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THE CONDITIONS OF STABILITY OF TWO-DIMENSIONAL QUANTUM SYSTEMS OF THREE CHARGED PARTICLES

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For a two-dimensional Coulomb system of three charged particles, among which two particles are identical and the third particle is of different nature, we study the conditions of existence for symmetric and antisymmetric bound energy states (conditions of stability) in the mass–charge (m, Z) plane. High-precision three-body numerical calculations based on a stochastic variational method with Gaussian bases are performed. Several anomalous effects in the behavior of the characteristic distances between particles are revealed, and the nonzero quadrupole moment is found in a two-dimensional polar-symmetric field. The systematic comparison of the results for two- and three-dimensional systems is performed. The values of energy and size, the density distributions, and the correlation functions for the various reference three-particle systems are obtained.

K e y w o r d s: three charged particles, two-dimensional systems, stability, variational method, structural functions

1. Introduction

Interest in two-dimensional quantum systems arises in the studies of defects in solids, physics of graphene, thin films consisting of one or few atomic layers, and various surface phenomena in condensed media. In general, the investigation of the dependence of fundamental physical characteristics on the space dimensionality and the difference of basic laws from those in three-dimensional problems is crucial for the deeper understanding of the various physical principles. Moreover, in different approaches, additionally to the basic Coulomb systems with fundamental particles, it is necessary to consider various quasiparticle and exciton systems, where the natural physical parameters of mass and charge can be varied. The dependence on the space dimensionality can be easily found for the simplest Coulomb systems of two charged particles, where the problem allows the explicit analytical solution. Increasing the complexity, the next step is to study the general problem of three charged particles such as trions XXY (see [1]), where it is possible to achieve highly accurate results. In the three-dimensional space, the general problem of three charged particles has been widely studied (see [2, 3]).

In the present work, we consider the general conditions of existence of bound states for three charged particles on a plane. We build the diagrams of stability thresholds and analyze some abnormal phenomena for two-dimensional Coulomb systems.

2. Statement of the Problem and Research Methods

Consider two-dimensional systems such as symmetric trions, consisting of two identical particles with masses $m_1 = m_2 = m$ and charges $Z_1 = Z_2 = 1$ and the third particle with mass $m_3 = M$ and charge $Z_3 = -Z$ (we use atomic units with $\hbar = e^2 = 1$). The Hamiltonian is

$$\hat{H} = \frac{\hat{p}_1^2 + \hat{p}_2^2}{2m} + \frac{\hat{p}_3^2}{2M} + \frac{1}{r_{12}} - Z\left(\frac{1}{r_{13}} + \frac{1}{r_{23}}\right). \qquad (1)$$

We consider here only the zero total angular momentum. For the most of subsequent calculations, we can put $M = 1$ without loss of generality. Assume similarly to the previous paper [3] that the conditions of stability of the quantum system in an appropriate state (conditions of existence of bound states) are defined by the fact that the energy of this state is below the ground-state energy (threshold) of the most stable subsystem. In the case of three particles with Hamiltonian (1), the conditions of stability

of the system in the n-th state with respect to the decay $(123) \to (23) + (1)$ are as follows:

$$E_n(3; m, Z) \le E_0(2; m, Z). \quad (2)$$

Here, $E_n(3; m, Z)$ is the estimated energy of the n-th state of three particles (1). The threshold energy of the two-particle subsystem has the obvious analytical form

$$E_0(2; m, Z) = -\frac{2mZ^2}{m+1}\frac{1}{(d-1)^2}, \quad (3)$$

where d is the space dimensionality. Note that the energy of two charged particles increases, as the dimensionality decreases, and becomes indefinite in the one-dimensional case (collapse occurs for the ground state). Moreover, for the potential $-1/r$, the ground state cannot be determined for the fractional dimensionality less than 1. For the 2D problem of two particles, the binding energy is 4 times higher than that for the 3D problem.

The investigation of bound states of the three-particle system (1) is performed, by using the variational Galerkin method with Gaussian basis (notation is similar to that for the three-dimensional problem [3]). We have

$$\phi_i(r_{12}, r_{13}, r_{23}) = \exp\left\{-a_i r_{12}^2 - b_i r_{13}^2 - c_i r_{23}^2\right\}. \quad (4)$$

Then the total wave function with zero angular momentum is defined as

$$\psi(r_{12}, r_{13}, r_{23}) = \sum_{i=1}^{K} N_i \hat{S}\phi_i(r_{12}, r_{13}, r_{23}), \quad (5)$$

where $\hat{S}$ is the symmetrization operator with respect to the permutations of identical particles, and K is the number of basis functions.

The energy spectrum and the corresponding symmetrized three-particle wave functions (rather, the linear coefficients N_i of the expansion or the state vectors) are solutions of the system of linear algebraic equations for the eigenvalues

$$\sum_{l=1}^{K} N_l \left\{\langle \hat{S}\phi_k \left| \hat{H} - E \right| \hat{S}\phi_l\rangle\right\} = 0, \quad k = \overline{1,K}, \quad (6)$$

where the energy matrix on the basis functions (4) for an arbitrary space dimensionality d is

$$\left\langle \hat{S}\phi_i | \hat{K} + V - E | \hat{S}\phi_j \right\rangle = \left(1 + s\hat{P}(b_i \leftrightarrow c_i)\right) \times$$
$$\times \left\{ d\frac{1}{D^{d/2+1}}\left[\frac{2}{m}a_i a_j(b+c) + \left(\frac{1}{m} + \frac{1}{M}\right) \times \right.\right.$$
$$\left. \times \big(b_i b_j(a+c) + c_i c_j(a+b)\big) + \frac{1}{m}\big(b(a_i c_j + a_j c_i) + \right.$$
$$\left. + c(a_i b_j + a_j b_i)\big) + \frac{1}{M}a(b_i c_j + b_j c_i)\right] +$$
$$+ \frac{\Gamma(d-1/2)}{\Gamma(d/2)}\frac{1}{D^{(d-1)/2}} \times$$
$$\left. \times \left[\frac{1}{\sqrt{b+c}} - Z\left(\frac{1}{\sqrt{a+c}} + \frac{1}{\sqrt{a+b}}\right)\right] - E\frac{1}{D^{d/2}}\right\}. \quad (7)$$

Here, D is the determinant of the corresponding quadratic forms that are diagonalized by integration with Gaussians

$$D = ab + ac + bc. \quad (8)$$

Here, $a = a_i + a_j$, $b = b_i + b_j$, $c = c_i + c_j$, and $\hat{P}(b_i \leftrightarrow c_i)$ is the permutation operator of corresponding parameters, $\Gamma(x)$ is the standard gamma function, $s = \pm 1$ for symmetric and antisymmetric states with respect to the permutations of coordinates of identical particles. All calculations were performed only for $d = 2$ (two-dimensional space) and partially for $d = 3$ (three-dimensional space). But, for generality, the energy matrix is presented for any dimensionality including its fractional values.

The next practically important step in variational calculations is the selection of optimal schemes to minimize the energy with respect to nonlinear variational parameters $\{a, b, c\}$. We systematically adopt certain variational stochastic techniques (see, e.g., [3–5]) that allow us to minimize the energy of any given state. It was found that the optimal strategy that keeps the balance of performance and accuracy of calculations is to increase the basis size by one function at every step and to perform a random sampling of variational parameters of the added basis function, keeping all the remaining nonlinear parameters frozen. The number of samples varies from few thousands (for a small-size basis) to few hundreds (when the basis is extended to several hundred functions). The maximal size of the basis varies from 600–700 to 1000 for the accuracy better than a fraction of percent. We emphasize also that, in order to obtain the best accuracy for the energy of each three-particle state, similar optimization schemes can be used for each state independently. This is very important from a practical point of view, if we are interested in the structure of the energy spectrum only. With this strategy, we get, of course, the best values for the energy levels, but somewhat violate the orthogonality condition for wave functions of different states.

3. Diagrams of Thresholds of Stability

First, we formulate the main result of this work, which consists of general conditions for the existence of bound states (diagram of stability) of 2D systems of three charged particles with Hamiltonian (1) depending on the mass m and the charge Z. We also compare the obtained diagrams of stability with those of 3D problem analyzed in [3].

We note that, in the 2D problem for $Z < 0$ (repulsion), there is no bound states. But, for $Z > 1$ and any mass $m > 0$, the number of bound states is infinite similarly to the 3D case. Indeed, in the polarizationless cluster variational approximation where the wave function (w.f.) of three particles is represented as the product of the ground-state w.f. of the two-particle subsystem (2 and 3) and the w.f. of the first particle relative to the center of mass of the other two ones, we have

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3,) \approx$$

$$\approx \exp\left\{-\sqrt{\frac{2m}{m+1}|E_0(2,m,Z)|}r_{23}\right\} f(r). \qquad (9)$$

Then the asymptotics of the effective potential on the coordinate $\mathbf{r} = \mathbf{r}_1 - \dfrac{m\mathbf{r}_2 + \mathbf{r}_3}{m+1}$ is the Coulomb attraction

$$V_{\text{eff.}}(r) \simeq -\frac{Z-1}{r} - \frac{(d+1)(3-d)(d-1)^2}{32Z^2}\times$$

$$\times\left(Z - \frac{1}{m^2}\right)\frac{1}{r^3} + ..., \qquad (10)$$

where d is the space dimensionality. Then the spectrum for $Z > 1$ is obviously unlimited even in this approximation from above (analog of the Kato theorem in the 3D space). It is worth to note that, for the 3D problem, the asymptotic potential $V_{\text{eff.}}(r)$ is Coulomb with exponential accuracy. In the 2D problem, the major corrections to the Coulomb asymptotics are *polynomial*, because the *quadrupole moment*

$$Q_2 = \langle(3z^2 - r^2)\rangle = (d+1)(3-d)(d-1)^2\times$$

$$\times\left(1 + \frac{1}{m}\right)^2 \frac{1}{16Z^2} \qquad (11)$$

(and all multipole momenta of even orders) has nonzero value even in a polar-symmetric field. It is also interesting that, in the molecular region $m \gg 1$, the correction of the order $1/r^3$ in (10) is attractive for $d < 3$ and repulsive for $d > 3$. In the atomic region $m \ll 1$, the result is opposite.

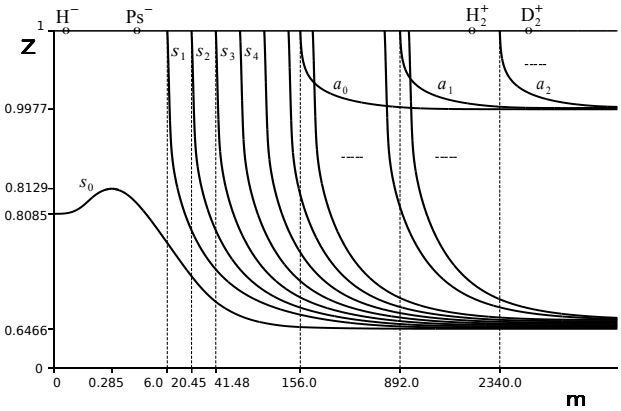

Fig. 1. Diagrams (given schematically) of the stability of the energy levels of two-dimensional systems of three charged particles

The region of intermediate charges $0 < Z < 1$ is more complicated (note that fractional values of charge are allowed, because we consider the relative charge of two kinds of particles or quasiparticles). There, we have performed high-accuracy calculations of stability thresholds, and the results are presented on the (m, Z)-plane (Fig. 1) in the form of threshold diagrams. The threshold lines of symmetric s_i and antisymmetric a_i (with respect to permutations of identical particles) states show (schematically) that these bound states exist above certain lines. From Fig. 1, we see that the systems in the atomic region (one-center problem) with $m \ll M = 1$, e.g., an atomic hydrogen ion H^- (we use the traditional notation for the (pee) bound system) or a positronium ion Ps^- ((eee^+) bound system), have only one symmetric bound state for $Z > Z_0 = 0.8085$ (and $m = 0$) in the two-dimensional case. Comparing to the 3D case where $Z_0 = 0.911$ [3], we see that, in the 2D case, three particles have more possibilities to form a bound state. The symmetric ground state exists for all values of mass m. To be more specific, we show some points for the curve s_0 obtained from our calculations in Table 1. Note that the threshold line of stability for the ground state is nonmonotonic with a maximum at $m = 0.285$, that is 1.93 times less than the similar value in the 3D problem. This value of Z_0 is by a factor of 1.14 less than that in the 3D

case. In the maximum of the s_0 curve, the formation of a bound state is least favorable. In the molecular region $m \gg 1$ (two-centered problem) where the domain of existence of bound states in 2D is wider, in the limit $m \to \infty$ and $Z > Z_{s(\text{crit.})}(2) = 0.64656$ (for the 3D problem, $Z_{s(\text{crit.})}(3) = 0.8101$), the number of symmetric vibrational bound states approaches infinity. Similarly, for states antisymmetric with respect to the permutations of identical particles in the molecular region, all threshold lines are located above the critical value $Z_{a(\text{crit.})} = 0.9977$, which is close enough to the corresponding three-dimensional value $Z_{a(\text{crit.})} = 0.9997$. We emphasize that vibrational antisymmetric bound states exist only in the region $Z \sim 1$.

Table 1. **Dependence of $Z_0(m)$ for the ground state threshold line (s_0)**

m	Z_0	m	Z_0
0	0.80853	0.5	0.81177
0.001	0.80857	1.0	0.80487
0.01	0.80890	2.0	0.78953
0.1	0.81136	5.0	0.75817
0.2	0.81262	10.0	0.73234
0.28	0.8128865	10^4	0.64835
0.285	0.8128868	10^6	0.64668
0.3	0.8128793	10^8	0.64656

Table 2. **Critical values of mass for symmetric states (with $Z = 1$)**

State index n	0	1	2	3	4	5
$m^{(s)}_{n(\text{crit.})}$	0.0	6.0	20.45	41.48	68.56	101.2
$\dfrac{m^{(s)}_{n(\text{crit.})(2D)}}{m^{(s)}_{n(\text{crit.})(3D)}}$	–	0.63	0.69	0.70	0.69	0.68

Table 3. **Critical values of mass for antisymmetric states (with $Z = 1$)**

State index n	0	1	2	3
$m^{(a)}_{n(\text{crit.})}$	156.0	892.0	2340.	4960.
$\dfrac{m^{(a)}_{n(\text{crit.})(2D)}}{m^{(a)}_{n(\text{crit.})(3D)}}$	0.47	0.51	0.51	0.55

Interesting behavior can be observed at the top part of the stability diagram when $Z = 1$. In this case, each new vibrational energy level appears at increasing critical values of the mass, which are presented for symmetric states in Table 2, and for the antisymmetric states in Table 3. It is worth noting that the general rule is that the accuracy of calculations listed in these tables decreases for higher excitations. To be more specific, we show the ratio of critical mass values for 2D and 3D in Table 2 (third line). All these values are close to 0.68, which shows a greater degree of connectedness in two-dimensional problems. Note that if the bound ground state exists for all masses m, then the 1-st excited state s_1 for $Z \leq 1$ and the 2D space appears only at $m \geq 6.0$. We note (see Table 2) that, for symmetric states, the threshold lines are significantly shifted to the region of lower masses comparing to the three-dimensional problem (similar result occurs for antisymmetric states as well). It is worth noting that the critical values of mass satisfy the quadratic rule similarly to the 3D case [3]. But, unlike 3D where the law was justified by quasiclassical quantization conditions, the quasiclassical formalism in the 2D case requires substantial modifications and cannot be used directly. We can present the approximation formulae for the critical masses, where new symmetric and antisymmetric states appear. We have

$$m^{(s)}_{n(\text{crit.})} \approx 3.4n(n+1),$$
$$m^{(a)}_{n(\text{crit.})} \approx 367n(n+1) + 156. \qquad (12)$$

Note that the higher the excited level, the more accurate are these quadratic approximations. Moreover, the approximation formulas like (12) for antisymmetric states in 2D and 3D contain coefficients that are almost two times different. This indicates the linear dependence of $m^{(a)}_{n(\text{crit.})}$ on $(d-1)$. It can be seen from the calculations (Table 3) and the approximate formulas (12) that the ratio of the critical masses for 2D and 3D problems for antisymmetric states is close to 0.51.

At the top part of Fig. 1, some reference systems are indicated, from which we can qualitatively see the number of bound states. From the approximating formulas (12), one can see that a hydrogen molecular ion H_2^+ ((*ppe*) bound system with the mass $m \sim 1836$) has 24 symmetric and 2 antisymmetric bound states. It is likely that, in 2D, the deuterium

molecular ion D_2^+ has about 33 symmetric and 3 antisymmetric bound states.

4. Mean-Square Distances and Structural Features

We define the mean-square distance R_{ik} (m.s.d.) between particles as

$$R_{ik} = \left(\langle\Psi \left|(\mathbf{r}_i - \mathbf{r}_k)^2\right| \Psi\rangle\right)^{1/2} \tag{13}$$

and mean-square radii R_j (m.s.r.) as

$$R_j = \left(\langle\Psi \left|(\mathbf{r}_j - \mathbf{R}_{\text{c.m.}})^2\right| \Psi\rangle\right)^{1/2}, \tag{14}$$

where $\mathbf{R}_{\text{c.m.}} = \dfrac{m(\mathbf{r}_1 + \mathbf{r}_2) + \mathbf{r}_3}{2m+1}$ is the coordinate of the center of mass of the three-particle system. In basis (5) with any space dimensionality d, we obtain the distance R_{12} between identical particles as

$$R_{12}^2 = \frac{d}{2N} \sum_{i,j=1}^{K} N_i N_j (b+c) \left(1 + s\hat{P}(b_i \leftrightarrow c_i)\right) \frac{1}{D^{d/2+1}} \tag{15}$$

and the distance

$$R_{13}^2 = \frac{d}{2N} \sum_{i,j=1}^{K} N_i N_j \left(1 + s\hat{P}(b_i \leftrightarrow c_i)\right) \times \\ \times \left(1 + s\hat{P}(b \leftrightarrow c)\right) \frac{a+c}{D^{d/2+1}}. \tag{16}$$

Here, the full normalization integral is defined as

$$N = \sum_{i,j=1}^{K} N_i N_j \left(1 + s\hat{P}(b_i \leftrightarrow c_i)\right) \frac{1}{D^{d/2}}, \tag{17}$$

and D is defined by (8). The permutation operator $\hat{P}(b_i \leftrightarrow c_i)$ in (15), (16), and (17) is the same as in (7).

Note that there are the general relations for any space dimensionality between m.s.r. of the system (the distance from the particle to the center of mass of the system) and m.s.d.

$$R_1^2 = R_2^2 = \frac{1}{(1+2m)^2} \left[m(m+1)R_{12}^2 + R_{13}^2\right], \tag{18}$$

$$R_3^2 = \frac{m^2}{(1+2m)^2} \left[4R_{13}^2 - R_{12}^2\right]. \tag{19}$$

It is easy to derive the inverse relation

$$R_{12}^2 = 4R_1^2 - R_3^2/m^2, \tag{20}$$

$$R_{13}^2 = R_1^2 + (1 + 1/m)\, R_3^2. \tag{21}$$

In a Gaussian basis, the expressions like (15) and (16) have a universal form for different excited states, and these expressions depend on the state only through linear $\{N_i\}$ and nonlinear $\{a_i, b_i, c_i\}$ variational parameters. By the way, (18) and (19) show also that this type of relationships does not depend explicitly on the space dimensionality, and the inequalities $R_{12} < 2R_{13}$ and $R_1 > R_3/2m$ are always satisfied. Additionally, relation (18) in case of infinite mass m yields the obvious relation $R_1 = R_2 \sim R_{12}/2$, since the center of mass of the three-particle system coincides with the center of mass of two heavy particles.

Consider the functional dependence of distances R_{12} and R_{13} on the mass and the charge. It is natural that, in the 3D case, distance R_{12} between identical particles that repel each other by Coulomb's law is greater than the distance R_{13} between particles with attraction [3] (triangle inequality). This result holds for all masses and, e.g., this is true for the structures of a molecular hydrogen ion H_2^+ and an atomic hydrogen ion H^-. In the 2D space where the coupling is significantly greater, the *abnormal* ratio in the ground symmetric state is observed for the distance between identical heavy particles and the distance between different particles that attract each other. From the calculations by (15) and (16), we obtain the inequality $R_{12} < R_{13}$: *distance between heavy identical particles is smaller than the distance between different particles* in the 2D space for symmetric states in molecular mode for sufficiently heavy masses m. In Fig. 2, the dependence of the distances between the particles on the mass of the heavier identical particles is presented for the ground state and $Z = 1$. In particular, the distance between protons in a molecular hydrogen ion (two fixed centers) is somewhat smaller than the distance between the electron and a proton. For $Z = 1$, the inequality $R_{12} < R_{13}$ holds for $m > 540$. In Fig. 3, we display the diagram, where the lines s_0 and s_1 for the ground state and the symmetric first excited state distances correspond to the equality $R_{12} = R_{13}$ and divide the whole area into two parts. These curves are displayed schematically, but with appropriate symbols

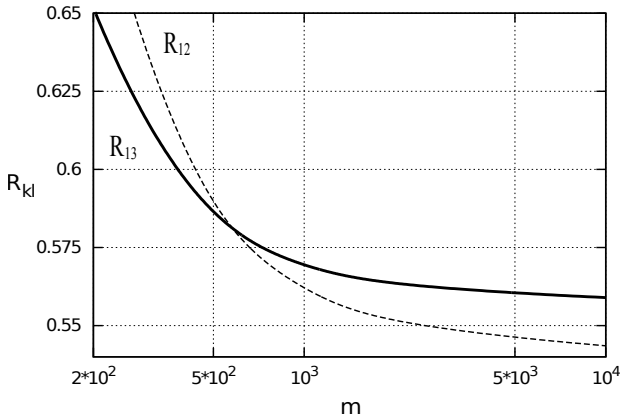

Fig. 2. Dependence of r.m.d. between particles on the mass m of identical particles ($Z = 1$, ground state)

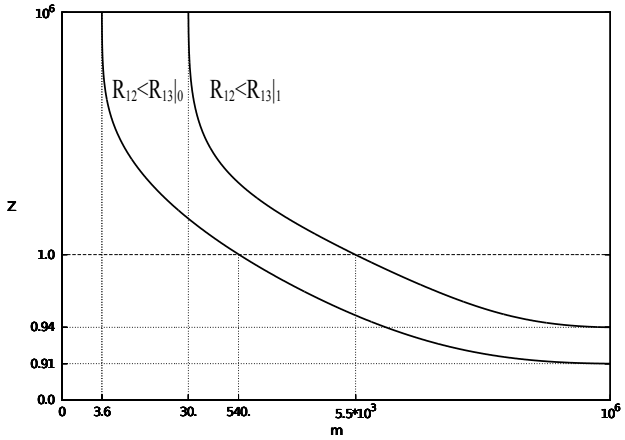

Fig. 3. Dependence of $Z_c(m)$ (schematically) under the condition $R_{12} = R_{13}$

for the asymptotics, on the (m, Z) plane in all important intervals of masses and charges. The abnormal inequality $R_{12} < R_{13}$ holds for the ground state above the line s_0 and the same is true for the first excited level. There is a similar picture for higher excited levels, where the corresponding line s_n is shifted to the right and upward, as the excitation increases. As for antisymmetric states, the normal structure with $R_{12} > R_{13}$ is observed in all reasonable regions of the (m, Z) plane.

The abnormal structure with $R_{12} < R_{13}$ can be interpreted as follows. For the 2D problem in the molecular region (e.g., molecular hydrogen ion H_2^+), where two heavy particles repel each other and are located, in fact, at a fixed distance R_{12} (this fixation of the distance is more significant comparing to the 3D space because of a much stronger binding), a light particle binding the system quickly moves only on the plane around one of the centers (every time, the light particle is at a considerable distance from another center). The mean value of these distances is R_{13}, which is greater than the distance between the fixed centers. For a light particle, there are much less possibilities for a maneuver, since it moves strictly in the plane. At the same time, if the mass m of heavy particles decreases, then the amplitude of motion of heavy particles increases (the distance between these particles increases as well), and the light particle spends more time between the centers. In this case, the distance R_{13} becomes equal to the distance R_{12} at some point and then gradually become less than R_{12} (see Fig. 2). Finally, if two identical particles are light (atomic hydrogen ion H^-), then the distance between them increases significantly due to the repulsion, and we observe a normal situation. For the 3D problem (and higher dimensions), the binding is much weaker, and the amplitude of a relative vibration of two heavy particles is higher, i.e., the result is normal. That the distance between identical particles is larger, than the distance between different particles for all values of mass m. In this case for the light particle, which binds the whole system, there is a significant probability to be located in the space between the heavy particles due to the significant space dimensionality. Therefore, $R_{13} < R_{12}$. Finally, if the space dimensionality d is the fractional and approaches 1, then the collapse occurs, and the third binding particle can be located only between the identical particles, and $R_{13} < R_{12}$ again. Thus, we see the nonmonotonicity in this anomalous effect for the relations between distances depending on the space dimensionality d.

It is useful to note some computational peculiarities of stochastic variational schemes with Gaussian basis. Indeed, the characteristic mean-square distances for the ground state monotonically decrease and approach the exact values, as the number of basis functions increases. The same is true for the energy of this state. The following natural law holds: the stronger the binding, the smaller is the system with the approximate relation $R \sim 1/\sqrt{|E|}$. Note also that, for excited states, only the energy monotonically approaches its exact value (variational prin-

ciple). At the same time, some minor fluctuations can occur for the size (or other average quantities), and these quantities converge to their exact values only on the average.

Consider now the basic structural functions such as particle density distributions and pair correlation functions for different bound states of three particles. The density distribution of particles,

$$\rho_i(r) = \langle\Psi|\delta\left(\mathbf{r} - \mathbf{r}_i + \mathbf{R}_{\text{c.m.}}\right)|\Psi\rangle, \tag{22}$$

determines the probability to find the i-th particle at a distance r from the center mass of the system. For the Gaussian basis functions (4) and for any space dimensionality d, they are defined by the expressions

$$\rho_3(r) = \frac{(1+2m)^d}{\pi^{d/2}m^dN}\sum_{i,j}^{K}\frac{N_iN_j}{(4a+b+c)^{d/2}}\times$$

$$\times\left(1+s\hat{P}(b_i\leftrightarrow c_i)\right)\exp\left\{-\frac{(1+2m)^2}{m^2}\frac{D}{4a+b+c}r^2\right\}, \tag{23}$$

$$\rho_1(r) = \frac{(1+2m)^d}{2\pi^{d/2}N}\sum_{i,j}^{K}N_iN_j\left(1+s\hat{P}(b_i\leftrightarrow c_i)\right)\times$$

$$\times\left(1+s\hat{P}(b\leftrightarrow c)\right)\frac{1}{(a+m^2b+(m+1)^2c)^{d/2}}\times$$

$$\times\exp\left\{-\frac{(1+2m)^2D}{a+m^2b+(m+1)^2c}r^2\right\}. \tag{24}$$

Similarly, the pair correlation functions

$$g_{kl}(r) = \langle\Psi|\delta\left(\mathbf{r}-\mathbf{r}_{kl}\right)|\Psi\rangle \tag{25}$$

determine the probability to find a pair of particles kl at a distance r and have the form

$$g_{12}(r) = \frac{1}{\pi^{d/2}N}\sum_{i,j}^{K}\frac{N_iN_j}{(b+c)^{d/2}}\left(1+s\hat{P}(b_i\leftrightarrow c_i)\right)\times$$

$$\times\exp\left\{-\frac{D}{b+c}r^2\right\}, \tag{26}$$

$$g_{13}(r) = \frac{1}{2\pi^{d/2}N}\sum_{i,j}^{K}N_iN_j\left(1+s\hat{P}(b_i\leftrightarrow c_i)\right)\times$$

$$\times\left(1+s\hat{P}(b\leftrightarrow c)\right)\frac{1}{(a+c)^{d/2}}\exp\left\{-\frac{D}{a+c}r^2\right\}. \tag{27}$$

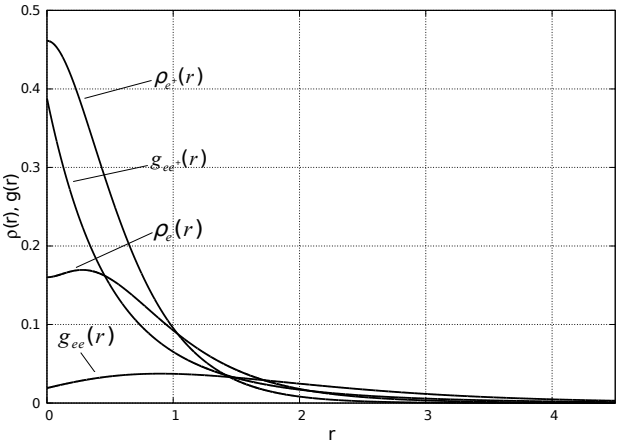

Fig. 4. Structural functions for the ground state of Ps^-

In all expressions (23), (24), (26), and (27), the full normalization integral is denoted by N (17), D is determined by (8), and the permutation operator $\hat{P}(b\leftrightarrow c)$ is similar to (7).

As an example of the radial dependence of the structural functions for two-dimensional systems, let us consider the particle density distributions and the correlation functions (Fig. 4) in a positronium ion Ps^- ($Z = 1$, and $m = 1$ corresponds to an intermediate case between the atomic and molecular regions). First, we note that the electron density distribution $\rho_e(r)$ (formula (24)) has a small dip at the origin (relative to the center of mass of the entire three-particle system) due to the repulsion between electrons. Second, the correlation functions have a much more extent asymptotic behavior in comparison with the density distributions. Consequently, m.s.d are always much larger than m.s.r. Third, the correlation function of two identical electrons $g_{ee}(r)$ (formula (26)) has a considerable dip at small distances because of their repulsion. Such behavior of the correlation functions is common for all systems, where the pair of particles has repulsion at small distances.

We now consider the density distributions of particles in a molecular hydrogen ion (H_2^+, $M = 1$, $m = 1836.152701$). As seen from Fig. 5, firstly, the heavy particles (protons p) are located almost at a fixed distance from the center of mass, which is located at the middle between the heavy particles. At the same time, the density distribution of the light particle (electron e) has a maximum at the origin (at the center of mass). Secondly, the figure shows the values of $r\rho(r)$ for greater clarity, which directly cor-

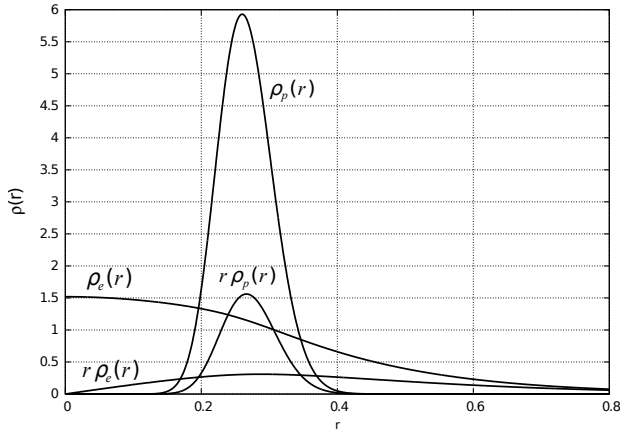

Fig. 5. Density distribution for the ground state of H_2^+

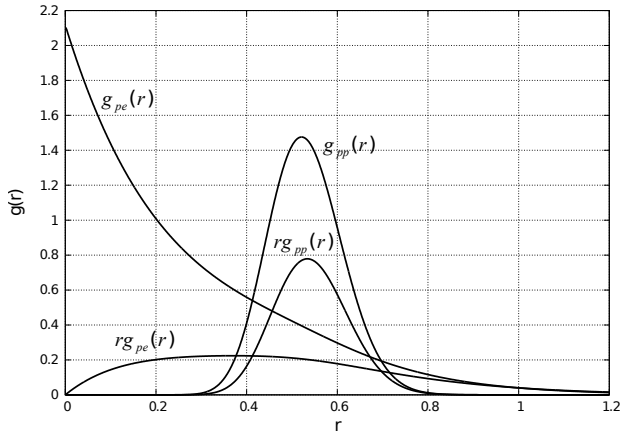

Fig. 6. Pair correlation functions for the ground state of H_2^+

respond to the probability of finding the corresponding particles at a distance r. One can see that m.s.r. of light particles is substantially larger than m.s.r. of heavy particles. The correlation functions are represented in Fig. 6 for H_2^+. This confirms again the fact that the heavy particles are located at a practically fixed distance, since $g_{pp}(r)$ is strongly localized around a distance of the order of 0.55. At the same time, the correlation function of different particles $g_{pe}(r)$, especially that multiplied by r, is more extent, and its typical radius can be larger than the distance between the identical particles, what have been discussed.

Finally, we indicate the general trends concerning the structural functions with a changing mass m (and for a fixed charge) from very small values in the atomic regime (or $m = 1$ and a very large mass of the third particle M) to significant m in the molecular regime. In the atomic regime (for example, atomic hydrogen ion), the heavy particle is strongly localized in a vicinity of the center of mass. The density distribution has a delta-like form, and two electrons are located at considerable distances from each other and from the fixed center. Meanwhile, the electronic density distribution monotonically decreases, as the distance increases. We emphasize that, in the atomic regime (single-centered problem), the correlation function between light and heavy particles is quite similar to the density distribution of a light particle. At the same time, the pair correlation function $g_{ee}(r)$ at small distances is suppressed significantly due to the repulsion and has a considerable tail at large distances. The extent of the correlations between light particles in the ground state is especially significant, when the system is close to the two-particle break-up (close to the threshold curve s_0 in Fig. 1). With increasing mass m (decreasing M), the center of mass becomes less fixed, and the amplitude of oscillations of two identical particles becomes smaller. For larger masses m, two identical particles become two fixed centers. If $Z > 1$, and if the mass M is large (e.g., helium atom), then two electrons in the ground state move in the field of a fixed center. In this case, the electron-electron repulsion becomes negligible, the electron distributions are monotonically decreasing, as the distance increases, and the density distribution radius decreases significantly.

5. Some Reference Three-Particle Systems

In this section, we briefly discuss the results of calculations of energies and sizes for some specific standard two-dimensional trions and compare them with other available results and with corresponding three-dimensional problems.

1. Consider firstly a molecular hydrogen ion H_2^+ ((ppe) with $m = 1836.152701$). In Table 4, we present the dissociation energy $D_n = E_0(2) - E_n(3)$ of several first symmetric vibrational (s) excited states (according to (12), the total number of symmetric states is 24) and two existing antisymmetric (a) states. Comparing to the 3D problem [3], the dissociation energy for symmetric states in the 2D space is larger by almost one order of magnitude (around 8 times). For the antisymmetric excited state, the difference is more by almost 4 orders. In Table 5 (second row), the results for the ground-state energy and the characteris-

tic distance are presented (the energy of the ground state of a hydrogen atom is $E_{0(2D)}(2) = -1.99891$). The data in this paragraph for the three-dimensional system are borrowed from [3]. It is useful to compare quantitatively the degree of stronger binding of two-dimensional systems comparing to three-dimensional ones. The following inequalities are satisfied:

$$\frac{E_{0(2D)}(3)}{E_{0(3D)}(3)} = 4.65 > 4, \tag{28}$$

$$\frac{R_{0(2D)}(3)}{R_{0(3D)}(2)} = 1/3.2 < 1/2\sqrt{2}. \tag{29}$$

They reflect more general patterns of relative growth due to the increased number of particles and the corresponding reduction in size. It is useful to note an abnormal ratio for m.s.d. for the molecular regime that has been discussed above: the distance R_{pe} between particles with attraction is slightly greater than the distance R_{pp} between identical heavy particles with repulsion.

2. For a positronium ion Ps^-, which is the most typical example of a system that corresponds to an intermediate case between the molecular and atomic regimes, we have only one weakly bound state, which is a demonstration of the stability diagram in Fig. 1. The energy and characteristic distances are shown in Table 5 (third line). It is also worth noting that the three-particle system is more bound than the two-particle one ($E_{0(2D)}(2)$=-1.0), and inequalities (28) and (29) are satisfied, although weaker than those for H_2^+.

Note that the ground-state energy of a positronium ion is obtained in work [6] coincides with the value from Table 5.

3. Consider the next trion with atomic nature, namely an atomic hydrogen ion H^-, for which there is also only one weakly bound energy level with parameters displayed in the 4-th row of Table 5. This system have one-center regularities, when the heavy proton is located almost in the center of mass (R_3 is very small), and the electron-electron distance R_{12} is significantly greater than the distance from the electron to the proton. In addition, inequalities (28) and (29) are even weaker than those for P_s^-. Note also that the energy of H^- depends slightly on the mass of the nucleus (proton). For the mass $M = \infty$, the energy $E_{0(2D)}(3) = -2.2402$, which is consistent with the result in [6].

4. Consider some results for a helium atom He ($Z = 2$, $m = 1$, $M = 7294.2995$) in the 2D space. First of all, we again recall that, since $Z > 1$, the discrete spectrum for this atom is infinite for both symmetric and antisymmetric states. Here, we present the data only for the first three (symmetric s_0 and s_1 and antisymmetric a_0) lowest states (Table 6), and the threshold energy of two particles $E_0(2) = -7.99891$. For a He atom, the role of a finite mass of the nucleus is else smaller. The calculated ground-state energy of a helium atom with infinite mass of the nucleus is $E_{0(2D)}(3) = -11.89982$, which is consistent with [7].

Note that the binding in the ground state of a helium atom in 2D is at least 4 times stronger than that in the 3D problem. But, for the excited levels, this ratio is somewhat smaller and decreases monotonically to 1, as the excitation increases. In particular, it holds for two particles, where the spectrum with zero angular momentum and dimension d is

$$E_n(2; m, Z) = -\big(2mZ^2/(m+1)\big)/(2n+d-1)^2. \tag{30}$$

Table 4. **Dissociation energies of the lowest energy states of He_2^+**

State n	s_0	s_1	s_2	a_0	a_1
D_n	0.779	0.696	0.615	1.97×10^{-4}	1.89×10^{-5}

Table 5. **Energy and characteristic distances for the ground states of H_2^+, Ps^-, and H^-**

$E_{0(2D)}(3)$	R_{12}	R_{13}	R_1	R_3	$E_{0(3D)}(3)$
−2.778	0.5489	0.5611	0.2747	0.4907	−0.59713682
−1.1215948	3.0178	2.1889	1.5988	1.0571	−0.26200507
−2.239	1.646	1.132	1.131	8.46×10^{-4}	−0.5274458

Table 6. **Energy and characteristic distances for an atom He**

$E_{0(2D)}(3)$ $E_{0(3D)}(3)$	R_{12}	R_{13}	R_1	R_3
s_0 −11.89811 −2.90330444	0.559954	0.386898	1.131	$7.3195 \cdot 10^{-5}$
a_0 −8.2948 −2.17493011	2.948	2.083	2.083	$4.04 \cdot 10^{-4}$
s_1 −8.2493 −2.14567849	3.437	2.429	2.429	$4.707 \cdot 10^{-4}$

Note that levels with different symmetries alternate in the energy spectrum of helium atoms, similarly to the 3D problem [3]. Moreover, the ground-state energy of an atom is separated from excited levels by a considerable interval or gap in the spectrum. This fact is characteristic of the atomic regime.

6. Conclusion

Our main result establishes the conditions of stability on the mass-charge plane for the ground and excited symmetric and antisymmetric states with zero angular momentum for the two-dimensional problem of three charged particles. The constructed diagrams of stability allow us to give the general pattern of bound states for trion systems in the 2D space.

There are the nontrivial structural features of some reference systems with three charged particles, and the general regularities depending on the mass and the charge of symmetric trions XXY in the 2D space. First, it is found that the quadrupole moment on the spherically symmetric wave functions is zero only in the 3D space. For the two-dimensional problem, the quadrupole moment is always positive, and it generates an attractive effective multipole interaction potential, which has the asymptotic behavior $-1/r^3$ even in a polar-symmetric field. Second, for three charged particles in the molecular regime, in particular for a molecular ion H_2^+ in the 2D space, it is found that the distance between two protons, which repel each other, is less than the distance between the proton and the electron, although they attract each other. It is generally known that such anomalies do not exist for the three-dimensional problems.

These issues will be further considered in the adiabatic approximation, where a proper justification on a transparent physical level can be provided.

The current research have a perspective to study the common problems of low-dimensional Coulomb systems with a few particles or centers with proper consideration of correlations, many-body effects, and corresponding symmetries of many-centered problems and specific Coulomb problems in spaces with any dimensionality d, including fractional ones.

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УМОВИ СТАБІЛЬНОСТІ
ДВОВИМІРНИХ КВАНТОВИХ СИСТЕМ
ТРЬОХ ЗАРЯДЖЕНИХ ЧАСТИНОК

Р е з ю м е

Досліджено умови існування симетричних та антисиметричних зв'язаних енергетичних рівнів (умови стабільності) на площині маса–заряд (m, Z) для двовимірних кулонівських систем трьох заряджених частинок, коли розглядаються дві тотожні частинки одного сорту, а третя частинка іншого сорту. Високоточні тричастинкові чисельні розрахунки виконано на основі стохастичного варіаційного методу з гаусоїдними базисами. Встановлено низку аномальних ефектів у поведінці характерних відстаней між частинками та наявності ненульового квадрупольного моменту у двовимірному полярно-симетричному полі. Виконано систематичне порівняння результатів дослідження для дво- та тривимірних систем. Для декотрих еталонних систем трьох частинок отримано енергії, розміри, розподіли густини та кореляційні функції.