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^{4}He tetramer and the Faddeev-Yakubovsky theory

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The Faddeev-Yakubovsky theory is applied to the system of $(^4He)_4$ interacting pairwise through a realistic He-He potential. The S-wave two-body t matrix is obtained using the unitary pole expansion method, while the S-wave $[3+1]$ and $[2+2]$ subamplitudes are obtained by the Hilbert-Schmidt and the energy-dependent pole expansion (EDPE) methods. The convergences of the latter subamplitudes are tested and the superiority of the EDPE over the Hilbert-Schmidt expansion (HSE) is confirmed. The present results also confirm the results of a previous calculation using the ATMS method (amalgamation of two-body correlations into the multiple-scattering process).

I. INTRODUCTION

Systems of helium atoms are of considerable interest as their study may clarify the clustering mechanism of quantum liquids. Thus, the $(^4He)_3$ trimer has been treated via ATMS-variational[1] (amalgamation of two-body correlations into the multiple-scattering process) and the Faddeev-UPE[2] (unitary pole expansion) methods. The resultant ground-state energies, -0.105 and -0.087 K, respectively, obtained assuming a realistic He-He interaction,[3] show good agreement with each other and, incidentally, establish the accuracy of the UPE method[4] for the S-wave part of the interaction and the relatively small contribution of $l\neq 0$ components.

Recently, various extensions of Faddeev's three-body theory to the four-, and, in general, n-body systems have been proposed. The first was that of Yakubovsky,[5] later clarified by Faddeev[6] so that the formalism is labeled Faddeev-Yakubovsky (FY). The second, and heuristically more appealing, is the Alt, Grassberger, and Sandhas (AGS) formalism[7] which embodies the generalization of the Lippman-Schwinger equation to the n-body system. Among others, we mention the formalisms of Sloan, Bencze, and Redish (SBR), and Baer, Kouri, Levin, and Tobocman (BKLT).[8]

Now although AGS is predated by FY, the first explicit derivation of a single-variable integral equation and thus the first opportunity for numerical solution, for the four-body problem was obtained through AGS.[9] Subsequently, Kharchenko, Kuzmichev, and Shadchin,[10] starting from FY and using a one-term separable two-body interaction and separable expressions for the $[3+1]$ and $[2+2]$ subsystems, reduced the problem to a set of single-variable integral equations which they solved. Later, Narodetsky[11] repeated the approach of Kharchenko *et al.* but employed the Hilbert-Schmidt expansion (HSE) method to obtain separable expressions for the subsystem amplitudes. Tjon[12] started from a local pairwise potential, found the UPE equivalent, then, just like Narodetsky, used the Hilbert-Schmidt technique to solve the problem. We did the same for the 4-α problem.[13] All these calculations were done with relevance only to the nuclear domain. An exception is Tjon's recent work on the $(^4He)_4$ tetramer which, however, is restricted to simple interactions and two dimensions.[14] Very recently, Sofianos *et al.*[15] proposed another separable expansion method for the $[3+1]$ and $[2+2]$ subsystems which is an analog of the UPE, but the form factors have an energy dependence so that the method is called the energy-dependent pole expansion (EDPE) method. It was reported by them that the convergence of the EDPE is faster than that of the HSE in some cases of simple N-N interactions.

The purpose of this paper is to improve on Tjon's calculation of $(^4He)_4$ by using a realistic local potential and to extend his work to three dimensions. At the same time, we are able to test the Hilbert-Schmidt and the energy-dependent pole separable expansion methods for the $[3+1]$ and $[2+2]$ sub-

system amplitudes, by comparing with previous ATMS-variational results. The He-He interaction is a very resonant force in the sense that whether it produces a bound dimer or not is yet an unresolved problem. In the few-particle systems with such a two-particle interaction, the higher partial-wave interactions than the S-wave ones have only a small effect.[16] Thus, in our calculations we have restricted ourselves to $l=0$ partial waves, but we have commented on $l\neq 0$ contributions also from direct comparison of our results with ATMS.

II. FORMALISM

Since the relevant equations forming the structure of our work are readily available elsewhere, we present here only the barest outline of the Faddeev-Yakubovsky equation for four bosons in the HSE and EDPE approximations as well as the UPE one.

A. Faddeev-Yakubovsky equation in the case of an S-wave separable two-body potential

In the Faddeev-Yakubovsky formalism, the bound-state wave function of a four-boson system is written as a sum of two kinds of amplitudes ψ and χ,

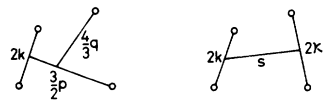

FIG. 1. Two kinds of Jacobi coordinates adopted in the momentum space.

$$\Psi=\sum_{\alpha}^{12}\psi(\vec{k}_\alpha\vec{p}_\alpha\vec{q}_\alpha)+\sum_{\beta}^{6}\chi(\vec{k}_\beta\vec{\kappa}_\beta\vec{s}_\beta)\ , \tag{1}$$

where α and β denote the 18 choices of Jacobi coordinates in the momentum space which are illustrated in Fig. 1.

In the case of a separable S-wave two-body potential

$$v(\vec{k},\vec{k}')=-\sum_i \frac{g_i(k)g_i(k')}{\lambda_i}\frac{1}{4\pi}\ , \tag{2}$$

the t matrix is also S-wave and can be written as

$$\begin{aligned} t(\vec{k},\vec{k}';z)&=\sum_{ij}g_i(k)\tau_{ij}(z)g_j(k')\frac{1}{4\pi}\ , \\ [\tau^{-1}(z)]_{ij}&=-\lambda_i\delta_{ij}-\int_0^\infty k^2dk\frac{g_i(k)g_j(k)}{z-\dfrac{k^2}{m}}\ , \end{aligned} \tag{3}$$

where m is the mass of the particle. Then, ψ and χ are written as

$$\begin{aligned} \psi(\vec{k}\vec{p}\vec{q})&=\frac{1}{z-\dfrac{1}{m}(k^2+\frac{3}{4}p^2+\frac{2}{3}q^2)}\sum_{ij}g_i(k)\tau_{ij}\left[z-\frac{3p^2}{4m}-\frac{2q^2}{3m}\right]A_j(\vec{p}\vec{q};z)\ , \\ \chi(\vec{k}\vec{\kappa}\vec{s})&=\frac{1}{z-\dfrac{1}{m}(k^2+\kappa^2+\frac{1}{2}s^2)}\sum_{ij}g_i(k)\tau_{ij}\left[z-\frac{\kappa^2}{m}-\frac{s^2}{2m}\right]B_j(\vec{\kappa}\vec{s};z)\ . \end{aligned} \tag{4}$$

Here, z is to be considered as the energy of the bound state, and A and B are what satisfy

$$\begin{aligned} A_j(\vec{p}\vec{q};z)=&\sum_{j'j''}\int d\vec{q}\,'X_{jj'}\left[\vec{p},\tfrac{1}{3}\vec{q}+\vec{q}\,';z-\frac{2q^2}{3m}\right]\tilde{\tau}_{j'j''}\left[z-\frac{3q^2}{4m}-\frac{3q'^2}{4m}-\frac{\vec{q}\vec{q}\,'}{2m}\right]A_{j''}(\vec{q}+\tfrac{1}{3}\vec{q}\,',\vec{q}\,';z) \\ &+\sum_{j'j''}\int d\vec{q}\,'X_{jj'}\left[\vec{p},-\tfrac{2}{3}\vec{q}-\vec{q}\,';z-\frac{2q^2}{3m}\right]\tilde{\tau}_{j'j''}\left[z-\frac{q^2}{m}-\frac{3q'^2}{4m}-\frac{\vec{q}\vec{q}\,'}{m}\right]B_{j''}(\vec{q}+\tfrac{1}{2}\vec{q}\,',\vec{q}\,';z)\ , \\ B_j(\vec{\kappa}\vec{s};z)=&2\sum_{j'j''}\int d\vec{s}\,'Y_{jj'}\left[\vec{\kappa},\tfrac{1}{2}\vec{s}+\vec{s}\,';z-\frac{s^2}{2m}\right]\tilde{\tau}_{j'j''}\left[z-\frac{3s^2}{4m}-\frac{s'^2}{m}-\frac{\vec{s}\vec{s}\,'}{m}\right]A_{j''}(-\vec{s}-\tfrac{2}{3}\vec{s}\,',\vec{s}\,';z)\ , \end{aligned} \tag{5}$$

where

$$\tilde{\tau}_{ij}(z)=\frac{1}{4\pi}\tau_{ij}(z)\ , \tag{6}$$

and X and Y, which can be seen as playing the role of effective potentials for A and B are, in turn, what satisfy

$$\begin{aligned} X_{jj'}(\vec{\mathrm{p}},\vec{\mathrm{p}}';z)&=V_{jj'}(\vec{\mathrm{p}},\vec{\mathrm{p}}';z)+\sum_{ll'}\int d\vec{\mathrm{p}}''V_{jl}(\vec{\mathrm{p}},\vec{\mathrm{p}}'';z)\tilde{\tau}_{ll'}\left[z-\frac{3p''^2}{4m}\right]X_{l'j'}(\vec{\mathrm{p}}'',\vec{\mathrm{p}}';z)\ , \\ Y_{jj'}(\vec{\kappa},\vec{\kappa}';z)&=W_{jj'}(\vec{\kappa},\vec{\kappa}';z)+\sum_{ll'}\int d\vec{\kappa}''W_{jl}(\vec{\kappa},\vec{\kappa}'';z)\tilde{\tau}_{ll'}\left[z-\frac{\kappa''^2}{m}\right]Y_{l'j'}(\vec{\kappa}'',\vec{\kappa}';z)\ , \end{aligned} \tag{7}$$

where V and W are defined by

$$\begin{aligned} V_{jj'}(\vec{\mathrm{p}},\vec{\mathrm{p}}';z)&=g_j(|\tfrac{1}{2}\vec{\mathrm{p}}+\vec{\mathrm{p}}'|)\frac{2}{z-\frac{1}{m}(p^2+p'^2+\vec{\mathrm{p}}\vec{\mathrm{p}}')}g_{j'}(|\vec{\mathrm{p}}+\tfrac{1}{2}\vec{\mathrm{p}}'|)\ , \\ W_{jj'}(\vec{\kappa},\vec{\kappa}';z)&=g_j(\kappa')\frac{1}{z-\frac{1}{m}(\kappa^2+\kappa'^2)}g_{j'}(\kappa)\ . \end{aligned} \tag{8}$$

Up to now, only the S-wave parts of X and Y are considered in the literature, so are they here:

$$\begin{aligned} &X_{jj'}(\vec{\mathrm{p}},\vec{\mathrm{p}}';z)=X_{jj'}(p,p';z)\frac{1}{4\pi}\ , \\ &Y_{jj'}(\vec{\kappa},\vec{\kappa}';z)=Y_{jj'}(\kappa,\kappa';z)\frac{1}{4\pi}\ , \\ &X_{jj'}(p,p';z)=V_{jj'}(p,p';z)+\sum_{ll'}\int_0^\infty p''^2dp''V_{jl}(p,p'';z)\tilde{\tau}_{ll'}\left[z-\frac{3p''^2}{4m}\right]X_{l'j'}(p'',p';z)\ , \\ &Y_{jj'}(\kappa,\kappa';z)=W_{jj'}(\kappa,\kappa';z)+\sum_{ll'}\int_0^\infty \kappa''^2d\kappa''W_{jl}(\kappa,\kappa'';z)\tilde{\tau}_{ll'}\left[z-\frac{\kappa''^2}{m}\right]Y_{l'j'}(\kappa'',\kappa';z)\ , \\ &V_{jj'}(p,p';z)=4\pi\int_{-1}^{1}dx\frac{g_j[(\frac{1}{4}p^2+p'^2+pp'x)^{1/2}]g_{j'}[(p^2+\frac{1}{4}p'^2+pp'x)^{1/2}]}{z-\frac{1}{m}(p^2+p'^2+pp'x)}\ , \\ &W_{jj'}(\kappa,\kappa';z)=4\pi\frac{g_j(\kappa')g_{j'}(\kappa)}{z-\frac{1}{m}(\kappa^2+\kappa'^2)}\ . \end{aligned} \tag{9}$$

In such a case, $A_j(\vec{\mathrm{p}},\vec{\mathrm{q}};z)$ and $B_j(\vec{\kappa},\vec{\mathrm{s}};z)$ of Eq. (4) are also S wave.

B. Separable expansion of [3 + 1] and [2 + 2] subamplitudes

Several methods have been proposed to obtain a separable representation of X and Y, among which we adopt in the present work the Hilbert-Schmidt (HSE) and the energy-dependent pole (EDPE) expansion methods.

(i) HSE.

In the HSE method, X and Y are expressed as

$$
\begin{aligned}
&X_{jj'}(p,p';z)=\sum_n x_j^n(p;z)H_n(z)x_{j'}^n(p';z)\ ,\\
&Y_{jj'}(\kappa,\kappa';z)=\sum_n y_j^n(\kappa;z)G_n(z)y_{j'}^n(\kappa';z)\ ,\\
&H_n(z)=\frac{1}{[\xi_n(z)-1]N_{nn}(z)}\ ,\\
&G_n(z)=\frac{1}{[\zeta_n(z)-1]M_{nn}(z)}\ ,\\
&N_{nn}(z)=\sum_{jj'}\int_0^\infty p^2dp\,x_j^n(p;z)\tilde{\tau}_{jj'}\left[z-\frac{3p^2}{4m}\right]x_{j'}^n(p;z)\ ,\\
&M_{nn}(z)=\sum_{jj'}\int_0^\infty \kappa^2d\kappa\,y_j^n(\kappa;z)\tilde{\tau}_{jj'}\left[z-\frac{\kappa^2}{m}\right]y_{j'}^n(\kappa;z)\ ,
\end{aligned}
\tag{10}
$$

where $[\xi_n(z),x_j^n(p;z)]$ and $[\zeta_n(z),y_j^n(\kappa;z)]$ are determined by an eigenvalue problem:

$$
\begin{aligned}
&x_j^n(p;z)=\xi_n(z)\sum_{j'j''}\int_0^\infty p'^2dp'V_{jj'}(p,p';z)\tilde{\tau}_{j'j''}\left[z-\frac{3p'^2}{4m}\right]x_{j''}^n(p';z)\ ,\\
&y_j^n(\kappa;z)=\zeta_n(z)\sum_{j'j''}\int_0^\infty \kappa'^2d\kappa'W_{jj'}(\kappa,\kappa';z)\tilde{\tau}_{j'j''}\left[z-\frac{\kappa'^2}{m}\right]y_{j''}^n(\kappa';z)\ .
\end{aligned}
\tag{11}
$$

Then, $A_j(\vec{\mathrm{p}},\vec{\mathrm{q}};z)$ and $B_j(\vec{\kappa},\vec{\mathrm{s}};z)$ are expressed in a separable series as

$$
\begin{aligned}
&A_j(\vec{\mathrm{p}},\vec{\mathrm{q}};z)=\sum_n x_j^n\left[p;z-\frac{2q^2}{3m}\right]H_n\left[z-\frac{2q^2}{3m}\right]\alpha_n(q;z)\frac{1}{4\pi}\ ,\\
&B_j(\vec{\kappa},\vec{\mathrm{s}};z)=\sum_n y_j^n\left[\kappa;z-\frac{s^2}{2m}\right]G_n\left[z-\frac{s^2}{2m}\right]\beta_n(s;z)\frac{1}{4\pi}\ ,
\end{aligned}
\tag{12}
$$

where $\alpha_n(q;z)$ and $\beta_n(s;z)$ are determined by

$$
\begin{aligned}
\alpha_n(q;z)=&\sum_{n'}\int_0^\infty q'^2dq'E_{nn'}(q,q';z)H_{n'}\left[z-\frac{2q'^2}{3m}\right]\alpha_{n'}(q';z)\\
&+2\sum_{n'n''}\int_0^\infty q'^2dq'\int_0^\infty q''^2dq''F_{nn'}(q,q';z)G_{n'}\left[z-\frac{q'^2}{2m}\right]F_{n''n'}(q'',q';z)H_{n''}\left[z-\frac{2q''^2}{3m}\right]\alpha_{n''}(q'';z)\ ,\\
\beta_n(s;z)=&2\sum_{n'}\int_0^\infty s'^2ds'F_{n'n}(s',s;z)H_{n'}\left[z-\frac{2s'^2}{3m}\right]\alpha_{n'}(s';z)\ ,\\
E_{nn'}(q,q';z)=&\tfrac{1}{2}\sum_{jj'}\int_{-1}^1 dx\,x_j^n\left[\left|\tfrac{1}{3}\vec{\mathrm{q}}+\vec{\mathrm{q}}'\right|;z-\frac{2q^2}{3m}\right]\\
&\times\tilde{\tau}_{jj'}\left[z-\frac{3q^2}{4m}-\frac{3q'^2}{4m}-\frac{qq'}{2m}x\right]x_{j'}^{n'}\left[\left|\tfrac{1}{3}\vec{\mathrm{q}}'+\vec{\mathrm{q}}\right|;z-\frac{2q'^2}{3m}\right]\ ,\\
F_{nn'}(q,q';z)=&\tfrac{1}{2}\sum_{jj'}\int_{-1}^1 dx\,x_j^n\left[\left|\tfrac{2}{3}\vec{\mathrm{q}}+\vec{\mathrm{q}}'\right|;z-\frac{2q^2}{3m}\right]\tilde{\tau}_{jj'}\left[z-\frac{q^2}{m}-\frac{3q'^2}{4m}-\frac{qq'}{m}x\right]y_{j'}^{n'}\left[\left|\vec{\mathrm{q}}+\tfrac{1}{2}\vec{\mathrm{q}}'\right|;z-\frac{q'^2}{2m}\right]\ .
\end{aligned}
\tag{13}
$$

The energy of the system is determined by the z value which satisfies the above equation for $\alpha_n(q;z)$.

(ii) EDPE.

In the EDPE method, X and Y are expressed as

$$
\begin{aligned}
&X_{jj'}(p,p';z)=\sum_{nn'}x_j^n(p;z)H_{nn'}(z)x_{j'}^{n'}(p';z)\ ,\\
&Y_{jj'}(\kappa,\kappa';z)=\sum_{nn'}y_j^n(\kappa;z)G_{nn'}(z)y_{j'}^{n'}(\kappa';z)\ ,\\
&x_j^n(p;z)=\sum_{j'}\int_0^\infty p'^2dp'V_{jj'}(p,p';z)f_{j'}^n(p')\ ,\\
&y_j^n(\kappa;z)=\sum_{j'}\int_0^\infty \kappa'^2d\kappa'W_{jj'}(\kappa,\kappa';z)h_{j'}^n(\kappa')\ ,\\
&[H^{-1}(z)]_{nn'}=\Gamma_{nn'}(z)-S_{nn'}(z)\ ,\\
&[G^{-1}(z)]_{nn'}=L_{nn'}(z)-T_{nn'}(z)\ ,\\
&\Gamma_{nn'}(z)=\sum_{jj'}\int_0^\infty p^2dp\int_0^\infty p'^2dp'f_j^n(p)V_{jj'}(p,p';z)f_{j'}^{n'}(p')\ ,\\
&L_{nn'}(z)=\sum_{jj'}\int_0^\infty \kappa^2d\kappa\int_0^\infty \kappa'^2d\kappa'h_j^n(\kappa)W_{jj'}(\kappa,\kappa';z)h_{j'}^{n'}(\kappa')\ ,\\
&S_{nn'}(z)=\sum_{jj'}\int_0^\infty p^2dp\,x_j^n(p;z)\tilde{\tau}_{jj'}\left[z-\frac{3p^2}{4m}\right]x_{j'}^{n'}(p;z)\ ,\\
&T_{nn'}(z)=\sum_{jj'}\int_0^\infty \kappa^2d\kappa\,y_j^n(\kappa,z)\tilde{\tau}_{jj'}\left[z-\frac{\kappa^2}{m}\right]y_{j'}^{n'}(\kappa;z)\ ,
\end{aligned}
\tag{14}
$$

where $f_j^n(p)$ and $h_j^n(\kappa)$ are determined by an eigenvalue problem:

$$
\begin{aligned}
&f_j^n(p)=\xi_n\sum_{j'j''}\tilde{\tau}_{jj'}\left[E_x-\frac{3p^2}{4m}\right]\int_0^\infty p'^2dp'V_{j'j''}(p,p';E_x)f_{j''}^n(p')\ ,\\
&h_j^n(\kappa)=\zeta_n\sum_{j'j''}\tilde{\tau}_{jj'}\left[E_y-\frac{\kappa^2}{m}\right]\int_0^\infty \kappa'^2d\kappa'W_{j'j''}(\kappa,\kappa';E_y)h_{j''}^n(\kappa')\ .
\end{aligned}
\tag{15}
$$

The values of E_x and E_y are chosen such that each of these equations has a solution which has an eigenvalue of unity.

Then, $A_j(\vec{p},\vec{q};z)$ and $B_j(\vec{\kappa},\vec{s};z)$ of Eq. (4) are expressed in a separable series as

$$
\begin{aligned}
&A_j(\vec{p},\vec{q},z)=\sum_{nn'}x_j^n\left[p;z-\frac{2q^2}{3m}\right]H_{nn'}\left[z-\frac{2q^2}{3m}\right]\alpha_{n'}(q;z)\frac{1}{4\pi}\ ,\\
&B_j(\vec{\kappa},\vec{s};z)=\sum_{nn'}y_j^n\left[\kappa;z-\frac{s^2}{2m}\right]G_{nn'}\left[z-\frac{s^2}{2m}\right]\beta_{n'}(s;z)\frac{1}{4\pi}\ ,
\end{aligned}
\tag{16}
$$

where $\alpha_n(q;z)$ and $\beta_n(s;z)$ are determined by

$$\alpha_n(q;z)=\sum_{n'n''}\int_0^\infty q'^2\,dq'$$
$$\times\left[E_{nn''}(q,q';z)+2\sum_{mm'}\int_0^\infty q''^2\,dq''F_{nm}(q,q'';z)G_{mm'}\left[z-\frac{q''^2}{2m}\right]F_{n''m'}(q',q'';z)\right]$$
$$\times H_{n''n'}\left[z-\frac{2q'^2}{3m}\right]\alpha_{n'}(q';z)\ ,$$

$$\beta_n(s;z)=2\sum_{n'n''}\int_0^\infty s'^2ds'F_{n'n}(s',s;z)H_{n'n''}\left[z-\frac{2s'^2}{3m}\right]\alpha_{n''}(s';z)\ , \tag{17}$$

$$E_{nn'}(q,q';z)=\tfrac{1}{2}\int_{-1}^{1}dx\sum_{jj'}x_j^n\left[\,|\,\tfrac{1}{3}\vec{q}+\vec{q}\,'\,|\,;z-\frac{2q^2}{3m}\right]$$
$$\times\tilde{\tau}_{jj'}\left[z-\frac{3q^2}{4m}-\frac{3q'^2}{4m}-\frac{qq'x}{2m}\right]x_{j'}^{n'}\left[\,|\,\tfrac{1}{3}\vec{q}\,'+\vec{q}\,|\,;z-\frac{2q'^2}{3m}\right],$$

$$F_{nn'}(s,q';z)=\tfrac{1}{2}\int_{-1}^{1}dx\sum_{jj'}x_j^n\left[\,|\,\tfrac{2}{3}\vec{q}+\vec{q}\,'\,|\,;z-\frac{2q^2}{3m}\right]$$
$$\times\tilde{\tau}_{jj'}\left[z-\frac{q^2}{m}-\frac{3q'^2}{4m}-\frac{qq'x}{m}\right]y_{j'}^{n'}\left[\,|\,\vec{q}+\tfrac{1}{2}\vec{q}\,'\,|\,;z-\frac{q'^2}{2m}\right].$$

The energy of the system is determined by the z value which satisfies the above equation for $\alpha_n(q;z)$.

C. UPE

We derive the form factors $g_i(k)$ of the separable two-body potential from a realistic local potential $v(r)$ by the UPE method, as Tjon did in his calculation of ^{4}He nucleus.[12] To obtain a separable potential in this scheme, we must perform a Fourier transformation from the configuration space to the momentum space. Every realistic He-He potential has a very strong repulsive core at small He-He distances. In such a case, it is better to transform the form factor $g_i(r)$ than to transform the potential $v(r)$, for greater numerical accuracy.

Thus, the form factors $g_i(k)$ are obtained by

$$g_i(k)=\left[\frac{2}{\pi}\right]^{1/2}\int_0^\infty r^2dr\,j_0(kr)g_i(r)\ ,$$

$$g_i(r)=\lambda_i v(r)u_i(r)\ , \tag{18}$$

$$j_0(x)=\sin x/x\ ,$$

where λ_i and u_i are determined by

$$su_i(r)=\left[-\frac{1}{m}\frac{d^2}{dr^2}+\lambda_i v(r)\right]u_i(r)\ ,$$
$$\lambda_i\int_0^\infty dr\,u_i(r)v(r)u_i(r)=-1\ . \tag{19}$$

We adopt the MDD-2 (Morse dipole-dipole) potential for He-He interaction:

$$v(r)=\epsilon(e^{2\alpha(1-x)}-2e^{\alpha(1-x)})\ ,$$
$$(0<r\le 3.6828\ \text{Å})$$
$$=-\frac{c_6}{r_6}-\frac{c_8}{r^8}\quad(r>3.6828\ \text{Å})\ , \tag{20}$$

where $x=r/3.024$ Å, $\alpha=6.12777$, $\epsilon=10.75$ K, $c_6=12014$ Å^{6}K, and $c_8=27670$ Å^{8}K. We take as $1/m=12.02$ K Å^2.

The MDD-2 potential assures a bound dimer at energy -0.0005 K. We choose for s this ground-state energy, so that the separable potential

$$v(k,k')=-\sum_i\frac{g_i(k)g_i(k')}{\lambda_i} \tag{21}$$

is the same in its operation on the two-body ground state as the original potential $v(r)$.

To determine λ_i and $u_i(r)$ (for $\lambda_i\neq 1$), we take a trial λ_i and solve an eigenvalue problem for s, and if the output value is the desired s, then the chosen λ_i is what we wanted. This determines $u_i(r)$ at the

same time. This procedure is superior in numerical accuracy to a direct solution of λ_i from the corresponding eigenvalue problem, because of the small values of $v(r)$ at larger r.

III. NUMERICAL METHOD

Since the integral-equation method of solving the four-body problem is "old stuff," we should stress the numerical aspects a little more to document the differences between the molecular and nuclear applications. (We did a part of it in Sec. II C.)

Numerical solution of the Faddeev-Yakubovsky equation for the $(^4\mathrm{He})_4$ system consists of three steps:

(I) A separable expansion of the interatomic potential through the UPE method, which means a separable two-body t matrix;

(II) a separable expansion of the $[3+1]$ and $[2+2]$ subamplitudes through the HSE or EDPE methods;

(III) the solution of the four-body equation which determines the four-body energy.

Each of these steps involves diagonalization of a matrix of finite rank. The diagonalization is performed in the configuration space in step I, while it is performed in the momentum space in steps II and III. We take the meshpoints for the variables by

$$r_i = r_1 + c_r \tan\frac{\pi}{2}x_i \quad \text{(step I)}$$

$$p_i = p_1 + c_p \tan\frac{\pi}{2}x_i \quad \text{(steps I, II, III)} \qquad (22)$$

$$x_i = (i-1)/N, \quad i = 1,2,\ldots,N$$

where N is the number of meshpoints. (We take $N=30$, $r_1=1.3$ Å, $c_r=1$ Å, $p_1=0.0001$ Å^{-1}, and $c_p=1$ Å^{-1} throughout the present calculation.) This type of transformation of variables was already adopted in our previous variational calculation of the $(^4\mathrm{He})_4$ system.[1] To represent the integration we adopt the Simpson weight.

In steps II and III, we need the values of the UPE form factors and those of the $[3+1]$ and $[2+2]$ subamplitudes at arbitrary values of the momentum variables. Then an interpolation is necessary which we perform by the Lagrange method of rank four. Further, if it is possible firstly to prepare this interpolation in a large number of meshpoints and approximate the values of the form factors at any arbitrary point by a Taylor expansion of order one, then it saves computer time considerably. We actually do this in step II.

TABLE I. Two-atom UPE eigenvalues. MDD-2 potential of McGee and Bruch is used. λ_A and λ_R denote the attractive and repulsive eigenvalues, respectively.

λ_A	λ_R
1	−0.000 128 846
7.044	−0.000 679 83
18.418	−0.001 673 02

To test the numerical accuracy of the present calculation, we varied N and c_p of Eq. (22) (N from 20 to 30 and c_p from 0.6 to 1.4 Å^{-1}), and found the resultant four-body energies are essentially unchanged in their absolute values up to the second digit.

IV. RESULTS AND DISCUSSIONS

In Table I, we list the UPE eigenvalues for the MDD-2 He-He potential. The extremely small values λ_R for the repulsive UPE terms come from the very strong short-range repulsion of the He-He potential. From the trend of the trimer energy (Table II) and the agreement with the results of Ref. 2, it seems that our most accurate results must be associated with UPE$=2A+1R$.

The resultant tetramer energy for each case of retaining various numbers of separable terms in the two-body t matrix and the $[3+1]$ and $[2+2]$ subamplitudes are listed in Table III and plotted in Fig. 2. These results show a tendency for convergence in both of HSE and EDPE, and indicate a converged value of some 0.37 K for the tetramer binding energy. When we compare this value with the ATMS value 0.49 K and consider the loosely-bound nature of small ^{4}He clusters (the small contributions coming from the higher partial waves than the S-wave ones, those of the two-body interaction and those of the $[3+1]$ and $[2+2]$

TABLE II. Behavior of the three-atom ground-state energy with respect to the two-atom UPE. $1A+1R$, for example, denotes that one attractive and one repulsive UPE term is retained in the calculation. In this three-body calculation, 50 meshpoints for the momentum variables are taken.

	$(2A)$ −0.0926 K	
$(1A)$ −0.0912 K		$(2A+1R)$ −0.0883 K
	$(1A+1R)$ −0.0838 K	

TABLE III. Four-atom ground-state energy obtained by retaining various numbers of two-atom UPE and the subamplitude HSE or EDPE terms. Energies are in K, and "a" means the attractive terms. To clarify how the four-body energy changes as we include the higher terms of the subamplitudes, we list the numbers to the third digit because for a fixed condition of numerical integration, the third digit can show the trend of the energy convergence (also the same for Table IV).

$T(2)$	$T(3+1)$	$T(2+2)$	E_4(HSE)	E_4(EDPE)
$1A$	$1a$	$1a$	−0.198	−0.405
	$2a$	$2a$	−0.380	−0.411
	$3a$	$3a$	−0.404	−0.413
$1A+1R$	$1a$	$1a$	−0.306	−0.364
	$2a$	$2a$	−0.351	−0.366
	$3a$	$3a$	−0.355	−0.366
$2A+1R$	$1a$	$1a$	−0.308	−0.371
	$2a$	$2a$	−0.356	−0.373
	$3a$	$3a$	−0.360	−0.373

subamplitudes), the agreement between the two calculations is good and shows the accuracies of the HSE and EDPE in this helium molecule system. This is the most important result of this work. The difference between the ATMS and the Faddeev-Yakubovsky energy is 2.6% of the potential energy (−4.62 K).

The first attempt to test the [3 + 1] and [2 + 2] subamplitude separable expansions was performed by Gibson and Lehman.[17] They directly solved the two-variable integral equations for X and Y by matrix inversion, and then solved the equations for the spectator functions A and B [Eq. (5)] by an iterative

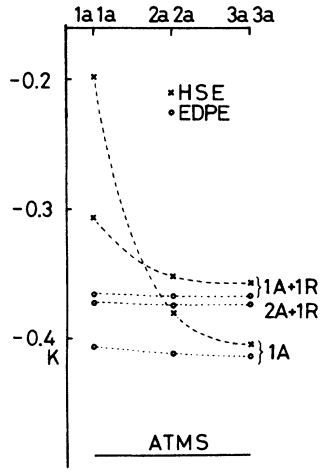

FIG. 2. Convergence behaviors of the four-body energy with respect to the S-wave HSE and EDPE. Dashed and dotted lines are drawn to guide the eye.

procedure. The resultant binding energies were compared with those obtained through the Bateman and the HSE methods. However, their value 89.6 MeV obtained for a one-term Yamaguchi triplet NN potential ($\lambda=0.415$ fm^{-3}, $\beta=1.45$ fm^{-1}) is smaller than that obtained by Narodetsky through HSE (90.10 MeV). This seems to be a contradiction because a further inclusion of the attractive HSE terms will increase the binding energy while the effect of including the repulsive terms is negligible. Our code also reproduced this HSE value and we found the numerical accuracy for this one-term Yamaguchi potential is fairly good. Probably, the 6-point Gaussian quadrature in the angular variable and the 12-point Gegenbauer quadrature in the momentum variables they adopted is insufficient in solving the two-variable integral equations. It should be emphasized that our present confirmation of the separable expansion methods is based on a comparison with an ATMS calculation and on the loose-binding characteristics of the helium molecule.

From Fig. 2, we can see clearly a superiority of the EDPE in convergence over the HSE; in the EDPE, the value for EDPE$=(1a,1a)$ reaches 98% of the converged value for UPE$=1A$ and larger than 99% for UPE$=1A+1R$, in contrast to the fact that in the HSE we need at least three attractive terms for each of the [3 + 1] and [2 + 2] subsystems [$(3a,3a)$] to estimate the converged value. This advantage amounts to a reduction of computer time by 15 to 20 times. The faster convergence of

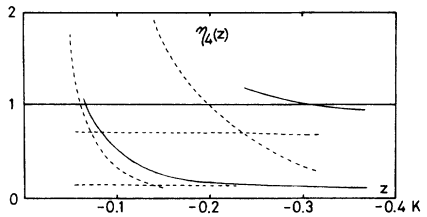

FIG. 3. Behavior of the Lagrange multiplier $\eta_4(z)$ which is introduced, in numerical calculation, on the right-hand side of the first equation in Eq. (13), with respect to trial four-body energy z.

EDPE was already pointed out by Sofianos *et al.* for cases of one-term Yamaguchi potentials. The significance of the present result lies in the fact that this feature is much enhanced in this helium molecule system.

It should also be noted that the convergence gets better in both of the HSE and EDPE when we include the repulsive terms in the two-body t matrix. To clarify this, we plot in Fig. 3 the values of the Lagrange multiplier η_4 introduced in the right-hand side of Eq. (4) to convert the equation into a form of matrix diagonalization which is performed by taking a trial z. When $\eta_4=1$, the trial z is representing the four-body energy E_4. We see that there appear two kinds of $\eta_4(z)$ in Fig. 3 for UPE$=1a$: "physical" ones and "unphysical" ones, the latter being quite insensitive to the variation of z. This shows that the four-body kernel obtained by UPE$=1A$ will involve an unphysical part. The unphysical $\eta_4(z)$ disappear when we consider the first repulsive term in the two-body t matrix.

Table IV shows separate convergence behaviors of the HS $[3+1]$- and $[2+2]$-separable expansions coupled with UPE$=1A+1R$. In the second column we fix the $[2+2]$ amplitude to $1a$ and increase the $[3+1]$ attractive terms, while we fix the $[3+1]$ amplitude to $1a$ and increase the $[2+2]$ attractive terms in the third column. We see that the effect of including higher $[2+2]$ terms is larger than that of including higher $[3+1]$ terms. The importance of the $[2+2]$ subsystem amplitude is also realized in Gibson and Lehman's calculations.[17]

Finally, we mention that we could not find an excited state below the $[3+1]$ threshold. This does not imply that such states do not exist; they may lie too close to the threshold to be "pulled out" for view.

TABLE IV. Separate convergence behavior with respect to the $[3+1]$ and $[2+2]$ subamplitudes. See the text.

	$[3+1]$ behavior	$[2+2]$ behavior
$1a$	-0.306	-0.306
$2a$	-0.319	-0.338
$3a$	-0.321	-0.343

V. CONCLUSION

The most important conclusion drawn from this work is that we could show the accuracy of the HSE and EDPE methods for the S-wave $[3+1]$ and $[2+2]$ subamplitudes. This is made possible by a comparison with an ATMS calculation and the loose-binding nature of the helium molecule. We found, however, the convergence rate of the HSE is rather slow, requiring much computer time, while that of the EDPE is clearly faster and one term for each of the $[3+1]$ and $[2+2]$ subsystems is sufficient in this helium molecule system. The present calculation is the first calculation using the EDPE in the case of realistic force, in particular, with inclusion of a strong short-range repulsion in the two-body interaction, and encourages the use of this expansion in other He molecule problems. With the EDPE and perhaps the separable expansion for subamplitudes suggested by Casel *et al.*,[18,19] calculations in the scattering domain should become more accessible.

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[1]S. Nakaichi, Y. Akaishi, H. Tanaka, and T. K. Lim, Phys. Lett. 68A, 36 (1978); S. Nakaichi, T. K. Lim, Y. Akaishi, and H. Tanaka, J. Chem. Phys. 71, 4430 (1979).
[2]H. S. Huber and T. K. Lim, J. Chem. Phys. 68, 1006 (1978).
[3]L. W. Bruch and I. J. McGee, J. Chem. Phys. 52, 5884

(1970).
[4]E. Harms, Phys. Rev. C 1, 1667 (1970).
[5]O. A. Yakubovsky, Yad. Fiz. 5, 1312 (1967) [Sov. J.—Nucl. Phys. 5, 937 (1967)].
[6]L. D. Faddeev, in *Three-Body Problem in Nuclear and Particle Physics,* edited by J. S. C. McKee and R. M. Rolph (North-Holland, Amsterdam, 1970).
[7]E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. B2, 167 (1967); P. Grassberger and W. Sandhas, *ibid.* 2, 181 (1967); W. Sandhas, Acta Phys. Austriaca Suppl. XIII, 679 (1974).
[8]I. H. Sloan, Phys. Rev. C 6, 1945 (1972); G. Bencze, Nucl. Phys. A210, 568 (1973); E. F. Redish, Phys. Rev. C 10, 61 (1974); D. Kouri and F. Levin, Phys. Lett. 50B, 421 (1974); W. Tobocman, Phys. Rev. C 9, 2466 (1974).
[9]E. O. Alt, P. Grassberger, and W. Sandhas, Phys. Rev. C 1, 85 (1970).
[10]V. F. Kharchenko and V. E. Kuzmichev, Nucl. Phys. A183, 606 (1972); V. F. Kharchenko, V. E. Kuzmichev, and S. A. Shadchin, *ibid.* A226, 71 (1924).
[11]Narodetsky, Nucl. Phys. A221, 191 (1974).
[12]J. A. Tjon, Phys. Lett. 56B, 217 (1975).
[13]S. Nakaichi, Y. Akaishi, and H. Tanaka, Prog. Theor. Phys. 64, 1315 (1980).
[14]J. A. Tjon, Phys. Rev. A 21, 1334 (1980).
[15]S. Sofianos, N. J. McGurk, and H. Fiedeldey, Nucl. Phys. A318, 295 (1979).
[16]J. Revai and J. Raynal, Lett. Nuovo Cimento 9, 461 (1974).
[17]B. F. Gibson and D. R. Lehman, Phys. Rev. C 14, 685 (1976); 15, 2257 (1977).
[18]A. Casel, H. Haberzettl, and W. Sandhas, contribution to the Proceedings of the 9th International Few-Body Conference, Eugene, Oregon, 1980 (unpublished); Phys. Rev. C 25, 1738 (1982).
[19]J. A. Tjon, Phys. Lett. 63B, 391 (1976).