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2003 J. Phys. A: Math. Gen. 36 L13

(http://iopscience.iop.org/0305-4470/36/1/103)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) L13–L20 PII: S0305-4470(03)52989-4

LETTER TO THE EDITOR

An example of three-body collapse

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Received 2 September 2002
Published 10 December 2002
Online at stacks.iop.org/JPhysA/36/L13

Abstract
The system of three identical bosons with s-wave inverse square interactions and zero total angular momentum is investigated within the Faddeev integrodifferential approach. It is proved that all three bosons can collapse, i.e. 'fall' into their centre of mass, if the constant of the interactions is sufficiently small, namely less than $-0.267\ldots$

PACS numbers: 21.45.+v, 02.60.Nm, 02.30.Mv, 02.70.Jn

In quantum mechanics [1], the problem of two particles interacting via the inverse square potential c/x^2, where c is an arbitrary real parameter and x is the interparticle distance, is completely solved. For example, the corresponding theorem for the existence of the solutions to the Schrödinger equation

$$\left(-\partial_x^2 + \frac{c}{x^2}\right)\psi(x;e) = e\psi(x;e) \qquad x \geqslant 0 \tag{1}$$

with zero angular momentum and an arbitrary real energy e can be formulated as the following three statements.

First, at any $e > 0$ and $c \in (-\infty, \infty)$ has the solution $\psi(x, e)$ describing the scattering state and having a physically acceptable ($\psi \to 0, x \to 0$) asymptotics at small distances

$$\psi(x;e) = O(x^q) \qquad q \equiv \tfrac{1}{2} + \sqrt{c + 1/4} \qquad x \to 0.$$

Second, at any $c < -1/4$ there is a solid spectrum of negative eigenvalues e and the corresponding square integrable eigenfunctions describing the bound states.

Finally, the ground state corresponds to the energy $e = -\infty$.

In this state the binding energy $|e|$ of two particles is infinitely large and, owing to the principle of uncertainty [1], the particles are located in an infinitesimal neighbourhood of their centre of mass ($x = 0$). Therefore, it is often said that at $c < -1/4$ the particles collapse, i.e. 'fall' at the point $x = 0$.

A sufficient condition for the collapse of N quantum-mechanical particles ($N > 2$) with two-body inverse square interactions is in general unknown [2] even if the interactions act

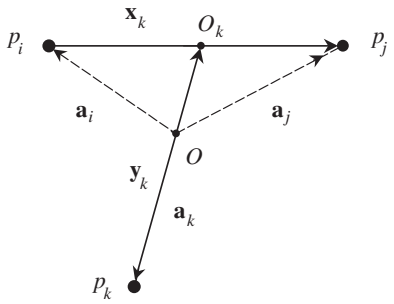

Figure 1. The radius vectors $\mathbf{a}_i, \mathbf{a}_j, \mathbf{a}_k$ of the bosons p_i, p_j, p_k and the corresponding Jacobi vectors $\mathbf{x}_k$ and $\mathbf{y}_k$.

only in the pairwise s-states. The main aim of the present work is to find this condition for three identical bosons p_1, p_2, p_3 having zero total angular momentum ℓ and interacting via S-wave inverse square potentials. To present these potentials we should first clarify the physical meaning of the three-body coordinates used. For this, we discuss some formulae.

So, in three-dimensional coordinate space $\mathcal{R}^3$ we introduce a fixed Cartesian system S_3 with the starting point O coinciding with the centre of mass of the three bosons. Let $\mathbf{a}_i$ be the radius vector of the boson p_i in the system S_3. Then we define three pairs of relative Jacobi coordinates $(\mathbf{x}_k, \mathbf{y}_k)$

$$\mathbf{x}_k \equiv \mathbf{a}_j - \mathbf{a}_i \qquad \mathbf{y}_k \equiv \frac{2}{\sqrt{3}}\left(\frac{\mathbf{a}_i + \mathbf{a}_j}{2} - \mathbf{a}_k\right) \tag{2}$$

where the indices i, j and k form a cyclic permutation of the triad of indices $(1, 2, 3)$: the index i becomes k, j becomes i and k becomes j. As one can see from figure 1, the Jacobi vector $\mathbf{x}_k$ connects the bosons p_i and p_j, and the Jacobi vector $\mathbf{y}_k$ is directed from the boson p_k to the centre of mass O_k of the pair (p_i, p_j). Finally, let (r, Ω_k) be the hyperspherical coordinates associated with the Jacobi vectors (2) by the formulae

$$r = \left(x_k^2 + y_k^2\right)^{1/2} \geqslant 0 \qquad \Omega_k = (\hat{x}_k, \hat{y}_k, \varphi_k)$$
$$\varphi_k = \operatorname{atan}(y_k/x_k) \in [0, \pi/2] \qquad k = 1, 2, 3.$$

Hence, the three-boson centre of mass is the point O with zero hyperradius ($r = 0$) and the distance between any two bosons vanishes, if and only if $r = 0$.

In our model each of the two bosons p_i and p_j interacts via the corresponding S-wave inverse square potential

$$V_k(\mathbf{x}_k) = \frac{c}{x_k^2} P_k^0 \qquad P_k^0 \equiv |Y_{00}(\hat{x}_k)\rangle\langle Y_{00}(\hat{x}_k)| \tag{3}$$

where Y_{00} is the spherical function and P_k^0 is the projector on the S-state of the bosons p_i and p_j. Due to the projectors P_k^0 these potentials are the nonlocal interactions. Hence, the total potential energy $V \equiv V_1 + V_2 + V_3$ is also the nonlocal and very complicated operator. Therefore, even in the case $\ell = 0$ the explicit and simple formula for the mapping $V\Psi$ of the three-boson wavefunction Ψ is unknown. But, if Ψ is expanded over the Legendre polynomials P_b,

$$\Psi(r, \varphi, u) = \sum_{b=2,4,\ldots} \sqrt{\frac{2b+1}{2}} P_b(u) \Psi_b(r, \varphi) \qquad \varphi \equiv \varphi_1 \qquad u \equiv \frac{(\mathbf{x}_1 \mathbf{y}_1)}{x_1 y_1} \tag{4}$$

then, according to the kinematic transformation theory [3], the mapping $V\Psi$ can be represented as a double infinite series

$$V\Psi(r,\varphi,u)=\frac{c}{r^2}\sum_{a,b=2,4,\ldots}P_a(u)\left[\sqrt{\frac{2a+1}{2}}\delta_{ab}\sec^2\varphi+\int_{-1}^{1}\mathrm{d}u\frac{P_a(u)A_b(\varphi')}{2-\cos 2\varphi+\sqrt{3}u\sin 2\varphi}\right]. \tag{5}$$

Here the angle $\varphi'\in[0,\pi/2]$ is the function of φ and u, $A_b(\varphi')$ is the integral

$$2\cos 2\varphi'=\sqrt{3}u\sin 2\varphi-\cos 2\varphi \qquad A_b(\varphi')=\int_{-1}^{1}\mathrm{d}u' P_b(u')P_b(u'')\Psi_b(r,\varphi'')$$

and in the integrand $\varphi''\in[0,\pi/2]$ and u'' are the functions of φ' and u':

$$-2\cos 2\varphi''=\sqrt{3}u'\sin 2\varphi'+\cos 2\varphi' \qquad 2u''\sin 2\varphi''=u'\sin 2\varphi'+\sqrt{3}\cos 2\varphi'.$$

By using expansions (4) and (5), the Schrödinger equation for Ψ

$$(H_0+V-E)\Psi=0 \qquad H_0\equiv-\left(\triangle_{x_k}+\triangle_{y_k}\right)$$

is reduced to the infinite system of coupled two-dimensional integrodifferential equations for the components Ψ_b. However, this system seems to be unsolvable even numerically.

In contrast to the Schrödinger equation, the Faddeev differential equations [2]

$$(H_0-E)\Psi_k=-V_k\Psi \qquad \Psi=\sum_{i=1}^{3}\Psi_i \quad k=1,2,3 \tag{6}$$

do not contain the total interaction V. In fact, each Faddeev equation contains only the corresponding two-body potential. Therefore, by the substitution of

$$\Psi_k(r,\Omega_k)=2r^{-5/2}\operatorname{cosec}2\varphi_k U(r,\varphi_k)Y_{00}(\hat{x}_k)Y_{00}(\hat{y}_k) \qquad k=1,2,3 \tag{7}$$

the Faddeev equations (6) are reduced to one integrodifferential equation:

$$\left(r^2\partial_r^2+\frac{1}{4}+Er^2\right)U(r,\varphi)=\left(-\partial_\varphi^2+\frac{c}{\cos^2\varphi}\right)U(r,\varphi)+\frac{c}{\cos^2\varphi}s\int_{C_-(\varphi)}^{C_+(\varphi)}\mathrm{d}\varphi' U(r,\varphi') \tag{8}$$

where $\varphi\equiv\varphi_1$, $s\equiv 4/\sqrt{3}$ and the integral limits are the break-lines

$$C_-(\varphi)=\left|\varphi-\frac{\pi}{3}\right| \qquad C_+(\varphi)=\frac{\pi}{2}-\left|\frac{\pi}{6}-\varphi\right|.$$

As one can see, on the left-hand side of equation (8) all the operators act only on the argument r, and on the right-hand side the operators act only on the other argument, i.e. on φ. Hence, the left and right sides are equal to a constant p^2. Therefore, as Avishai first noted in [4], the arguments r and φ are separated from each other by the substitution

$$U(r,\varphi)=f(r)g(\varphi).$$

As a result, one gets two equations connected only by the constant, p^2, of separation of independent variables r and φ. It should be emphasized that the first equation

$$\left(-\partial_r^2+\frac{p^2-1/4}{r^2}\right)f(r)=Ef(r) \tag{9}$$

is similar in form to equation (1) and the other equation

$$\left(-\partial_\varphi^2+\frac{c}{\cos^2\varphi}\right)g(\varphi)+\frac{c}{\cos^2\varphi}s\int_{C_-(\varphi)}^{C_+(\varphi)}\mathrm{d}\varphi' g(\varphi')=p^2g(\varphi) \tag{10}$$

has to be added by the boundary conditions

$$g(\varphi) = 0 \qquad \partial_\varphi^2 g(\varphi) = 0 \qquad \varphi = 0, \pi/2 \tag{11}$$

providing the regularity of the Faddeev components (7) at the points $\varphi = 0$ and $\varphi = \pi/2$.

Note that the problem (10), (11) was solved numerically by Avishai [4], but only for $c = 0, -1, \ldots, -6$ and, unfortunately, the author used a wrong value $s = 1$ for the coefficient $s = 4/\sqrt{3}$. This is a reason to re-examine this problem and investigate it in more detail.

The plan of our further study can be formulated as follows.

First, we compare equation (1) with equation (9) and, as a result, we prove that a three-boson collapse can take place only if $p^2 < 0$.

Second, we clarify why the well-known method [5, 6] based on the representation

$$g(\varphi) = \sum_{n=1}^{N} b_n \sin 2n\varphi \tag{12}$$

is inconvenient for numerical study of the problem (10), (11) when $c < 0$ or $p^2 < 0$.

Finally, as a result of solving this problem by the modified spline-function [7] method [8] we prove that $p^2 < 0$ if c is sufficiently small, namely $c < c_b = -0.267\ldots$

So, the three-particle equation (9) studied differs from the two-particle equation (1) only by notation: r plays the role of x, $p^2 - 1/4$ stands for c and E stands for e. Therefore, the above-mentioned theorem can be applied to equation (9). Hence, under the condition $p^2 - 1/4 < -1/4$ or $p^2 < 0$, equation (9) has the solution describing the three-boson bound state with an infinitely large binding energy $B = -E = \infty$. In other words, all three bosons can collapse when p is a pure imaginary number, as we wished to prove.

Now, let us analyse the eigenvalue problem (10), (11) in which p^2 and g are, respectively, the eigenvalue and eigenfunction. For any c and $p^2 = 16$ there is the solution $g = \sin 4\varphi$ generating the spurious ($\Psi_1 + \Psi_2 + \Psi_3 \equiv 0$) solution [3, 9] to the Faddeev equations (6). In what follows this solution is not considered because it corresponds to the trivial three-boson wavefunction ($\Psi \equiv 0$). At $c = 0$ all the eigenvalues are positive and integer numbers, namely, $p_1^2 = 4$, $p_{\nu-1}^2 = (2\nu)^2$, $\nu = 3, 4, \ldots$, and for each eigenvalue p_ν^2 there is only one eigenfunction $g = g_\nu$: $g_1 = \sin 2\varphi$, $g_\nu = \sin(2(\nu+1)\varphi)$, $\nu = 2, 3, \ldots$.

By the well-known criterion [5], the exact solution, representable as a finite sum (12), exists if and only if $p^2 = (t+2)^2$, $N = t/2 + 1 < \infty$, where $t = 4, 6, \ldots$, and the nonzero constant c and the coefficients b_n obey the well-defined algebraic eigenvalue problem.

For example, at $c = 4$ and $p^2 = p_1^2 = 36$ the exact solution reads [5]

$$g(\varphi) = \sin 2\varphi - \tfrac{4}{5} \sin 4\varphi - \sin 6\varphi \tag{13}$$

and the simple methods to calculate the other exact solutions are presented in [5, 6].

The criterion has an important corollary [3]: for any $p^2 \neq (t+2)^2$, $t = 0, 2, \ldots$, and hence for $p^2 \leqslant 0$, all the solutions of the problem (10), (11) are the infinite ($N = \infty$) expansions (12) whose convergence is not proven analytically.

For a numerical analysis of the convergence of these expansions, we assume that $p^2 \neq t^2$ at any odd positive t. Therefore, $4n^2 - p^2 \neq 0$ for any natural n, and the infinite sum (12) can be rewritten in a more convenient form for our purpose,

$$g(\varphi) = \sum_{n=1}^{\infty} \frac{X_n}{4n^2 - p^2} \sin 2n\varphi \qquad b_n = \frac{X_n}{4n^2 - p^2} \qquad n = 1, 2, \ldots. \tag{14}$$

Now, we multiply equation (10) by the function $\cos^2 \varphi$ and substitute the ansatz (14) in the equation thus obtained. Then, using for any φ and integer n the trigonometric identity

$$4 \cos^2 \varphi \sin 2n\varphi = \sin 2(n-1)\varphi + 2 \sin 2n\varphi + \sin 2(n+1)\varphi$$

and the well-known spectral formulae [3]

$$\int_{C_-(\varphi)}^{C_+(\varphi)} \mathrm{d}\varphi' \sin 2n\varphi' = K_n \sin 2n\varphi \qquad K_n = \frac{\sin 2n\pi/3}{n \sin 2\pi/3} \tag{15}$$

we reduce the equation to the infinite but algebraic linear system of homogeneous equations for the unknown coefficients X_n:

$$\left(2 + \frac{12c}{4 - p^2}\right) X_1 + X_2 = 0$$

$$X_{n-1} + \left(2 + \frac{4c(1 + 2K_n)}{4n^2 - p^2}\right) X_n + X_{n+1} = 0 \qquad n = 2, 3, \ldots.$$

As one can see, only the second ($n = 2$) equation does not contain the constant c because, owing to (15), $1 + 2K_n = 0$ only for $n = 2$. Let us exclude $X_2 = -(X_1 + X_3)/2$ from the infinite system and then study the finite subsystem

$$3\left(\frac{1}{2} + \frac{4c}{4 - p^2}\right) X_1 - \frac{1}{2} X_3 = 0$$

$$-\frac{1}{2} X_1 + \left(\frac{3}{2} + \frac{4c}{36 - 4p^2}\right) X_3 + X_4 = 0$$

$$X_{n-1} + \left(2 + \frac{4c(1 + 2K_n)}{4n^2 - p^2}\right) X_n + X_{n+1} = 0 \qquad n = 4, 5, \ldots, N - 1$$

$$X_{N-1} + \left(2 + \frac{4c(1 + 2K_N)}{4N^2 - p^2}\right) X_N = 0 \qquad N < \infty.$$

As is well known [10], this homogeneous system has a nontrivial solution if and only if the determinant $\det \mathbf{A}$ of its matrix $\mathbf{A}$ is equal to zero which is impossible when $\mathbf{A}$ has a dominant main diagonal, in other words, when all the following relations hold:

$$|A_{nn}| > |A_{n-1,n}| + |A_{n,n+1}| \qquad n = 1, \ldots, N - 1.$$

Owing to (15) $|K_n| \leqslant 1/n$ for all n and by definition c is a real number. Therefore, at least one of these relations is not valid only for a real p^2 in two cases: $c > 0$, $p^2 > 4$ or $c < 0$, $p^2 < 4N^2$, and only in these cases may $\det \mathbf{A}$ vanish. Hence, p^2 may be negative only for negative c when interactions (3) are attractive ones. As $\mathbf{A}$ depends on c and p^2, the relation $\det \mathbf{A}(c, p^2) = 0$ means that the allowed p^2 is a function of c: $p^2 = p^2(c)$, or vice versa $c = c(p^2)$. Then, the matrix $\mathbf{A}$ has dimension $N - 1$ and is the Jacobi matrix [10]. For any fixed $p^2 < 4N^2$ the determinant of this matrix is a polynomial of c of degree $N - 1$ and has exactly $N - 1$ simple zeroes $c = c_1, c_2, \ldots, c_{N-1}$. Hence, for any fixed c the determinant has $N - 1$ different zeroes $p^2 = p_\nu^2(c)$ that we arrange as $p_1^2(c) < p_2^2 < \cdots < p_{N-1}^2(c)$.

As we have established, to calculate the root p_1^2 of the equation $\det \mathbf{A} = 0$ with one per cent relative accuracy, one can use a comparatively small N if $c > 0$ and N should be too large if $c < 0$. For example, $N = 30$ for $c = 0.2$ while $N = 5 \times 10^7$ for $c = -0.3$ when $p^2 < 0$. In other words, at $c < 0$ expansions (12) converge too slowly as $N \to \infty$. Therefore, to calculate p^2 and g we have applied another method in which these expansions are not used.

In this method the nodes φ_j of the uniform grid $\triangle_\varphi$ with the step h

$$\triangle_\varphi : \varphi_j = hj \qquad j = 0, 1, \ldots, M \quad h = \pi/2M$$

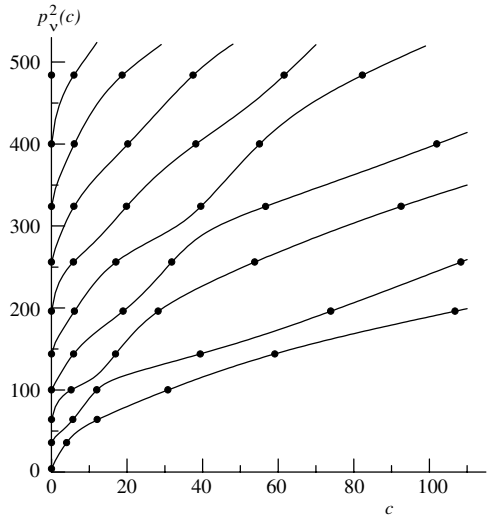

Figure 2. The solid curves are the eigenvalues $p_1^2(c) < p_2^2(c) < \cdots < p_9^2(c)$ as functions of the non-negative parameter c of interactions (3) and each dot is the point (c, p_ν^2) with the abscissa c and ordinate $p_\nu^2 = (t+2)^2$, such that the exact solution (12) with $N = t/2 + 1$ exists.

are used as collocation nodes, the searched function g is approximated by the cubic spline $S(\varphi) = S_{3,1}(\varphi)$ of C^2-class [7] and, instead of the second-order accuracy approximation

$$\partial_\varphi^2 g(\varphi)|_{\varphi=\varphi_j} = S_j'' + O(h^2) \qquad S_j'' \equiv \partial_\varphi^2 S(\varphi)|_{\varphi=\varphi_j} \qquad j = 1, 2, \ldots, M-1$$

that we have applied in [8], a more accurate fourth-order approximation [7] is used

$$\partial_\varphi^2 g(\varphi)|_{\varphi=\varphi_j} = \frac{1}{12h^2}(S_{j-1}'' + 10S_j'' + S_{j+1}'') + O(h^4) \qquad j = 1, 2, \ldots, M-1.$$

For this reason, the method described has fourth-order accuracy. To demonstrate its power, we have solved the problem (10), (11) at $c = 4$ and $M = 1000$ and then compared the calculated eigenvalue $\tilde{p}^2 = 36.0 + 2 \times 10^{-10}$ and the eigenfunction S with the exact eigenvalue $p^2 = 36$ and eigenfunction (13), respectively. Thus, we have found

$$\left|\frac{\tilde{p}^2}{p^2} - 1\right| = O(10^{-12}) \qquad \left|\frac{S(\varphi_j)}{g(\varphi_j)} - 1\right| = O(10^{-6}) \qquad j = 1, \ldots, M-1.$$

Hence, for the uniform grid formed by one thousand nodes ($M = 1000$), one may expect comparatively high relative accuracy. Therefore, we have used this grid for the calculation of the eigenvalues $p^2 = p_\nu^2(c)$, $\nu = 1, 2, \ldots$, plotted by the solid lines in figures 2 and 3 as well as for the calculation of the corresponding eigenfunctions $g(\varphi) = S(\varphi) = g_\nu(\varphi)$.

As was numerically established, for $c \in [-10, 100]$ each ($\nu = 1, 2, \ldots, M-1 = 999$) eigenvalue $p^2 = p_\nu^2(c)$ is a monotonically increasing function of c, i.e. $p_\nu^2(c) < p_\nu^2(c+\varepsilon)$ for any c and $\varepsilon > 0$, and all $M-1$ eigenvalues p_ν^2 form the monotonically growing set: $p_\nu^2(c) < p_{\nu+1}^2(c)$ for any c and $\nu = 1, 2, \ldots, M-1$. Therefore, the zeroes c^ν of these eigenvalues form the monotonically decreasing set: $c^{\nu+1} < c^\nu$ for any $\nu = 1, 2, \ldots, M-1$. In particular, $c^1 \approx -0.267$, $c^2 \approx -0.532$ and $c^3 \approx -1.167$ and only the last significant digits of these numbers change when M is chosen larger than 1000. Hence, at least at one per cent accuracy, the desired relation $p^2 < 0$ takes place for any c less than zero $c_b \equiv c^1 = -0.267\ldots$ of the minimal (first) eigenvalue $p^2 = p_1^2(c)$. Therefore, at this c there is a special three-boson state $|\nu\rangle$ with $\nu = 1$ and the Faddeev hyperangular component $g = g_1$ corresponding to the

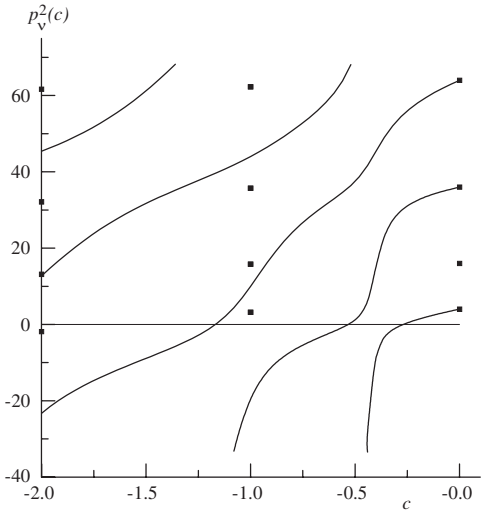

Figure 3. The thin solid line is the level $p^2 = 0$, the solid curves are the eigenvalues $p_1^2(c) < p_2^2(c) < \cdots < p_5^2(c)$ as functions of the negative parameter c of interactions (3) when $s = 4/\sqrt{3}$ in equation (10), and each square is the point (c, p_ν^2) with the abscissa $c = 0$, $c = -1$ or $c = -2$ and the corresponding ordinate $p_\nu^2 = \lambda$ calculated in [4] for $s = 1$.

value $p^2 = p_1^2(c)$. In this state all three bosons collapse. At $c^2 < c < c^1$ all eigenvalues p_ν^2 with $\nu \geqslant 2$ are positive and, therefore, in the corresponding states $|\nu\rangle$ three bosons do not collapse. Thus, for $c^{n+1} < c < c^n$, $n = 1, 2, \ldots, M-1$ the eigenvalues p_ν^2 with $\nu < n$ are negative, while all the other eigenvalues are positive. Therefore, for this c all three bosons collapse in the states $|\nu\rangle$ with $\nu = 1, 2, \ldots, n$ and do not collapse in all other states with $\nu \geqslant n+1$.

So, we have attained our main aim, and now we can formulate the main result as follows: at zero total angular momentum and sufficiently small constant c of interactions (3), namely $c < -0.267\ldots$, all three bosons collapse in the state $|1\rangle$.

In conclusion, we discuss a possible application of our method to the investigation of exotic three-atom clusters having a very large (about a few tens of ångstroms) size [11].

In the cited paper [11] two statements were proved.

First, if the binding energy in an 'electron+atom' pair is sufficiently small, three-atom clusters may arise in the four-body systems formed by three identical atoms bounded by a single electron.

Second, in these systems the effective 'atom+atom' interaction has the leading term c/x^2, in which x is the distance between two atoms and the constant c is negative.

Hence, the model of three identical bosons with interactions (3) and our spline-algorithm seem to be applicable for the calculation of the wavefunctions and binding energies of the S-states of three-atom clusters.

Acknowledgments

The author is grateful to Dr V A Roudnev, Dr F M Pen'kov and Professor S I Vinitsky for useful discussions.

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