy of the solutions obtained by the numerical method.

Let us consider the geometrical (topological, spatial) characteristics of the above-mentioned peculiar resonant states. Since it is quite difficult to study these characteristics experimentally in the case of electron collisions with molecules, we will consider the systems that are accessible for experimental studies, viz., clusters of molecules of inert gases [28].

It should be noted that these molecular clusters consisting of atoms of helium, lithium, and a number of inert gases attract attention of both theoreticians [29] and experimentalists [28] primarily due to applied studies such as superfluidity, superconductivity, Bose condensation, chemistry and physics of clusters, laser physics (i.e., the possibility of developing He_2^+ molecular laser), as well as the possibility of observing such a peculiar quantum effect in real systems.

However, a direct theoretical analysis of even the simplest of the above systems, viz., He_3 consisting of three helium nuclei and six electrons, is an extremely complicated problem.

To analyze the He_3 system, we consider the cluster approximation in which this system is replaced by a simpler system consisting of three force centers (helium atoms). The validity of this approximation for calculations of bound states is obvious since the difference between the binding energy of the system and the ionization energy of the atom is several orders of magnitude. It is well known that helium atoms are bosons; consequently, the problem boils down to analysis of three pairwise identical neutral spinless particles. To solve this problem, we propose mathematically correct model-free methods in the theory of scattering in the three-body system [13-15].

It should be emphasized that virtual levels in paired subsystems in the case of complex many-particle systems do not lead to the emergence of resonant states in a many-particle system [1]. This, however, does not mean that this effect is absent in these systems since it can be due to many-particle and not two-particle virtual states.

For this reason, we will consider the interpretation of a number of peculiar properties of systems He_3, Ar_3, Kr_3, Ne_3, Xe_3, Li_3, and Rn_3 precisely on the basis of the three-particle approximation. It should be noted that a large number of theoretical and experimental methods exist for studying clusters consisting of atoms of helium and a number of inert gases. Most methods are intended for studying bound states; however, scattering states [28-31], which are most informative for confirming the existence of peculiar resonant states, were practically ignored.

It was stated by a number of authors [30] that the main difficulties in studying the He3 system are associated with its low binding energy (1 mK), an unusually large size of the excited state ($\sim\ 150A^o$), and a strong repulsion at small distances. However, the results obtained in [15, 31], where an analogous three-particle approximation was used for calculating the He_3 system, differ from the statements made in [30].

For this reason, it would be also interesting to verify the conclusions drawn in [30] on the basis of the three-particle approximation with the short-range pair potentials used in [32]. The main purposes of this investigation are

(i) determining the number of possible resonant states;

(ii) clarifying the role of pair interaction potentials in the characteristics of these states;

(iii) estimating the effect of repulsion at short distances, which can be approximated by a hard core in the model for the boundary conditions [13-15] imposed on the characteristics of these peculiar states.

Thus, the theoretical analysis of the He_3 system is reduced to solving equations in the quantum theory of scattering in a three-body system, which makes it possible to use the well-known methods [13-15]. In contrast to [30], where resonances in a three-particle system were studied using the Faddeev equations on the basis of analytic continuation of the scattering matrix to the range of complex energy values, we are using here direct numerical solution without an analytic continuation.

In this case, after the separation of angular variables, the Faddeev equations (6) in the coordinate space for the He_3 system in the three-particle approximation with pair short-range potentials [32] have the form [13-15]

$$[H_{\lambda,l} - z]\Psi_{aL}(x,y) = -V(x)(\Psi_{aL}(x,y) + \sum_{a'} \int_{-1}^{+1} \Psi_{a'L}(x',y') h^L_{aa'}(x',y',\eta) d\eta), \qquad (9)$$

where

$$H_{\lambda,l} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \frac{l(l+1)}{x^2} + \frac{\lambda(\lambda+1)}{y^2}$$

$$z = E + i0, \qquad L = l + \lambda, \qquad a = (l,\lambda),$$

For calculations with a hard core in the model of boundary conditions, the right-hand side is equal to zero for $x < c$, where c is the core size. To obtain an unambiguous solution to the equations, we must preset boundary conditions (7), (8),

$$\Psi_{aL}(x,y)\mid_{x=0}=0, \qquad \Psi_{aL}(x,y)\mid_{x=0}=0, \qquad (10)$$

which assume the following form in the boundary-condition model:

$$\Psi_{aL}(c,y)+\sum_{a'}\int_{-1}^{+1}\Psi_{a'L}(x',y')h_{aa'}^{L}(x',y'),\eta d\eta=0$$

$$x'=\sqrt{x^2/4+3y^2/4-\sqrt{3}xy\eta/2}, \quad y'=\sqrt{3x^2/4+y^2/4+\sqrt{3}xy\eta/2},$$

For $\rho\to\infty$ the boundary conditions in the case of short-range pair potentials can be written in the form [13]

$$\Psi_{aL}\sim_{\rho\to\infty}a_{aL,v}\sum_{v}\psi_{l,v}(x)H_v(\sqrt{E-E_{2,l,v}})+A_{aL}(\theta)\frac{expi\sqrt{E}\rho+i\pi L/2}{\sqrt{\rho}} \qquad (11)$$

where $\psi_{l,v}(x)$ are the partial components of the wave functions of paired subsystems with binding energy $\epsilon_{l,v}$; $\rho=\sqrt{x^2+y^2}$; $\theta=\arctan y/x$; $a_{aL,v}$ and $A_{aL}(\theta)$ are the scattering amplitudes of processes with two or three particles, respectively, in the final state; and $H_v(x)$ are the Hankel spherical functions.

In calculations of bound states, the wave functions decrease quite rapidly at infinity; consequently, at a large distance $x=R_x$, $y=R_y$, the asymptotic boundary conditions can be replaced by the conditions

$$\frac{\partial_x\Psi_{aL}\mid_{x=R_x}}{\Psi_{aL}\mid_{x=R_x}}=i\sqrt{\epsilon_v}$$

$$\frac{\partial_y\Psi_{aL}\mid_{y=R_y}}{\Psi_{aL}\mid_{y=R_y}}=i\sqrt{\epsilon_v-E}$$

For the He_3 system in the three-particle approximation with angular momentum $L=0$, we have

$$H_{\lambda,l}=H_{0,l}=-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)(1/x^2+1/y^2),$$

where partial components l assume even values. $l=0,2,4,...$; and the expression for functions $h_{aa'}^{L}(x,y,\eta)$ is given in [13-15].

The asymptotic behavior of the components of Eqs. (9) for scattering processes with short-range potentials can be described by the function [13-15]

$$\Psi_l(x,y;z)=\delta_{l0}\psi_d(x)[\sin(\sqrt{z-\epsilon_d}y)+\exp(i\sqrt{z-\epsilon_d}y)[a_0(z)+o(y^{-1/2})]]$$

$$+\frac{\exp(i\sqrt{z}\rho)}{\sqrt{\rho}}[A_l(z,\theta)+o(\rho^{-1/2})], \qquad (12)$$

where $a_0(z)$, $z=E+i0$ is the elastic scattering amplitude for $E>\epsilon_d$, and $A_l(E,\theta)$ is the decay amplitude for $E>0$.

We also assume that the helium molecule He_2 has only one bound state with binding energy $\epsilon^d<0$ and with the corresponding wave function $\psi_d(x)$.

For processes of scattering, the scattering matrix for $z=E+i0$, $E>\epsilon^d$, the scattering phases and lengths in the s state can be expressed with help of the following formulas

$$S_0(z)=1+2ia_0(z),$$

$$\delta_0(p)=\frac{1}{2}Im\ln S_0(\epsilon_d+p^2+i0), \quad p>0,$$

$$L_{sl}=-\sqrt{3}/2\lim_{p\to 0}a_0(p)/p$$

To solve the system of equations (9) with boundary conditions (10), (12) numerically, we used the standard method described in detail in [13-15, 17]. For pair interaction potentials, we used potentials HFDHE2, HFD-B, HFDID, LM2M1, LM2M2, and TTYPT with appropriate parameters [32], which reproduce in detail the main parameters of the corresponding molecules [18].

The results of calculation of the energy of bound states in systems He_3 and He_3^* with and without taking into account the hard core are given in Tables 1-4.

The results of calculation of the scattering states in systems He_3 and He_3^* with and without taking into account the hard core are given in d Fig.4 (dependence of fase shifts on energy).

For interpreting the geometrical characteristic of the He_3 molecule in both graund and exiting ststes was given in [31].Using the method devtloped in these paper, let us consider the geometric characteristics of Ne_3 and Ne_3^* molecules which are considerable interest in context of investigations into Bose condensation, supercondactivity and superfluidity. The results of calculation of the density function difined as [31]

$$\varrho(\boldsymbol{r}_1) = \int |F(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)|^2 d\boldsymbol{r}_2 d\boldsymbol{r}_3,$$

where

$$F(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \Psi(x, y, z') + xy[\frac{\Psi(x^+, y^+, z'^+)}{x^+y^+} + \frac{\Psi(x^-, y^-, z'^-)}{x^-y^-}]/2\pi xy,$$

$$z' = (\boldsymbol{x}, \boldsymbol{y})/xy,$$

$$x^{+-} = (x^2/4 + 3y^2/4 -_+ \sqrt{3}xyz'/2)^{1/2}, \quad y^{+-} = (3x^2/4 + y^2/4 -_+ \sqrt{3}xyz'/2)^{1/2},$$

are presented in Fig.2,3. This function has the form

$$\varrho(r) = \frac{\sqrt{3}}{4\pi^2 r^2} \int |F(x, r\sqrt{3}, z')|^2 dx dz'$$

A sufficiently clear representation of the geometrical characteristics of theinert gases is provided be plotting thes function in coordinates r_i, r_a, where $r_l = rz'$ $r_a = \frac{z'}{|z'|} r(1 - z'^2)^{1/2}$.

Note that here, for excited state of the inert gas molecules as well for the molecules He_3^*, [31] and Ne_3^* (Fig.2,3), this function has two peaks, which corresponds to a linear structure of the He_3^* system. This corresponds to the situation when the third particle in the excited state is located with a high probability between two other particles (as if this state corresponded to two combined paired subsystems). It is precisely this configuration that corresponds to the conditions for the emergence of the Efimov effect in a three-particle system, when the scattering length in one of the paired subsystems is quite large. This conclusion is confirmed by calculations of the clusterization coefficient defined by the formula [31]

$$f_c = \int \Psi(x, y, z') \phi_2(x) dz' dx$$

The results of such calculations are given in Table 1. It can be seen that two-particle states dominate in the excited state Ne_3^* , while their role in the ground state is insignificant. In the ground state, system He_3 forms a nearly equilateral triangle, while in the excited state, one of the atoms is at a large distance from the other two atoms. Other excited states can be obtained by the similitude method [1, 13, 15].

An analogous structure is formed in the calculation of the ground states of the systems Ne_3, Ar_3, Kr_3, Xe_3, and Re_3 using the three-particle approximation. The results of calculation of these systems in the given approximation with the HFD-B potential and the parameters borrowed from [32] are presented in Tables 5-6.

In calculations based on the boundary-condition model, the value of core c was chosen so that even a slight change in this quantity did not affect the binding energy of paired subsystems. In our calculations, $c = 1.5A^o$, the value of binding energy for the helium molecule was 1.69 mK, and the value of r_0 was 100 A^o. A detailed description of the numerical method for solving system of equations (9) with asymptotic boundary conditions (11), and (12) is given in [13-15].

It should be noted that, according to our calculations, the size of the ground state of the He_3 system is smaller than the size of the He_2 molecule. However, the size of the excited state He_3^* of the three particle system is much larger than that of the two-particle system He_2. The experimental data [28] confirm this statement. Thus, in the given approximation, the results of calculations indicate that peculiar resonant states can exist in the He_3 system, the number of such states being not more than two.

To study the scattering processes occurring during the collision of an atom with a helium molecule and to determine the role of pair interaction potentials, we calculated the amplitudes of elastic scattering and decay as well as phase shifts with and without taking into account the hard core.

The results are almost independent of the form of pair interaction potentials and on whether or not the hard core was taken into account both for bound states and for scattering state. Thus, it can be concluded that the form of pair interaction potentials and allowance for a hard core in the boundary-condition model in the given approximation does not substantially affect the results of calculations.

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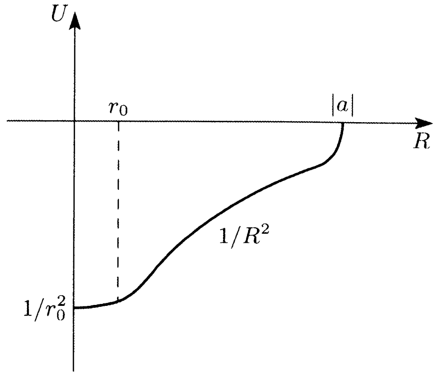

Figure 1. Effective potential responsible for resonances in a three-body system.

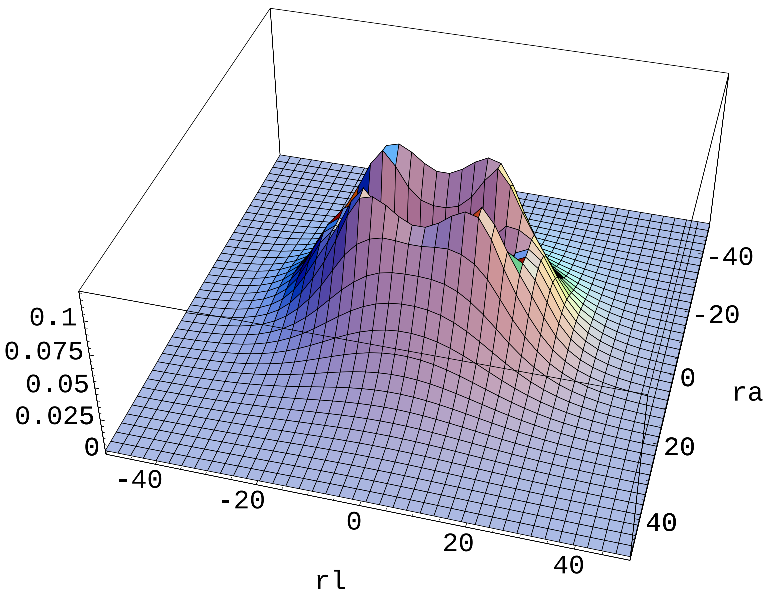

Figure 2. The density functions for Ne_3^* molecule in ground states.

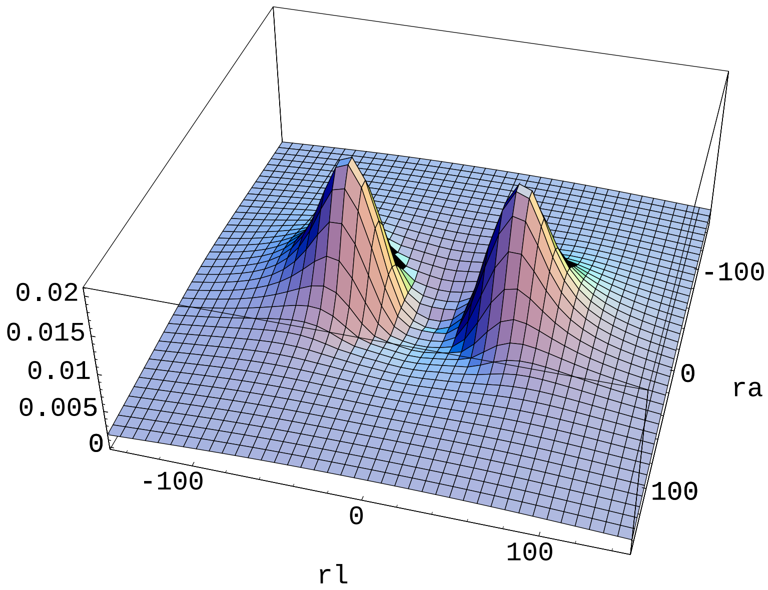

Figure 3. The density functions for Ne_3^* molecule in exited states.

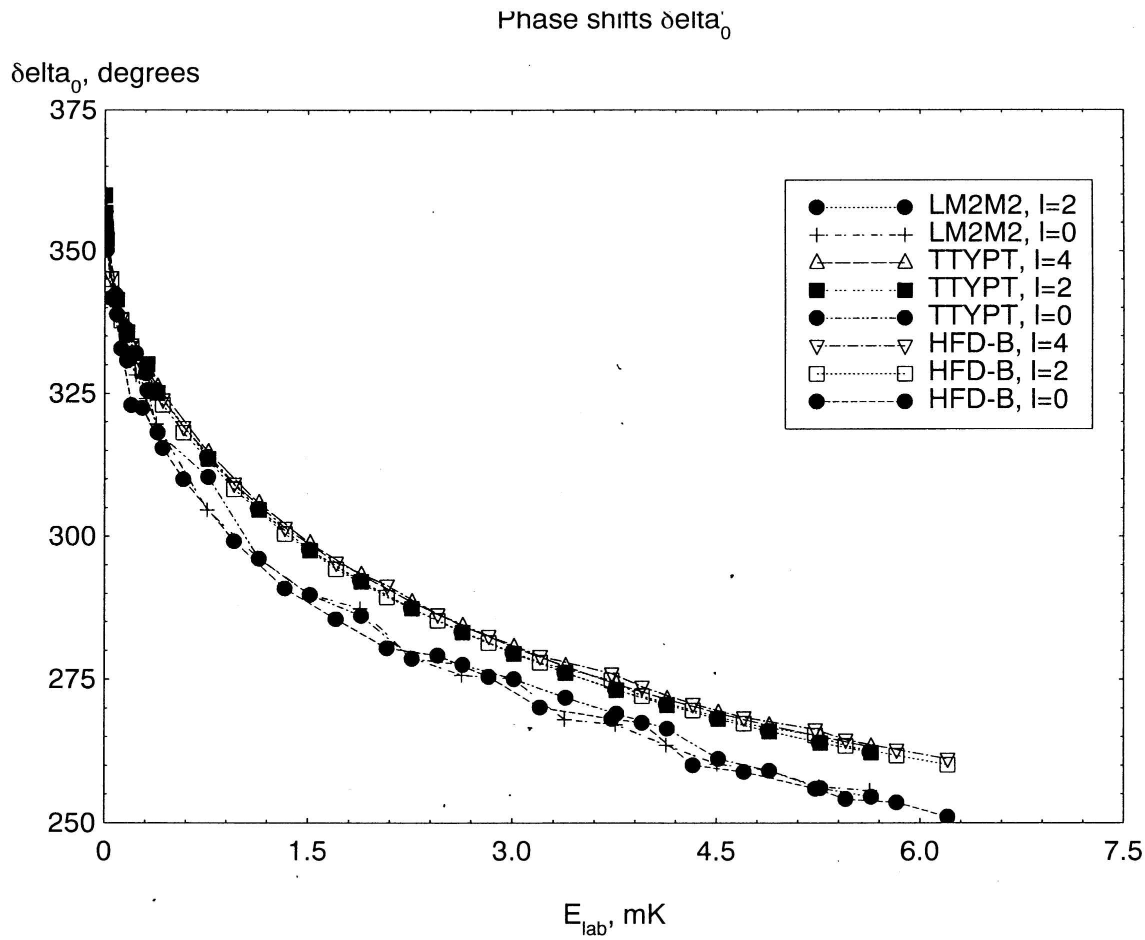

Figure 4. Dependence of fase shifts on energy for the collisions between helium atom and molecule for potentials $HFD-B$, $LM2M2$, $TTYP$[32] calculated (a) without and (b) with taking into account the hard core.

Table 1. Binding energy, coefficient of clasterization, scattering length, mean radius and square of mean raduius for He_3

Potential	E_{He_3}, mK	$\|f_c\|^2$	L_{sl}, Å	$< r_{He_3} >$, Å	$< r^3_{He_2} >^{1/2}$, Å
HFDHE2	-0.1171	0.2094	140	5.65	6.46
HFD-B	-0.1330	0.2717	137	5.48	6.23
HFD-ID	-0.1061	0.1555	139	5.80	6.64
LM2M1	-0.1247	0.2412	132	5.57	6.35
LM2M2	-0.1264	0.2479	131	5.55	6.32
TTYPT	-0.1264	0.2487	130	5.56	6.33

Table 2. Binding energy, coefficient of clasterization, scattering length, mean radius and square of mean raduius for He_3 in boundary-condition model

Potential	E_{He_3}, mK	$\|f_c\|^2$	L_{sl}, Å	$< r_{He_3} >$,Å	$< r^3_{He_2} >^{1/2}$,Å
HFDHE2	-0.1170	0.2095	138	5.65	6.46
HFD-B	-0.1329	0.2717	135	5.48	6.23
HFD-ID	-0.10612	0.1555	134	5.80	6.64
LM2M1	-0.12465	0.2412	130	5.57	6.35
LM2M2	-0.12641	0.2479	131	5.55	6.32
TTYPT	-0.12640	0.2487	131	5.56	6.33

Table 3. Binding energy, coefficient of clasterization, scattering length, mean radius and square of mean raduius for He_3^*

Potential	$E_{He_3^*}$, mK	$\|f_c^*\|^2$	L_{sl}, Å	$< r_{He_3^*} >$,Å	$< r^3_{He_3^*} >^{1/2}$,Å
HFDHE2	-1.6653	0.9077	134	55.26	66.25
HFD-B	-2.743	0.9432	135	48.33	57.89
HFD-ID	-1.0612	0.8537	140	62.75	75.38
LM2M1	-2.1550	0.9283	129	51.53	61.74
LM2M2	-2.2713	0.9319	131	50.79	60.85
TTYPT	-2.2806	0.9323	131	50.76	60.81

Table 4. Binding energy, coefficient of clasterization, scattering length, mean radius and square of mean raduius for He_3^* in boundary condition model

Potential	$E_{He_3^*}$, mK	$\|f_c^*\|^2$	L_{sl}, Å	$< r_{He_3^*} >$,Å	$< r^3_{He_3^*} >^{1/2}$,Å
HFDHE2	-1.6765	0.9078	135	56.22	67.11
HFD-B	-2.7458	0.9439	135	48.31	58.00
HFD-ID	-1.1061	0.8597	136	62.87	76.13
LM2M1	-2.2585	0.9323	132	52.41	62.04
LM2M2	-2.2801	0.9319	131	50.79	61.05
TTYPT	-2.2885	0.9339	131	51.23	60.89

Table 5. Binding energies of inert gas molecules calculated by using HFD-B potential, a.u. 10^{-6}

$Energy$	Ne_2	Ar_2	Kr_2	Xe_2	Rn_2
E_{thr}	178	394	619	854	9268
E_{exp}	135	446	629	874	-

Table 6. Binding energies of the ground state and the first excited state of the inert gas molecules calculated by using HFD-B potential

Ne_3	Ne_3^*	Ar_3	Ar_3^*	Kr_3	Kr_3^*	Xe_3	Xe_3^*	Rn_3	Rn_3^*
398	330	1278	1215	1885	1811	2509	2438	30875	30801

