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On the algebraic solution of the non-relativistic three-body problem: bound states

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Abstract. It is shown that the Schrödinger equation for a non-relativistic three-body system can be written in closed form by using only nine generators of three independent $O(2, 1)$ algebras and a few physical parameters (three masses and potential characteristics). In the case of Coulomb three-body systems such a form contains only a finite number of terms and six physical parameters (three masses and three charges). For a number of Coulomb three-body systems with unit charges (i.e. $X^+X^+Z^-$ and $X^+Y^+Z^-$), optimized parameters for simple approximate wavefunctions have been obtained.

1. Introduction

It is known that three-body systems play a unique role in non-relativistic quantum mechanics. Such systems are of interest in atomic, nuclear and plasma physics, as well as in condensed matter theory. From the theoretical point of view, three-body systems have a small number of degrees of freedom and, therefore, their properties can be found from the first quantum-mechanical principles. However, in contrast with two-body systems, they seem quite complicated and, therefore, as a rule, they have been investigated by applying numerical procedures.

The main goal of the present article is to develop an alternative method for the analytical consideration of three-body systems. We will show that the Schrödinger equation for a three-body system can be written as an equation in terms of generators of three independent $O(2, 1)$ algebras. This makes it possible to find analytical solutions or to investigate its properties without direct solution of the Schrödinger equation. Also, by using the commutation relations of the $O(2, 1)$ algebra, one can simplify significantly the Schrödinger equation and thereby, in principle, achieve greater accuracy of numerical solution. It should be mentioned here that such a procedure was used for the first time in [1] to consider Coulomb three-body systems. It was shown that in such a case the appropriate Schrödinger equation contains only nine generators of three $O(2, 1)$ algebras and six physical parameters (the masses and charges of each of the three particles). Unfortunately, these nine generators could not be chosen as independent. Now we have overcome this and related problems and wish to present a closed form for this method.

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2. Theory

Let us consider a non-relativistic three-body system. The three point particles have the masses m_1, m_2, m_3 and interact with each other by the scalar pair-potentials $V_{31}(r_{31})$, $V_{32}(r_{32})$, $V_{21}(r_{21})$, respectively. Without loss of generality we shall restrict ourselves to the case of central potentials $V_{ij}(r_{ij}) = V_{ij}(r_{ij})$. Also, for simplicity, we shall consider the case when the three-dimensional angular momentum L equals zero (S-states), since the generalization to cases when $L \geqslant 1$ or when the potential contains the $L \cdot S$, L^2 and S^2 operators is straightforward but non-trivial (for more details see [1]). For $L = 0$ the Hamiltonian has the form (in units where $\hbar = 1$)

$$\begin{aligned} H = &-\frac{1}{2\mu_{21}}\left(\frac{\partial^2}{\partial r_{21}^2}+\frac{2}{r_{21}}\frac{\partial}{\partial r_{21}}\right)-\frac{1}{m_3}\frac{r_{31}\cdot r_{32}}{r_{31}r_{32}}\frac{\partial^2}{\partial r_{31}\partial r_{32}} \\ &-\frac{1}{2\mu_{31}}\left(\frac{\partial^2}{\partial r_{31}^2}+\frac{2}{r_{31}}\frac{\partial}{\partial r_{31}}\right)-\frac{1}{m_2}\frac{r_{21}\cdot r_{32}}{r_{21}r_{32}}\frac{\partial^2}{\partial r_{21}\partial r_{32}} \\ &-\frac{1}{2\mu_{32}}\left(\frac{\partial^2}{\partial r_{32}^2}+\frac{2}{r_{32}}\frac{\partial}{\partial r_{32}}\right)-\frac{1}{m_1}\frac{r_{21}\cdot r_{31}}{r_{21}r_{31}}\frac{\partial^2}{\partial r_{21}\partial r_{31}} \\ &+V_{21}(r_{21})+V_{31}(r_{31})+V_{32}(r_{32}) \end{aligned} \tag{2.1}$$

where $\mu_{ij}^{-1} = m_i^{-1} + m_j^{-1}$, and $(i, j, k) = (1, 2, 3)$. We wish to find solutions of the appropriate Schrödinger equation which corresponds to the bound state spectra. The metric in the function space of the relative coordinates is determined by the following scalar product

$$\int\int\int \psi_1(r_{31}, r_{32}, r_{21})\psi_2(r_{31}, r_{32}, r_{21}) r_{31}r_{32}r_{21}\, dr_{31}\, dr_{32}\, dr_{21}. \tag{2.2}$$

The r_{ij} are relative coordinates, which are not independent (since e.g. $|r_{31} - r_{32}| \leqslant r_{21} \leqslant r_{31} + r_{32}$) and a number of difficulties arise from this (see, e.g., [1]). However, there are three independent 'perimetric' coordinates u_1, u_2, u_3 [2] which are related to the relative coordinates by

$$\begin{aligned} u_1 &= \tfrac{1}{2}(r_{21} + r_{31} - r_{32}) \\ u_2 &= \tfrac{1}{2}(r_{21} + r_{32} - r_{31}) \\ u_3 &= \tfrac{1}{2}(r_{32} + r_{31} - r_{21}) \end{aligned} \tag{2.3}$$

with the inverse relations $r_{ij} = u_i + u_j$, where $i \neq j = (1, 2, 3)$. All three perimetric coordinates are independent and non-negative (i.e. $0 \leqslant u_i \leqslant \infty$, where $i = 1, 2, 3$ [1, 2]). The metric in the function space of the perimetric coordinates is

$$\int\int\int \psi_1(u_1, u_2, u_3)\psi_2(u_1, u_2, u_3) u_1^{-1}u_2^{-1}u_3^{-1}\, du_1\, du_2\, du_3. \tag{2.4}$$

In terms of this metric the original Schrödinger equation can be rewritten in the form

$$\begin{aligned} 0 &= u_1u_2u_3r_{32}r_{31}r_{21}(H - E)\psi(u_1, u_2, u_3) \\ &= u_1u_2u_3(u_1 + u_2)(u_1 + u_3)(u_2 + u_3)(H - E)\psi(u_1, u_2, u_3). \end{aligned} \tag{2.5}$$

We wish to prove that this equation can be written in closed form in terms of the following nine generators

$$S_k = \frac{1}{2}u_k\left(-\frac{\partial^2}{\partial u_k^2}+1\right)$$
$$T_k = -\mathrm{i}u_k\frac{\partial}{\partial u_k} \tag{2.6}$$
$$U_k = \frac{1}{2}u_k\left(-\frac{\partial^2}{\partial u_k^2}-1\right)$$

where i is the imaginary unit and $k = 1, 2, 3$. Each set k of three operators conforms to a $O(2, 1)$ algebra with the following commutation relations

$$[S_k, T_k] = -\mathrm{i}U_k \qquad [T_k, U_k] = \mathrm{i}S_k \qquad [U_k, S_k] = -\mathrm{i}T_k \tag{2.7}$$

where $k = 1, 2, 3$. For each k, the Casimir operator $C_2 = S_k^2 - T_k^2 - U_k^2$ has the value 0. All pairs of generators from $S_1, T_1, U_1; S_2, T_2, U_2; S_3, T_3, U_3$ with different indices commute with each other. This means that these three O(2, 1) algebras are completely independent (in contrast with the choice in [1]).

Now, we rewrite the Schrödinger equation (equation (2.5)) in closed form in terms of only these nine generators and a few physical parameters

$$\begin{aligned}
&2u_1u_2u_3(u_1+u_2)(u_1+u_3)(u_2+u_3)(H-E)\psi(u_1,u_2,u_3)\\
&\quad=\Sigma_{(ijk)}[[(\mu_{ij}^{-1}+\mu_{ik}^{-1})A+m_i^{-1}B_{ijk}](S_j-U_j)(S_k-U_k)(S_i+U_i)\\
&\qquad+[\mu_{ij}^{-1}A+m_1^{-1}B_{123}+m_2^{-1}B_{231}+m_3^{-1}B_{312}](S_k-U_k)T_iT_j\\
&\qquad+2\mathrm{i}(\mu_{ij}^{-1}C_{ijk}+\mu_{ik}^{-1}C_{ikj})(S_j-U_j)(S_k-U_k)T_i]\\
&\qquad+2\ A\times P\times[V_{21}(S_1-U_1+S_2-U_2)+V_{31}(S_1-U_1+S_3-U_3)\\
&\qquad+V_{32}(S_2-U_2+S_3-U_3)+E]\psi(S_1-U_1,S_2-U_2,S_3-U_3)=0
\end{aligned} \tag{2.8}$$

where $(ijk) = (123)$, (231) or (312), and A, B_{ijk}, C_{ijk} and P designate the following operator expressions

$$A = (S_1-U_1+S_2-U_2)(S_2-U_2+S_3-U_3)(S_1-U_1+S_3-U_3)$$

$$\begin{aligned}
B_{ijk} &= (S_j-U_j+S_k-U_k)\\
&\quad\times[(S_i-U_i)(S_k-U_k)+(S_i-U_i)(S_j-U_j)-(S_j-U_j)(S_k-U_k)+(S_i-U_i)^2]
\end{aligned}$$

$$C_{ijk} = (S_i-U_i+S_k-U_k)(S_j-U_j+S_k-U_k)$$

$$P = (S_1-U_1)(S_2-U_2)(S_3-U_3) \tag{2.9}$$

which are finite polynomials in the powers of the nine generators for the three different $O(2, 1)$ algebras (S_i, T_i, U_i), $(i = 1, 2, 3)$.

3. Applications and discussion

We have shown that the Schrödinger equation (2.5) (or equation (2.8)) may be represented as a finite sum of terms, each of which has a closed form in terms of generators of three independent $O(2, 1)$ algebras as well as a few physical characteristics of the system (masses of particles, parameters of the potentials, etc). Therefore, to solve this equation one can use a number of algebraic methods and find its solution, in principle, without computation [3]. Let us consider briefly the three following applications of this approach to various three-body problems.

3.1. On the formal solutions in the three-body problem

First, consider the situation when each pair potential is a regular (analytic) function of the respective relative distance, i.e.

$$V_{ij}(S_i - U_i + S_j - U_j) = \Sigma_{n',k'} C_{ij;n',k'} (S_i - U_i)^{n'} (S_j - U_j)^{k'}$$

where the $C_{ij;n',k'}$ are determined from the explicit form of the potential $V_{ij}(r_{ij})$.

In this case, from equation (2.8), by applying the commutation relations (2.7), we can try to find the general solution of equation (2.8) in the form of a simple series

$$\begin{aligned}\psi(S_1 - U_1, S_2 - U_2, S_3 - U_3) &= \Sigma_{n,m,l} c_{n,m,l} (S_1 - U_1)^n (S_2 - U_2)^m (S_3 - U_3)^l \varphi \\ &= \Sigma_{n,m,l} c_{n,m,l} u_1^n u_2^m u_3^l \end{aligned} \tag{3.1}$$

where φ is the constant 'vacuum vector' which does not depend upon the $(S_i - U_i)(i = 1, 2, 3)$ generators and can be chosen, in principle, without loss of generality, to be equal to 1.

The wavefunction ψ in the form of equation (3.1) is a so-called 'formal solution' of the Schrödinger equation, i.e. an 'expansion that is capable of satisfying the Schrödinger equation term by term, without requiring the physical boundary conditions to be satisfied' [4]. (In the Coulomb case, such boundary conditions would be e.g. the coalescence conditions [5] for two or more particles.) Discussion about the existence (absence) of such formal solutions for the three-body problem (mainly in the case of the Coulomb three-body He-like (or two-electron) systems) has been of great value since the early years of quantum mechanics (see, e.g., [6–8]). The construction of formal solutions was used intensively later [2, 9–12] to obtain very accurate numerical solutions in three-body Coulomb systems.

The coefficients $c_{n,m,l}$ in the formal solution ψ, equation (3.1), can be determined by using only the commutation relations of the $O(2, 1)$ algebras, equations (2.7) and the Hamiltonian in the form of equation (2.8). Therefore, these coefficients only depend analytically upon the parameters of the problem which are included in equation (2.8). Moreover, to find the linear equations for the coefficients $c_{n,m,l}$ a further simplification can be made. To do this the following six creation–annihilation operators are introduced as in [13]

$$\begin{array}{lll} U_1 = \frac{1}{2}(a_2^+ a_1 + a_1^+ a_2) & T_1 = \frac{i}{2}(a_2^+ a_1 - a_1^+ a_2) & S_1 = \frac{1}{2}(a_2^+ a_2 - a_1^+ a_1) \\ U_2 = \frac{1}{2}(b_2^+ b_1 + b_1^+ b_2) & T_2 = \frac{i}{2}(b_2^+ b_1 - b_1^+ b_2) & S_2 = \frac{1}{2}(b_2^+ b_2 - b_1^+ b_1) \\ U_3 = \frac{1}{2}(c_2^+ c_1 + c_1^+ c_2) & T_3 = \frac{i}{2}(c_2^+ c_1 - c_1^+ c_2) & S_3 = \frac{i}{2}(c_2^+ c_2 - c_1^+ c_1) \end{array} \tag{3.2}$$

where

$$\begin{array}{lll} a_i^+ a_j - a_j a_i^+ = -\mathrm{i}\delta_{ij} & a_i^+ a_j^+ - a_j^+ a_i^+ = 0 & a_i a_j - a_j a_i = 0 \\ b_i^+ b_j - b_j b_i^+ = -\mathrm{i}\delta_{ij} & b_i^+ b_j^+ - b_j^+ b_i^+ = 0 & b_i b_j - b_j b_i = 0 \\ c_i^+ c_j - c_j c_i^+ = -\mathrm{i}\delta_{ij} & c_i^+ c_j^+ - c_j^+ c_i^+ = 0 & c_i c_j - c_j c_i = 0 \end{array} \tag{3.3}$$

for $i = 1, 2$ and $j = 1, 2$. By substituting equation (3.2) into equation (2.8), we obtain the equation

$$\Sigma W^{n_1,n_2,m_1,m_2,l_1,l_2}_{n_1',n_2',m_1',m_2',l_1',l_2'} (a_1^+)^{n_1}(a_1)^{n_1'}(a_2^+)^{n_2}(a_2)^{n_2'}(b_1^+)^{m_1}(b_1)^{m_1'}(b_2^+)^{m_2}(b_2)^{m_2'} \times (c_1^+)^{l_1}(c_1)^{l_1'}(c_2^+)^{l_2}(c_2)^{l_2'}\psi = 0 \tag{3.4}$$

where

$$\psi = \Sigma C_{k_1,k_2,k_3,k_4,k_5,k_6}(a_1^+)^{k_1}(a_2^+)^{k_2}(b_1^+)^{k_3}(b_2^+)^{k_4}(c_1^+)^{k_5}(c_2^+)^{k_6}|0,0,0,0,0,0\rangle \tag{3.5}$$

In the last equation $|0, 0, 0, 0, 0, 0\rangle$ is the 'vacuum vector', i.e.

$$p|0,0,0,0,0,0\rangle = 0 \tag{3.6}$$

where p is any one of the operators a_1, a_2, b_1, b_2, c_1 and c_2.

In fact, this means that the original Schrödinger equation for the Coulomb three-body problem in the coordinate representation has been reduced to the equivalent problem of three boson complex (charged) fields. Likewise, in principle, we have made a second quantization for an arbitrary non-relativistic three-body system. The solution of the second quantized equations may be easier than the original one in the coordinate representation (see, e.g., [14]).

3.2. Coulomb three-body systems

For a Coulomb three-body system, the potential energy component in equation (2.8) is

$$(S_1 - U_1)(S_2 - U_2)(S_3 - U_3)(q_1q_2C_{123} + q_1q_3C_{312} + q_2q_3C_{231}) \tag{3.7}$$

where the C_{ijk} are the three previously defined (equations (2.9)) finite (quadratic) polynomials of the $(S_i - U_i)$, $(i = 1, 2, 3)$ generators. q_1, q_2 and q_3 are the charges of the particles (in the system of units where $\hbar = 1, m_e = 1$ and $e = 1$ (Hartree atomic units)). In this case each term in the right-hand side of equation (2.8) contains a finite number of $O(2, 1)$ generators. Therefore, one can try to find the exact solution (or to approximate it with high accuracy) by applying rotations (and complex rotations) which are determined with the help of unitary (non-unitary, respectively) transformations Φ such as

$$\Phi(\alpha, \beta, \gamma) = \exp[-\mathrm{i}\alpha T_1 - \mathrm{i}\beta T_2 - \mathrm{i}\gamma T_3] \tag{3.8}$$

where α, β, γ are complex variables.

From the commutation relations (2.7) it follows that

$$(S \pm U)^n F(T) = F(T \mp \mathrm{i} \times n)(S \pm U)^n \tag{3.9}$$

where $F(x)$ is an arbitrary holomorphic (analytic) function on x and n is an integer. If we choose $F(x) = \exp(-i\beta x)$ where β is a real or complex number and $n = 1$, we obtain the Hausdorff–Campbell–Baker [15] formula

$$\exp(-i\beta T)(S \pm U)\exp(i\beta T) = \exp(\pm\beta)(S \pm U). \tag{3.10}$$

Therefore, in the general case we find the following formulae for the Φ transformation (equation (3.8))

$$\Phi^{\dagger}(\alpha,\beta,\gamma)(S_1 \pm U_1)^{n_1}(S_2 \pm U_2)^{n_2}(S_3 \pm U_3)^{n_3}\Phi(\alpha,\beta,\gamma)$$
$$= \exp(\pm n_1\alpha \pm n_2\beta \pm n_3\gamma)(S_1 \pm U_1)^{n_1}(S_2 \pm U_2)^{n_2}(S_3 \pm U_3)^{n_3} \tag{3.11}$$

and

$$\Phi^{\dagger}(\alpha,\beta,\gamma)T_1^{n_1}T_2^{n_2}T_3^{n_3}\Phi(\alpha,\beta,\gamma) = T_1^{n_1}T_2^{n_2}T_3^{n_3} \tag{3.12}$$

where n_1, n_2 and n_3 are non-negative integers, and $\Phi^{\dagger}$ is the complex conjugate of Φ.

The last two equations mean that the real or complex numbers α, β and γ are the free parameters of the 'rotation' Φ. Their choice in a definite manner can be used to significantly simplify the original Schrödinger equation with the Hamiltonian equation (2.8) and even to solve it analytically. It should be mentioned that this procedure is a generalization of the Foldy–Wouthuysen 'rotation' (in quantum electrodynamics) (see, e.g., [16]).

Let us consider only real values of α, β and γ. Our first goal is to reduce the Hamiltonian, equation (2.8), for the Schrödinger equation to the diagonal form by applying the unitary transformation Φ, equation (3.8), with the optimized values of α, β and γ. In fact, this means solving the appropriate eigenvalue problem analytically. However, it is easy to show that this problem is not solvable exactly in terms of only three real parameters α, β and γ.

Another related problem is to obtain the 'best approximate solution' by a complete and very careful optimization of the three real parameters for the non-unitary transformation $\Psi(\alpha,\beta,\gamma)$.

$$\Psi(\alpha,\beta,\gamma) = \exp[-\alpha(S_1 - U_1) - \beta(S_2 - U_2) - \gamma(S_3 - U_3)].$$

By the variational principle this problem can be reformulated as follows. Consider the basis functions in the form

$$\phi = \exp(-(\beta' + \gamma')(S_1 - U_1) - (\alpha' + \gamma')(S_2 - U_2) - (\alpha' + \beta')(S_3 - U_3))\varphi \tag{3.13}$$

where φ is the 'vacuum vector' which can be chosen to be equal to 1. In this case the coordinate representation equation (3.13) takes the form

$$\phi = \exp(-(\beta' + \gamma')u_1 - (\alpha' + \gamma')u_2 - (\alpha' + \beta')u_3) = \exp(-\alpha' r_{32} - \beta' r_{31} - \gamma' r_{21}). \tag{3.14}$$

It should be noted that these functions have the factorized form in both the relative coordinates r_{31}, r_{32}, r_{21} and in the perimetric coordinates u_1, u_2, u_3. Our main question is: how many such functions $\{\phi\}$ are needed to produce the lowest bound state in the Coulomb three-body system? This question presents specific interest for the systems with unit charges, i.e. for the $X^+Y^+Z^-$ ions.

After very careful optimization of the α', β', γ' parameters in the functions ϕ, the answer is that except for the extremely weakly bound (so-called pre-threshold) systems (e.g. the $d^+t^+p^-$ or $\mu^+\pi^+\pi^-$ ions) one needs only one function (three parameters) for symmetric (i.e. such as $X^+X^+Z^-$), and two functions (six parameters) for non-symmetric systems (i.e. such as $X^+Y^+Z^-$). Our optimized values of the α', β', γ' parameters for a number of such systems are presented in table 1, together with the energy in quasi-atomic units ($e = 1, \hbar = 1$ and $m_{\min} = 1$, where $m_{\min} = \min(m_X, m_Y, m_Z)$). We considered the symmetric systems from $^{\infty}H^-$ up to $^{\infty}H_2^+$ and a few non-symmetric systems. All mass values can be found elsewhere (see, e.g., [17]). For comparision the 'exact' energies from the recent literature are listed for each system in table 1: $^{\infty}H^-$ [18], $^1H_2^+$ [19] and $^{\infty}H_2^+$ [20]. The variational results for the other (intermediate) three-body systems with unit charges in table 1 are from [21]. Our highly accurate variational results for the $(t\mu\mu)^-$ and $(d\mu\mu)^-$ ions in table 1 are published here for the first time.

Table 1. The carefully optimized values of the three non-linear parameters and the total energies E_t and the best 'exact' energies E_{ex} (known from the literature) for the lowest bound states of Coulomb three-body systems with unit charges in quasi-atomic units ($m_{\min} = 1, \hbar = 1, e = 1$).

system	α'	β'	γ'	E_t	E_{ex}
$^{\infty}H^-$	1.075 018	0.483 7428	−0.146 5637	−0.523 865 929 78	−0.527 750 165 4431
T^-	1.074 801	0.483 5586	−0.146 4767	−0.523 762 830 28	−0.527 649 048 182
D^-	1.074 693	0.483 4670	−0.146 4335	−0.523 711 544 22	−0.527 598 324 665
$^1H^-$	1.074 368	0.483 1917	−0.146 3035	−0.523 557 410 56	−0.527 445 881 093
Mu^-	1.069 273	0.478 8893	−0.144 2731	−0.521 139 938 74	−0.525 054 806 223
$t^+\mu^-\mu^-$	1.032 008	0.448 2164	−0.129 8856	−0.503 443 123 67	−0.507 544 602 642
$d^+\mu^-\mu^-$	1.011 947	0.432 2761	−0.122 4746	−0.493 906 140 66	−0.498 103 091 755
$p^+\mu^-\mu^-$	0.956 3414	0.390 1085	−0.103 1240	−0.467 424 326 25	−0.471 866 342 087
$3^+1^-1^-$	0.788 8136	0.279 7721	−0.054 8906	−0.387 146 313 77	−0.392 141 012 853
$2^+1^-1^-$	0.697 8110	0.229 4157	−0.034 6167	−0.343 193 301 20	−0.348 371 665 880
$Ps^-(1^+1^-1^-)$	0.520 1386	0.147 9152	−0.005 9907	−0.256 692 004 87	−0.262 005 070 2326
$p^+p^+\mu^-$	0.939 0592	0.197 3986	0.080 087 95	−0.465 047 703 98	−0.494 386 820 2486
$d^+d^+\mu^-$	0.991 9291	0.201 8128	0.098 944 01	−0.491 122 435 57	−0.531 111 135 402
$t^+t^+\mu^-$	1.011 036	0.203 3346	0.106 3759	−0.500 516 617 00	−0.546 374 225 598
$^1H_2^+$	1.051 496	0.206 4299	0.123 3115	−0.520 346 395 58	−0.597 139 0625
$^{\infty}H_2^+$	1.052 118	0.206 4762	0.123 5856	−0.520 650 797 64	−0.602 634 2140
$p^+d^+\mu^-$	0.972 7714	0.115 4430	0.108 2796		
	0.311 3552	0.960 2925	0.048 185 17	−0.480 834 863 68	−0.512 711 796 5008
$p^+t^+\mu^-$	0.986 1977	0.095 043 93	0.113 0547		
	0.352 5432	0.967 2839	0.034 437 78	−0.487 600 188 87	−0.519 880 089 7819
$d^+t^+\mu^-$	1.003 480	0.169 3369	0.111 9977		
	0.239 3984	0.999 8013	0.090 454 43	−0.496 157 998 83	−0.538 594 975 058

The optimized values of the nonlinear parameters are of great value, since by using these one can very easily estimate properties of such systems, e.g. the expectation value of the $\langle\delta_{+-}\rangle$ function for the Ps^- ion is $\sim 0.020\,076\,8859$, and by following [22] the total annihilation rate for the Ps^- ion is $\sim 2.020\,0857\ ns^{-1}$. The 'exact' result is $\approx 2.086\,12\ ns^{-1}$ [21, 22]. However, in the cases of other properties the agreement is not as good, e.g. for the electron–electron cusp. The same approach may also be very useful for the cases of the harmonic oscillator potential, the spherically symmetric square well potential and in other even more general and complex cases.

3.3. The virial theorem

Finally, let us consider the virial theorem for three-body systems. As is well known, the virial theorem is of great value as an independent test of the results of numerical solution for the appropriate Schrödinger equation. The physical meaning of the virial theorem is that the real physical state must be optimal with respect to distance variation [23]. However, in the independent perimetric coordinates the distance variations are determined by the T_i ($i = 1, 2, 3$) generators. We can write the following three independent hypervirial relations [23–25]

$$(\psi, (H - E)T_i - T_i(H - E)\psi) = (\psi, A_i\psi) = 0 \tag{3.15}$$

where $i = 1, 2, 3$ and ψ is the eigenfunction which corresponds to the eigenvalue E. To obtain the explicit form of the A_i operators the following commutation relations are useful

$$[T_j, (S_k \pm U_k)^n] = \pm in\delta_{jk}(S_k \pm U_k)^n \qquad [T_j, (T_k)^n] = 0 \tag{3.16}$$

where $j = 1, 2, 3$; $k = 1, 2, 3$ and n is a non-negative number.

By using the explicit form of the operator $(H - E)$ (equation (2.8)) and the commutation relations (equations (3.16)) it is possible to find each hypervirial operator A_i. By summing equations (3.15) on $i (i = 1, 2, 3)$ one obtains the relation between the expectation values of the kinetic energy and potential energy which is often called the 'virial theorem' [7, 26–7].

In conclusion we wish to mention that the same algebraic approach can be extended to the case of Dirac-type equations as well as to the cases of non-local potentials (e.g. Hartree–Fock equations).

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