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Importance of two-body correlations in the ^{4}He molecules(*)

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Summary. — We investigated whether the recently developed Integrodifferential Equation Approach to Few- and Many-body systems, known as IDEA, can be used to study the ground-state properties of He-molecules. Using two realistic ^{4}He-^{4}He interactions of Aziz and collaborators, the binding energies and the root mean-square radii for small molecules are calculated and the results obtained are compared with those previously obtained by other methods. The principal result of this study is that the practically hard-core and the short-range attraction of the molecular potentials give rise to strong many-body correlations and an increased importance of higher partial waves which cannot be, adequately, handled with S-wave projected formalisms.

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1. – Introduction

Various methods have been used in the past to study the ground-state properties of ^{4}He molecules. We mention here the Variational Method (VM) [1-3], the Variational Monte Carlo method (VMC) [4, 5], the Green Function Monte Carlo method (GFMC) [5-10], the Faddeev method in momentum space [11, 12], and the Faddeev-Noyes method (FN) in configuration space [13]. In all these calculations use was made of the dominant pairwise structure of the intermolecular force in the many-body environment and in this way various properties of the system such as the ground-state properties, mean-square radii, and density distributions, were studied.

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The variational-type calculations have the advantage that they can handle any number of atoms in the molecule. On the other hand, the Faddeev-type methods are exact and they include the two-body forces in their formalism in an unambiguous way. They have, however, the disadvantage that they can be used for calculations, with the present-day computing power, only up to four-body systems.

In this work, the Integrodifferential Equation Approach (IDEA) for few-body systems [14-18] is employed. In this method the A-body bound-state wave function is expanded in Faddeev-type components (*i.e.* sum of pairwise components). A further expansion in potential harmonics and projection on the r_{ij} space results in an integrodifferential equation in two variables describing the bound state of systems with the number of particles $A \geq 3$. The IDEA for the three-body case and for S-wave projected potentials is equivalent to the exact Faddeev equation. However, for $A > 3$ systems the IDEA becomes approximate since it takes into account only two-body correlations. In the nuclear case the method has been successfully applied in bound-state calculations and good results, for systems with $A \leq 16$, were obtained [16-19]. The method, is computationally appealing since an equation of the same form is employed for different number of particles.

It will, therefore, be of interest if these equations can be also successfully used to study molecular systems with any number of particles. The main difference between the nuclear and molecular systems lies in the nature and characteristics of the two-body force, the latter having a hard core and long-range characteristics which make the many-body calculations cumbersome. In this investigation, two semi-empirically constructed realistic ^{4}He-^{4}He interactions of Aziz and collaborators, namely the $HFDHE2$ potential [20] and the new HFD-B potential [21], were used to test the method by studying the ground state properties of systems with $3 \leq A \leq 5$.

We used the Finite Element (FE) method [22] in the two-dimensional space, to calculate the binding energies and the root mean square radii (r.m.s.) for the molecules and the results are compared with those previously obtained via the aforementioned variational methods as well as with those obtained via the Faddeev-Noyes (FN) equations in configuration space [13] and the Faddeev equation [11, 12]. Furthermore, we employed the Extreme Adiabatic Approximation (EAA) [15, 16] in order to study its applicability to these systems. The application of the EAA to many-body systems with such peculiar forces, is not only interesting by itself, as it simplifies tremendously the numerical calculations, but also exhibits properties for the underlying interactions, *e.g.*, via the study of the eigenpotentials.

This paper is organised as follows. In sect. **2** we briefly describe the IDEA method. In the same section a different form of it more suitable in molecular calculations is given together with the adiabatic approximation. In sect. **3** we briefly describe the two potentials used and present our main results. Our conclusions are drawn in sect. **4**.

2. – The method

The bound state of an A-body system can be calculated using the IDEA [15]. Although the formalism has been previously described in detail, we will briefly recall the main formulae for convenience and in order to transform them into new Cartesian-type coordinates.

In this method the A-body bound-state wave function is expanded in components characterizing the pairs,

$$\Psi(\mathbf{r}) = \sum_{i<j\leq A} \psi_{ij}(\mathbf{r}). \tag{1}$$

They satisfy the Faddeev-type equation

$$(T-E)\psi_{ij}(\mathbf{r}) = -V(r_{ij}) \sum_{k<l\leq A} \psi_{kl}(\mathbf{r}). \tag{2}$$

Here $\mathbf{r}$ represents all the coordinates, $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_A)$ and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, if $\mathbf{r}_i$ is the coordinate of particle i. The reason for adopting such an expansion is the assumption, that the pairwise nature of the intermolecular force is dominant in the many-body environment. The $\psi_{ij}(\mathbf{r})$ are assumed to be of the form

$$\psi_{ij}(\mathbf{r}) = H_{[L_m]}(\mathbf{r}) F(\mathbf{r}_{ij}, \rho), \tag{3}$$

where ρ is the hyperradius, $\rho = \left[2/A \sum r_{ij}^2\right]^{1/2}$, and $H_{[L_m]}(\mathbf{r})$ is a suitable harmonic polynomial of minimal degree $[L_m]$ [23]. For A-boson systems in a ground state $[L_m] = 0$ and $H_{[L_m]}(\mathbf{r}) = 1$. This is the case of the S-wave projected potentials considered here. The IDEA is then defined via

$$(T - \frac{A(A-1)}{2} V_0(\rho) - E) F(\mathbf{r}_{ij}, \rho) = -[V(r_{ij}) - V_0(\rho)] \sum_{k<l\leq A} F(\mathbf{r}_{kl}, \rho). \tag{4}$$

The $V_0(\rho)$ is the hypercentral potential [15, 16] and is given by the average of the two-body potential over the unit hypersphere, *i.e.* for $\rho = 1$. In the case of molecular forces the $V_0(\rho)$ is highly repulsive causing failure of the method, and thus we set it equal to zero. This amounts to the S-wave projected Integrodifferential Equation (SIDE) [15, 16]. In order to solve this equation, two further steps are required. In the first step we write

$$F(\mathbf{r}_{ij}, \rho) = P(z_{ij}, \rho)/\rho^{(D-1)/2}, \tag{5}$$

where $z_{ij} = 2r_{ij}^2/\rho^2 - 1$, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, and $D = 3(A-1)$; in a second step we project eq. (4) on the r_{ij} space to obtain, for spin-independent two-body potentials, an integrodifferential equation given by

$$-\left[\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial\rho^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{\rho^2} + \frac{4}{\rho^2}\frac{1}{W(z)}\frac{\partial}{\partial z}(1-z^2)\frac{\partial}{\partial z}\right) + E\right] P(z,\rho) = -V(r_{ij})\Pi(z,\rho), \tag{6}$$

where $\mathcal{L} = (D-3)/2$. The weight function $W(z)$ is given by

$$W(z) = (1-z)^\alpha (1+z)^\beta, \tag{7}$$

with $\alpha = (D-5)/2$ and $\beta = 1/2$. The function $\Pi(z,\rho)$ results from the projection on the r_{ij} space, $\Pi(z,\rho) = \sum_{k<\ell\leq A} \langle \vec{r}_{ij} | F(\vec{r}_{k\ell}, \rho) \rangle$, and is given by

$$\Pi(z,\rho) = P(z,\rho) + \int_{-1}^{+1} f(z,z') P(z',\rho) \mathrm{d}z'. \tag{8}$$

The $f(z,z')$ is the so-called projection function given by

$$f(z,z') = W(z') \sum_K \frac{f_K^2 - 1}{h_K} P_K^{\alpha,\beta}(z) P_K^{\alpha,\beta}(z'), \tag{9}$$

$P_K^{\alpha,\beta}(z)$ being the Jacobi polynomial and

$$f_K^2 = 1 + \frac{2(A-2)P_K^{\alpha,\beta}(-\frac{1}{2}) + [(A-2)(A-3)/2]P_K^{\alpha,\beta}(-1)}{P_K^{\alpha,\beta}(1)} . \tag{10}$$

The h_K is a normalization constant for the Jacobi polynomials,

$$h_K = \int_{-1}^{+1} [P_K^{\alpha,\beta}(z)]^2 W(z) \mathrm{d}z. \tag{11}$$

The calculation of the projection function cannot in general be performed analytically, except for bosons in S-states [15, 23]. It has the general structure

$$f(z,z') = 2(A-2) f(z,z',-1/2) + \frac{(A-2)(A-3)}{2} f(z,z',-1), \tag{12}$$

where $f(z,z',-1/2)$ is the projection function for connected pairs such as $(12),(13)$ and $f(z,z',-1)$ the one for disconnected pairs such as $(12),(34)$, which occur only for $A \geq 4$ [15, 23]. Further details concerning the derivation of these equations can be found in refs. [15, 23].

In the nuclear case the above equations gave excellent results without major numerical or computational difficulties. However, for the molecular case where there is a strong repulsion in the interaction, amounting to a hard sphere, the coordinates ρ and z turned out to be unsuitable especially for $A > 3$. Therefore, we transformed the SIDE equation using the variables

$$x = \rho \sqrt{\frac{1+z}{2}} \tag{13}$$

and

$$y = \rho \sqrt{\frac{1-z}{2}}, \tag{14}$$

which for $A = 3$ are identical to the usual Jacobi coordinates. For $A > 3$, y is the hyperradius with respect to all Jacobi coordinates except x. In these coordinates the SIDE reads

$$\begin{aligned} \left[\frac{\hbar^2}{m}\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \frac{\mu(\mu+1)}{y^2}\right) + V(x) - E\right] \Phi(x,y) = \\ = V(x) x y^\lambda \int_{-1}^{+1} f(z,z') \frac{\Phi(x,y)}{x' y'^\lambda} \mathrm{d}z', \end{aligned} \tag{15}$$

where

$$\Phi(x,y) = xyP(x,\sqrt{x^2+y^2}), \tag{16}$$

$$\lambda = \frac{3A-7}{2}, \tag{17}$$

and

$$\mu = \lambda - 1\,. \tag{18}$$

This equation has a much simpler left-hand side as compared to the one for ρ and z coordinates, but the integral on the right-hand side is not along a coordinate. For $A = 3$ it is similar to the Faddeev-Noyes equation [24]. In general it has the advantage that the choice of the mesh points which are needed to solve the equation is directly related to the physical dimensions of the system.

It is customary to solve the above equations by employing piecewise polynomials in both coordinates (ρ, z) (or, alternatively, in (x,y)). This method is quite accurate since only numerical approximations are used. The EAA [15], however, can also be employed. In this approach the orbital and the radial motion are decoupled, *i.e.* one assumes $P(z,\rho) \approx u(r)\widetilde{P}(z,r)$, where the component $\widetilde{P}(z,\rho)$ satisfies the equation

$$\left[\frac{\hbar^2}{m}\left(\frac{4}{\rho^2}\frac{1}{W(z)}\frac{\partial}{\partial z}(1-z^2)\frac{\partial}{\partial z}\right) - U_\lambda(\rho)\right]\widetilde{P}(z,\rho) = V(r_{ij})\widetilde{\Pi}(z,\rho), \tag{19}$$

while the radial function $u(\rho)$ satisfies

$$\frac{\hbar^2}{m}\frac{\partial^2}{\partial\rho^2}u_\lambda(\rho) + [E - \frac{\mathcal{L}(\mathcal{L}+1)}{\rho^2} - U_\lambda(\rho)]u_\lambda(\rho). \tag{20}$$

$U(\rho)$ is the so-called eigenpotential for the system.

Once the components $P(z_{ij},\rho)$ are found, one can construct the full wave function by using the relevant A-body Jacobi coordinates (see ref. [17] for more details).

3. – Results

The construction of an accurate ^{4}He-^{4}He potential is a long-standing problem in molecular physics. As a consequence, there are several potentials, which can be employed in many-body calculations. In this work two different atom-atom interactions were used. These are:

a) The $HFDHE2$ potential.

Of all potentials, the empirically constructed $HFDHE2$ potential of Aziz *et al.* [20], was considered in the past to be the most realistic one giving the best agreement with the two-body measurements. In the many-body environment, where the molecular forces are assumed to be acting in a pairwise manner, this potential predicts the condensed-phase properties reasonably well [9]. It has the form

$$V(r) = \varepsilon\left\{A\exp[-\alpha x] - \left[\frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}}\right]F(x)\right\}\,, \tag{21}$$

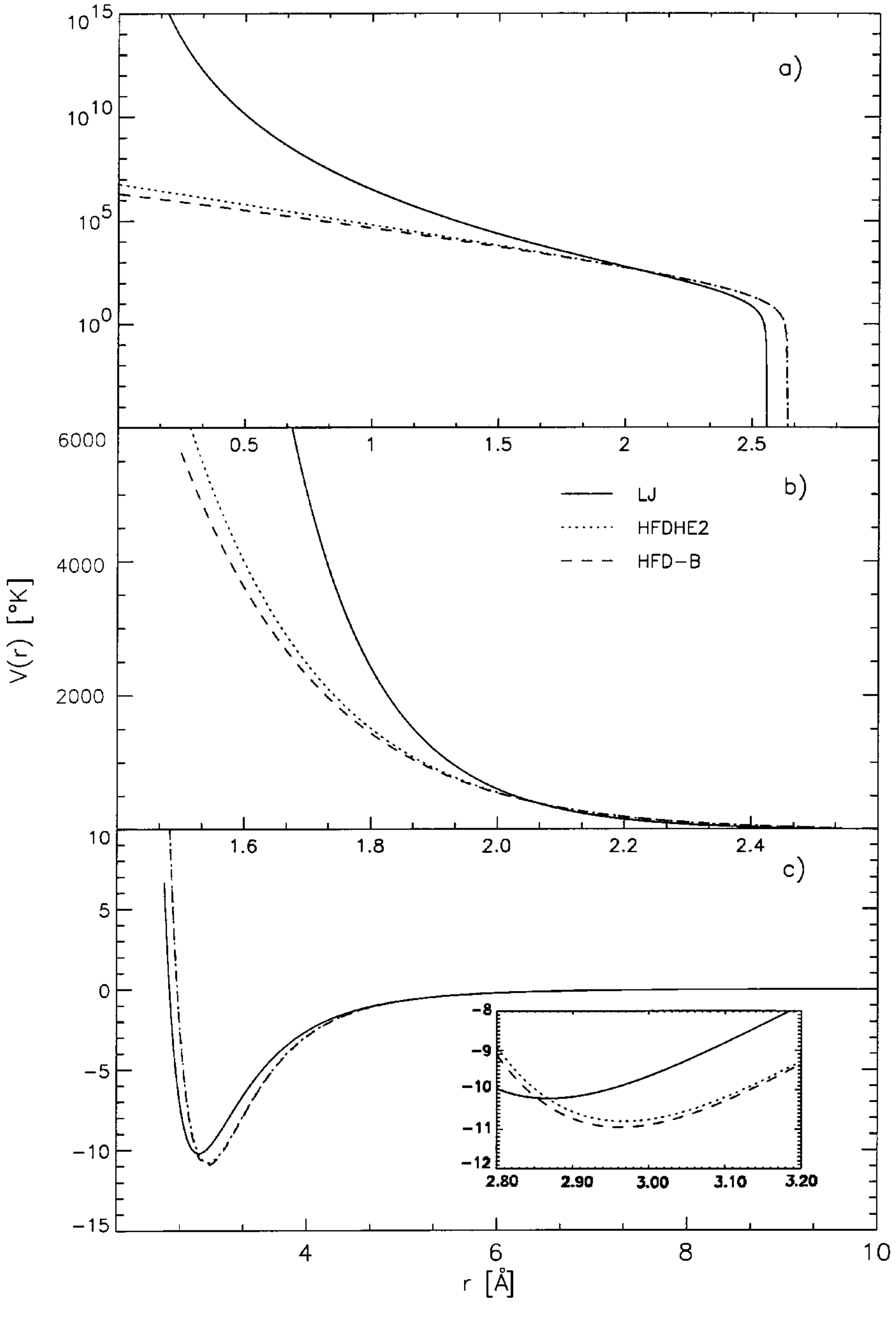

Fig. 1. – The two realistic $HFDHE2$ and $HFD\text{-}B$ and the Lennard-Jones 6-12 potentials; a) short-range hard-core , b) intermediate and c) attractive region. The region around the minima of the potentials is shown in the inset of c).

TABLE I. – *The* He-He *interactions HFD-B and HFDHE2 of Azizit et al.*

Parameter	*HFD-B* [21]	*HFDHE2* [20]
ε(K)	10.948	10.8
r_m (Å)	2.963	2.9673
$A \times 10^6$	0.184 431 01	0.544 850 4
α	10.43329537	13.353 384
β	−2.279 651 05	...
C_6	1.367 452 14	1.377 324 12
C_8	0.421 238 07	0.425 378 5
C_{10}	0.174 733 18	0.178 100
D	1.482 6	1.241 314

where $x = r/r_m$. The function $F(x)$ is given by

$$F(r) = \begin{cases} \exp\left[-\left(\dfrac{D}{x} - 1\right)\right]^2, & \text{if } x \leq D\,, \\ 1, & \text{if } x > D\ . \end{cases}$$

b) The HFD-B potential.
Since the introduction of the $HFDHE2$ potential, new virial coefficients experimental data for ^{4}He became available, new *ab initio* calculations of the dispersion coefficients have appeared, and new measurements of transport properties have been done (see ref. [21] and references therein). This necessitated the modification of the previous potential to reproduce the latest data. The new semi-empirical potential is known as the HFD-B potential and is given by

$$V(r) = \varepsilon \left\{ A \exp[-\alpha x + \beta x^2] - \left[\frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}}\right] F(x) \right\}. \tag{22}$$

The function $F(x)$ has the same structure as in the $HFDHE2$ potential. The parameters for these two potentials are given in table I. The potentials are plotted in fig. 1. In the same figure the Lennard-Jones 6-12 (LJ) potential [25] is also plotted for comparison purposes. The LJ potential is one of the earliest potentials used in ^{4}He molecule studies [1,2]. It is in many respects inferior to the realistic potentials of Aziz *et al.*, and variational calculations with this potential in polyatomic molecules were unsatisfactory [1, 2, 9]. In this figure the three regions, short, medium, and attractive, are shown for comparison purposes. The hard-core behaviour of the three potentials is clearly seen in fig. 1*a*). The LJ has hard-core characteristics and an attractive well which differ considerably from the other two. On the other hand, the two realistic forces are exhibit only small differences both at short distances and in the attractive well region. Nevertheless, these small differences are essential in reproducing the two-body data. It will be of interest to know how these differences are manifested in polyatomic systems.

We use the above Aziz *et al.* potentials to calculate the binding energies, the mean-square radii, the eigenpotentials and the Faddeev components for molecules with $3 \leq A \leq 5$. Two methods of solution of eq. (6) (and its equivalent equation (16)) are used. In

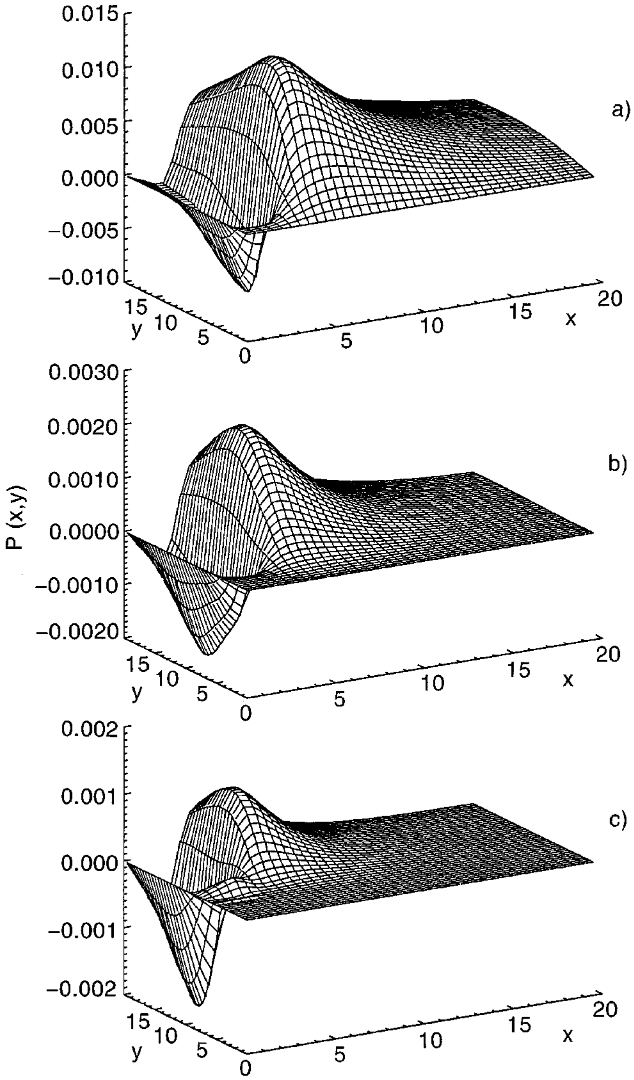

Fig. 2. – The Faddeev-components for a) $A = 3$, b) $A = 4$ and c) $A = 5$ resulting for the *HFD-B* potential.

the first the FE method has been employed [22], while in the second B-splines together with the Extreme Adiabatic Approximation are used [15].

In order to determine $\Phi(x, y)$ by the FE method, we expand it on a rectangular grid of $N \times M$ intervals in x and y, using quintic Hermite splines [26], which guarantee continuity of $\Phi(x, y)$ and its first and second derivatives with respect to x and y. Denoting the splines in the x-coordinate by $X_i(x),\ i = 1, 2, , \cdots, 3M + 1$, and the splines in the y-coordinate by

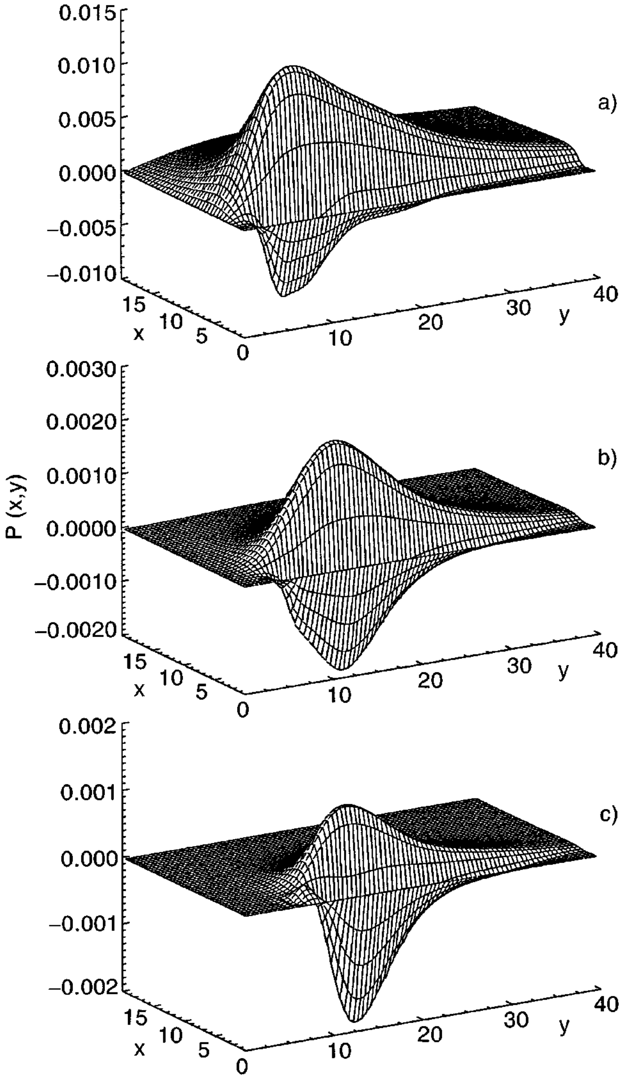

Fig. 3. – The Faddeev-components for a) $A = 3$, b) $A = 4$ and c) $A = 5$ with the x and y coordinates exchanged and the y range extended up to 40 Å.

$Y_i(y),\ i = 1, 2, , \cdots, 3N + 1$, the expansion reads

$$\Phi(x, y) = \sum_{i=1}^{3M+1} \sum_{j=1}^{3N+1} p_{ij} X_i(x) Y_j(y) \,. \tag{23}$$

To determine the expansion coefficients we use the Galerkin method. This amounts to the following: we use the above expansion in the SIDE equation and multiply by a function $Q(x, y)$ satisfying the same boundary conditions as Φ, integrate over x and y and require that the resulting expression holds for all $Q(x, y)$ that are linear combinations

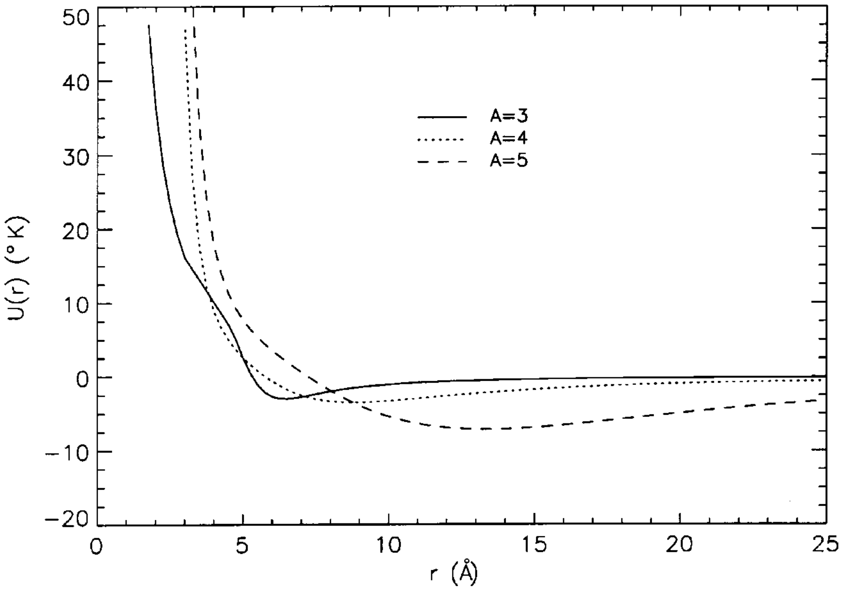

Fig. 4. – The eigenpotentials resulting from the $HFDHE2$ potential for a) $A = 3$, b) $A = 4$ and c) $A = 5$.

of $X_i(x)Y_j(y)$. This leads to a generalized non-symmetric eigenvalue problem, which is solved using the non-symmetric Lanzcos method [27]. In order to facilitate the convergence we furthermore apply a spectral transformation.

To obtain the solution in the EAA, we use the B-splines as defined by Cox [28]. Once more, the use of the Galerkin method reduces eq. (19) to an eigenvalue problem for each ρ and thus the matrices are of much smaller size and easy to handle. The eigenpotential $U(\rho)$ is then used in eq. (20) to obtain the binding energy of the molecule.

The Faddeev components for the $A=3$, 4, and 5 systems are shown in fig. 2. It is seen that the shape of all three components is similar. This demonstrates that as the number of atoms in the molecule increases, the pairwise nature of the inter-molecular force remains dominant. The x-range of the wave function, *i.e.* the range of the effective interaction, is reduced. This is clearly visible in the figure where for $A=3$, fig. 2a), the wave function is extended out to 15 Å, while for $A=5$, fig. 2c), the wave functions is confined in the region of less than 10 Å.

The Faddeev components are shown with x and y exchanged in fig. 3. As mentioned earlier, the y-coordinate is the hyperradius for the $(A-1)$-system. The hard-core repulsion at short distances is shifted outwards and the Faddeev components are stretched out up to about 40 Å. This reflects the growing of the spatial extension of the molecule as the number of particles is increased.

In fig. 4 we present the eigenpotentials obtained in the EAA. In this figure the same behaviour is exhibited, *i.e.* an increase of the distance where the hard-core appears and an increase of the range of the effective force. It is noted here that the eigenpotentials go asymptotically to one of the $(A-1)+1$ scattering states with the depth of the asymptotic tail corresponding to the bound state of the $(A-1)$-molecule. However, to obtain reliable numerical results is difficult, as one needs to describe the $(A-1)$-bound state, which for

TABLE II. – *The binding-energy results (in K). The first line for each molecule corresponds to the HFDHE2 and the second to HFD-B.*

A	Exact	EAA	Faddeev	VMC	GFMC
3	0.083 0.096	0.188 0.211	0.11 [12], 0.092 [11] 0.096 [13] (^{a})		0.1173 [5]
4	0.399 0.431	0.523 0.570	0.394 [11]	0.512 [5]	0.5332 [5]
5	0.926 0.990	1.329 1.388			

(a) $l = 0,\ \lambda = 0$ partial wave.

large ρ is concentrated near $z = -1$. The non-monotonous slope of the eigenpotential for $A = 3$ around 4 Å should be noted. This behaviour is due to the crossing of the adiabatic potential curves.

The binding energy results are given in table II. It is seen that using the FE method we obtain results for the $HFDHE2$ potential and for the $A = 3$ case, which are lower than those obtained via the Faddeev equations [11, 12] and the GFMC method [5]. They are, however, in agreement with the $l = 0$, $\lambda = 0$ result of the Faddeev-Noyes-calculation of Carbonell *et al.* [13]. The same is true for the $A=4$ case where the results for the HFDHE2 potential are about 20% less than those of the VMC and GFMC methods [5], but in good agreement with the results of ref. [11]. To the best of our knowledge, there are no results available with either of the Aziz potentials for the $A = 5$ case and therefore no comparison can be made.

The root mean square (r.m.s.) radii results are presented in table III together with the results of ref. [5]. It is seen that our results are up to 20% higher than the GFMC results, indicating that the bound-state wave function obtained by SIDE has a larger spatial range which reflects the underbinding.

The EAA results are rather unsatisfactory. Better results could have been obtained using the Uncoupled Adiabatic Approximation (UAA) [15]. However, crossing of the adiabatic potential curves made the resulting improvement unstable and therefore the EAA can only be used for interpretation purposes.

The differences in the binding energies between the two potentials are, depending on A, between 7% and 16%. Given the small differences between the two potentials, shown

TABLE III. – *Same as in table II for the root mean-square radii results (in Å).*

A	Exact	GFMC
3	7.59 7.29	5.98 ([5])
4	6.11 6.02	5.16 ([5])
5	5.62 5.55	

in fig. 1, this is a surprising result which explicitly exhibits how small differences in the two-body forces are enhanced in the many-body environment.

4. – Conclusions

We started our investigation using the basic assumption that the dominant interaction within the molecule is the two-body ^{4}He-^{4}He force. To obtain a stable solution for molecules with $A > 3$, we then transformed the original SIDE equation in terms of a new set of coordinates of Cartesian type which are more suitable for molecular calculations and physical interpretation.

The binding energies obtained by solving this equation via the FE method are considerably smaller than the exact GFMC results, while the r.m.s.-radii are larger than those obtained by the Monte Carlo methods. There are mainly two sources for such a discrepancy. The first is due to the omission of the higher-order partial waves. These are expected to be important due to the effective hard-core nature of the interatomic force, which in the semi-classical picture corresponds to large impact parameters and large relative angular momenta. In cases where the potential is not as repulsive as the Aziz *et al.* potentials, the higher partial wave effects can be included, to a good approximation, via the hypercentral potential, *i.e.* via the IDEA method [15, 16]. In the present case, however, this is not possible, since the hypercentral potential is highly repulsive resulting in failure of the IDEA. The second reason is the importance of the higher-order correlations which can only be included variationally, using for example a Jastrow-type correlation function. It is, therefore, of utmost importance that the integrodifferential equations used in this investigation be modified to take higher partial waves and many-body correlations into account.

A surprising result of this investigation is the differences found between the two realistic forces, namely the $HFDHE2$ and the $HFD\text{-}B$ potential. Although the differences between the two potential are rather small (see fig. 1), they, nevertheless, gave binding energy results which differ by up to 16%. This indicates that in future calculations the $HFD\text{-}B$ potential should be given a preference over the HFDHE2, which was employed in the Monte-Carlo calculations.

For $A > 5$ molecules the results were not stable and the SIDE should be modified to handle them. Such a modification of the equations was carried out and calculations are in process.

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