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LIPPMAN-SCHWINGER EQUATION IN THE HARMONIC-OSCILLATOR BASIS FOR THE TRINUCLEON BOUND-STATE PROBLEM

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Уравнение Липпмана-Швингера в осцилляторном базисе для задачи на связанное состояние трех нуклонов

Матричный элемент n -частичной свободной функции Грина в осцилляторном базисе представлен в виде одномерного интеграла, удобного для практических вычислений. Исходя из уравнения Липпмана-Швингера, получена более быстрая сходимость в расчёте энергии связи трех нуклонов по сравнению с методом диагонализации энергетической матрицы. Новым методом рассматривается асимптотическое поведение волновой функции трех частиц при использовании ее явного представления.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Lippman-Schwinger Eqation in the Harmonic-Oscillator Basis for the Trinucleon Bound-State Problem

The matrix element of the n -body free Green function between the harmonic-oscillator states has been brought into the form of a one-dimensional integral which is useful for practical calculations. Using the explicit expansion for the three-body wave function, its asymptotic form is derived by a new method. Starting with the Lippman-Schwinger equation, better convergence for the binding energy calculations is obtained as compared with the method of the diagonalization of the energy matrix.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

Several years ago the problem of the trinucleon ground-state was extensively studied[1] by the method of the diagonalization of the energy matrix (DEM) built up from the Reid soft-core interaction[2] in a harmonic-oscillator basis. Strayer and Sauer[3] improved these calculations by enlarging the basis considerably. Their results are compatible with those derived by other methods[3]. The convergence of some of the basic three-nucleon bound-state quantities like the binding energy and s-state probability was lacking, however.

It is known, that this trouble lies in the form of the spatial dependence of the oscillator wave functions. A great number of them is needed to build up a realistic three-nucleon wave function which (a) is strongly suppressed at small relative distances and (b) decreases exponentially at large relative distances[4]. The complications arising from (a) can be partly avoided by using the super-soft-core two-nucleon potentials[5].

Nunberg, Pace and Prosperi[6] attempted to solve the problem by introducing two oscillator radii instead of the usual one.

The employment of another nonlinear parameter gave them a tool to change once more the radial form of the oscillator wave functions so that the convergence would be better. They estimated that they improved it by ≈ 0.2 MeV in the binding energy, at the maximum number of oscillator quanta $Q_{max} = 36$.

In this paper we attempt to make the convergence of the three-nucleon binding energy calculations better using the Lippman-Schwinger (LS) equation. This approach is based on the observation [7,8] that the incorrect asymptotic behaviour of the wave function from the DEM method is due to the truncation of the basis in which the kinetic energy operator is acting. Quite recently, this method has been used [9] to solve the two-centre problem with realistic potentials. A potential V was expanded in terms of harmonic oscillator functions $V \to \sum_{i,j}^{N} |i\rangle\langle i|V|j\rangle\langle j|$. Thus, the resulting approximation to V is a rank-N separable potential, and the well-known methods can be applied to solve the problem.

Here, we consider the problem more formally and use rather the completeness of the basis to simplify the treatment of the kernel of the LS equation. The formalism needed for practical calculations is described in sec. 2. The numerical results for the triton binding energy are given in sec. 3.1. Our main results concerning the three-body wave function properties are presented and discussed in sect. 3.2.

2. FORMALISM

Let us write down the LS equation for the trinucleon bound-state problem

$$|\Psi> = -G_0(E)V|\Psi> . \qquad (1)$$

In eq. (1) the Green function $G_0(E)$ is

$$G_0(E) = (H_0 - E)^{-1}, \qquad (2)$$

where E is the energy eigenvalue and H_0 is the kinetic energy operator of the system. Further, V stands for the operator of the potential energy and is equal to the sum of the two-nucleon potentials. Using the completeness of the basis constructed[10,3] from the harmonic oscillator functions $<r|n\ell> = b^{-3/2}R_{n\ell}(r/b)$ (b is the oscillator length parameter, $b = (\hbar/\omega M)^{1/2}$ where ω is the oscillator frequency and M is the nucleon mass), we write eq. (1) as

$$|\Psi> = -\sum_{i,j} G_0(E)|i><i|V|j><j|\Psi> . \qquad (3)$$

We define the basis states $|k>(k=i,j)$ according to eq. (2) of ref.[3].

In principle, the sums in eq. (3) contain an infinite number of terms. We take the first N_i (N_j) of them for the sum over i(j). We do not demand that $N_i = N_j$. The reason is that the sum over i may turn out to be saturated easier than the sum over j. The equality $N_i = N_j$ would just mean waste of the computer time when performing the sum over i numerically.

Now we transform eq. (3) into the system of homogeneous equations for the coefficients $c_k = <k|\Psi>$

$$c_k = -\sum_{j=1}^{N_j}\sum_{i=1}^{N_i} \langle k|G_0(E)|i\rangle\langle i|V|j\rangle c_j , \quad k=1,\ldots,N_j . \qquad (4)$$

It is immediately seen that the problem of solution of eq. (1) is simplified considerably. In eq. (4) the potential energy matrix $\langle i|V|j\rangle$ is the same as in the DEM method. Here we use the Eikemeier-Hackenbroich potential/11/. This potential has the core of $\approx$ 800 MeV and reproduces satisfactorily the nucleon-nucleon phase shifts in the singlet-even and triplet-even states up to 300 MeV and the binding energy of the deuteron.

We restrict ourselves to the trinucleon symmetric S-state. In this case the matrix element of the Green function $G_0(E)$ between the oscillator states $|i\rangle$ and $|k\rangle$ is

$$\langle k|G_0(E)|i\rangle = \sum_{\substack{\dot{n}_1\dot{n}_2\dot{n}'_1\dot{n}'_2\dot{\ell} \\ \dot{\ell}\ \text{even}}} (-1)^{\dot{n}_2+\dot{n}'_2} \frac{2}{[(1+\delta_{n_1 n_2})(1+\delta_{n'_1 n'_2})]^{1/2}} \times \langle \dot{n}_1\dot{\ell}, \dot{n}_2\dot{\ell}, 0|n_1\ell, n_2\ell\rangle\langle \dot{n}'_1\dot{\ell}, \dot{n}'_2\dot{\ell}, 0|n'_1\ell', n'_2\ell'\rangle F^{\dot{\ell}}_{\dot{n}_1\dot{n}_2,\dot{n}'_1\dot{n}'_2}(\omega,a). \qquad (5)$$

The sum in eq. (5) is restricted by the conditions

$$n_1+n_2+\ell = \dot{n}_1+\dot{n}_2+\dot{\ell} = \frac{Q}{2}$$
$$n'_1+n'_2+\ell' = \dot{n}'_1+\dot{n}'_2+\dot{\ell} = \frac{Q'}{2}. \qquad (6)$$

The numbers of the oscillator quanta Q and Q' are related to the states $|k\rangle$ and $|i\rangle$, respectively. The sum over i in eq. (4) is different from zero, only if the selection rule

$$\frac{1}{2}(Q+Q') + \ell + \ell' = \text{even} \qquad (7)$$

is satisfied. Due to this restriction about one half of the terms is ruled out.

The symbols of the type $\langle \dot{n}_1 \dot{\ell}_1, \dot{n}_2 \dot{\ell}_2, L | n_1 \ell_1, n_2 \ell_2 \rangle$ stand for the Moshinsky transformation coefficients [10].

The function $F^{\dot{\ell}_1 \dot{\ell}_2 \ldots \dot{\ell}_r}_{\dot{n}_1 \dot{n}_2 \ldots \dot{n}_r, \dot{n}_1' \dot{n}_2' \ldots \dot{n}_r'}(\omega, a)$ (in our case $r=2$ and $\ell_1 = \ell_2 = \ell$) is the r-dimensional integral

$$F^{\dot{\ell}_1 \dot{\ell}_2 \ldots \dot{\ell}_r}_{\dot{n}_1 \dot{n}_2 \ldots \dot{n}_r, \dot{n}_1' \dot{n}_2' \ldots \dot{n}_r'}(\omega, a) = \frac{2}{\omega \hbar} \int_0^\infty \int_0^\infty \ldots \int_0^\infty \frac{\left(\prod_{k=1}^{r} R_{n_k \ell_k}(p_k) R_{n_k' \ell_k}(p_k) p_k^2 \, dp_k \right)}{\left(\sum_{k=1}^{r} p_k^2 \right) + a^2} . \qquad (8)$$

In eq. (8) $p_k \; (k=1,2,\ldots,r)$ are the absolute values of the Jacobi momenta of the $(r+1)$-body problem [10] and

$$a^2 = - \frac{2E}{\omega \hbar} . \qquad (9)$$

For the practical calculations the following integral representation of the function F is useful

$$F^{\dot{\ell}_1 \dot{\ell}_2 \ldots \dot{\ell}_r}_{\dot{n}_1 \dot{n}_2 \ldots \dot{n}_r, \dot{n}_1' \dot{n}_2' \ldots \dot{n}_r'}(\omega, a) =$$

$$= \frac{2}{\omega \hbar} \frac{\prod_{k=1}^{r} \Gamma\left(\dot{n}_k + \dot{n}_k' + \dot{\ell}_k + \frac{3}{2} \right)}{\left[\prod_{k=1}^{r} \dot{n}_k ! \, \Gamma\left(\dot{n}_k + \dot{\ell}_k + \frac{3}{2} \right) \Gamma\left(\dot{n}_k' + \dot{\ell}_k + \frac{3}{2} \right) \right]^{1/2}}$$

$$\times\int_0^\infty dz\, e^{-\alpha^2 z}\,\frac{z^{\sum_{k=1}^{r}(\dot{n}_k+\dot{n}_k')}}{(1+z)^{\sum_{k=1}^{r}(\dot{n}_k+\dot{n}_k'+\dot{\ell}_k+\frac{3}{2})}}\prod_{k=1}^{r}F\left(-\dot{n}_k,-\dot{n}_k';-\dot{n}_k-\dot{n}_k'-\frac{1}{2};1-\frac{1}{z^2}\right). \qquad (10)$$

Here $\Gamma(\alpha)$ and $F(\alpha,\beta;\gamma;x)$ are the gamma and hypergeometric functions [12], respectively.

In order that the system of equations, eq. (4) be solvable, the condition

$$\mathrm{Det}\left|\delta_{jk}+\sum_{i=1}^{N_i}\langle k|G_0(E)|i\rangle\langle i|V|j\rangle\right|=0,\quad j,k=1,\ldots,N_j. \qquad (11)$$

must hold. This equation defines the energy eigenvalues of the problem.

3. RESULTS AND DISCUSSION

3.1. The three-nucleon binding energy

We found numerically the lowest energy eigenvalue as the function of three non-linear parameters b, N_i and N_j. The results are presented in tables 1 and 2.

The convergence for $Q_{max} = 20$ ($N_j = 67$) is similar to the case when $Q_{max} = 16$ (table 1). It is seen from table 1 that the sum over i in eq. (4) is saturated for $N_i = 53$ (18 oscillator quanta).

In table 3 we present the results derived within the DEM method for the same potential [11] (see also ref. [13]). The comparison of tables 2 and 3 shows that the convergence in the binding energy for the LS equation is better.

Table 1

The triton ground-state energy $-E$ (in MeV) from eq. (4) as a function of the number N_i of the intermediate states $|i\rangle$ and of the oscillator length b (in fm); the dimension of the determinant is 41 (Q_{max} = 16).

b	N_i 37	41	45	49	53
.7	6.38	6.31	6.37	6.40	
.8	6.42	6.47	6.50	6.51	6.51
.9	6.33	6.38	6.37	6.35	

Table 2

The triton ground-state energy E_{min} (in MeV) from eq. (4) as a function of the number N_j of the basis states corresponding to the total number of oscillator quanta Q_{max} ; b = = 0.8 fm and the number of intermediate states $|i\rangle$, taken into account, N_i = 53 (18 oscillator quanta).

N_j (Q_{max})	41(16)	67(20)
$-E_{min}$	6.51	6.65

Table 3

The triton gorund-state energy E_{min} (in MeV) from the DEM method as a function of the total number of oscillator quanta Q_{max}; b = = 0.9 fm

Q_{max}	16	20	24	28
$-E_{min}$	5.93	6.40	6.64	6.76

The other investigations of the triton ground-state energy E_{min} with the potential used here give 6.98 MeV [14], 7.00 MeV [14], and 7.03 MeV [16].

Strayer and Sauer[3] estimated that due to the lack of convergence their computed binding energy was about 0.5 MeV too small than the extrapolated ground-state energy (this extrapolated value is in agreement with the value from other calculations). Here we see, that using the super-soft-core potential, the rate of convergence in the DEM method is better.

3.2. The three-nucleon wave function

Solving eq. (4) for the coefficients c_k we obtain the wave function of the problem

$$|\Psi\rangle = -\sum_{i=1}^{N_i} G_0(E)|i\rangle d_i \,, \qquad (12)$$

with

$$d_i = \sum_{j=1}^{N_j} \langle i|V|j\rangle\, c_j \,. \qquad (13)$$

The coefficients c_j are also restricted by the normalization of the function $|\Psi>$.

In the coordinate representation, the wave function from both the LS equation and the DEM method is of the form

$$\Psi(\vec{x}_1,\vec{x}_2)=\sum_{k=1}^{N_k} D_k \left(\frac{2}{1+\delta_{n_1 n_2}}\right)^{1/2} \sum_{\ell \text{ even}} \frac{(-1)^{n_1+\frac{\ell}{2}}}{(2\ell+1)^{1/2}} Y_{\ell m}(\hat{x}_1) Y^*_{\ell m}(\hat{x}_2)$$

$$\times <n_1\ell, n_2\ell, 0 | n_1\ell, n_2\ell> I^{\ell}_{n_1 n_2}(x_1,x_2)\theta(\tfrac{1}{2},\tfrac{1}{2}). \qquad (14)$$

In eq. (14) $N_k = N_i$ for the wave function from the LS equation and $N_k = N_j$ for the DEM method. The sums over $k=(n_1 n_2 \ell)$ and $(n_1 n_2 \ell)$ are restricted by the conditions of eq. (6); the coefficients $D_k = -(2/\hbar\omega) d_k$ with d_k from eq. (13) for the LS equation. For the DEM method D_k result from the diagonalization procedure. Further, $\theta(S,T)$ is the spin-isospin wave function. We choose the dimensionless internal coordinates $\vec{x}_1, \vec{x}_2$ according to refs.[10,3]

$$\vec{x}_1 = \frac{1}{\sqrt{2}}(\vec{x}_1 - \vec{x}_2),$$
$$\vec{x}_2 = \frac{1}{\sqrt{6}}(\vec{x}_1 + \vec{x}_2 - 2\vec{x}_3). \qquad (15)$$

At last for the wave function from the LS equation

$$I^{\ell}_{n_1 n_2}(x_1,x_2) = \int_0^{\infty} G^{\ell}_{n_1 n_2}(x_1,x_2;z)\,dz, \qquad (16)$$

where

$$G^{\dot{\ell}}_{\dot{n}_1\dot{n}_2}(\dot{x}_1,\dot{x}_2;z)=Ne^{-\alpha^2 z}\frac{(1-2z)^{\dot{n}_1+\dot{n}_2}}{(1+2z)^{\dot{n}_1+\dot{n}_2+2\dot{\ell}+3}}\,e^{-\frac{\dot{x}_1^2+\dot{x}_2^2}{2(1+2z)}}$$

$$\times L^{\dot{\ell}+\frac{1}{2}}_{\dot{n}_1}\left(\frac{\dot{x}_1^2}{1-4z^2}\right)L^{\dot{\ell}+\frac{1}{2}}_{\dot{n}_2}\left(\frac{\dot{x}_2^2}{1-4z^2}\right), \qquad (17)$$

and

$$N=2\left[\frac{\dot{n}_1!\,\dot{n}_2!}{\Gamma(\dot{n}_1+\dot{\ell}+\frac{3}{2})\Gamma(\dot{n}_2+\dot{\ell}+\frac{3}{2})}\right]^{1/2}(\dot{x}_1\dot{x}_2)^{\dot{\ell}}. \qquad (18)$$

The function $L^{\alpha}_{n}(t)$ is the Laguerre polynomial /12/. For the DEM method

$$I^{\dot{\ell}}_{\dot{n}_1\dot{n}_2}(\dot{x}_1,\dot{x}_2)=G^{\dot{\ell}}_{\dot{n}_1\dot{n}_2}(\dot{x}_1,\dot{x}_2;0)=Ne^{-\frac{1}{2}(\dot{x}_1^2+\dot{x}_2^2)}\dot{x}_1^{\dot{\ell}+\frac{1}{2}}\dot{x}_2^{\dot{\ell}+\frac{1}{2}}L^{\dot{\ell}+\frac{1}{2}}_{\dot{n}_1}(\dot{x}_1^2)L^{\dot{\ell}+\frac{1}{2}}_{\dot{n}_2}(\dot{x}_2^2), \qquad (19)$$

with N from eq. (18).

It is the factor $\exp[-(\dot{x}_1^2+\dot{x}_2^2)/2]$ in eq. (19) which dictates the asymptotic behaviour of the wave function from the DEM method and forces it to go down too rapidly. In eq. (17) the effect of this factor is reduced by the denominator $(1+2z)$.

Consider now the asymptotics of the function $I^0_{00}(\dot{x}_1,\dot{x}_2)$ from eqs. (16)-(18)

$$I^0_{00}(\dot{x}_1,\dot{x}_2)\approx\int_0^\infty e^{-\alpha^2 z-\frac{\rho^2}{2(1+2z)}}\frac{dz}{(1+2z)^3}, \quad \rho^2=\dot{x}_1^2+\dot{x}_2^2. \qquad (20)$$

After some simple transformations we obtain

$$I^{0}_{00}(\vec{x}_1,\vec{x}_2) \approx \frac{e^{-\alpha\rho}}{\rho^{5/2}}, \qquad \alpha = (-\frac{2E}{\hbar\omega})^{1/2}. \tag{21}$$

Generally it can be shown that the function from the LS equation (eqs. (14), (16)-(18)) has the asymptotic form, eq. (21). The proof will be given elsewhere.

The asymptotic shape of the type $\exp(-\alpha\rho)/\rho^{5/2}$ for the trinucleon bound-state function was derived from the Faddeev equations by Merkuriev /4/ (true three-body asymptotic form).

It follows that the wave function build up here from the LS equation is more correct than that obtained by the DEM method (eqs. (14), (19)). Consequently, the convergence in the binding energy calculations is also better (see tables 2 and 3).

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