CALCULATION OF DEUTERON BINDING ENERGY WITH AND WITHOUT PARTIAL WAVE DECOMPOSITION METHODS

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Abstract

In this paper, the binding energy of deuteron is calculated by using both with and without partial wave decomposition methods. Firstly, the time independent Schrödinger equation is transformed into Lippmann-Schwinger equation for two-body bound system. This equation is solved by using Gauss-Legendre integration method. In this calculation, Malfliet-Tjon III potential is used and derived the potential matrix element in momentum space. The binding energy of deuteron is calculated by using iterative method. From this research, it is found that our calculated deuteron binding energy by using with partial wave decomposition method is 2.2283 MeV and it is about 4 keV greater than the experimental result. Our calculated deuteron binding energy by using without partial wave decomposition method is 2.2335 MeV and it is about 9 keV greater than the experimental result. The experimental deuteron binding energy is 2.2245 MeV.

Keywords: Gauss-Legendre integration method, iterative method, Malfliet-Tjon III potential

Introduction

In 1931, Brige and Menzel suggested the existence of the first isotope of hydrogen. After a few months later American scientist H.C. Urey and his co-worker investigated the distilled sample of natural hydrogen for the optical atomic spectrum of ${}^{1}_{1}H$ in a discharge tube. Isotopic separation to study the properties of deuterium quickly became an intense activity. The discovery of deuterium in 1932, coming before the discovery of neutron, was an experimental shock to theory. Deuteron, the simplest system of bound nucleon, the nucleus of deuterium atom contains one proton and one neutron. In 1932, it is discovered by Urey and his co-workers. The properties of deuteron in nuclear theory are as important as the hydrogen atom in atomic theory. It was shortly after the discovery of deuteron, Chadwick discovered neutron devoted in deuteron while he studied the deuterium. There is no man who immediately eliminates the confusion of proton and neutron. Because the previous model is persistent as a bound system of a proton and an electron. Based on this assumption, Heisenberg produced the first model of proton-neutron force. He assumed that the phenomenological potential could describe the proton-neutron force, and the neutron was a spin ½ particle like proton. The first idea about the nature of the nucleon-nucleon interaction came from Yukawa in 1935. He assumed that the strong interaction between two nucleons is carried by an interaction in quantum.

Deuterium is one of the only four stable nuclides with an odd number of protons and neutrons. Most odd-odd nuclei are unstable with respect to beta decay because the decay product are even-even, and are therefore more strongly bound, due to nuclear paring effects. Its benefits from having its proton and neutron coupled to a spin 1 state, which gives a stronger nuclear interaction. The corresponding spin 1 state does not exist in the two-nucleon or two-proton system due to Pauli's exclusion principle which would require one or the other identical particle

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with the same spin to have some other different quantum number, such as orbital angular momentum.

The standard approach in conventional nuclear theory is to treat the two-nucleon interaction in a phenomenological manner, that is, assume it to be derivable from a potential, and then set up a reasonable form for it in agreement with general theoretical considerations and experimental data. Most experimental data providing direct information on the potential concern with the two-nucleon system: neutron-proton (n-p), proton-proton (p-p) and neutron-neutron (n-n). The n-p system produces a bound state, whereas no bound state exists in p-p and n-n systems.

Calculations by Using Partial Wave Decomposition Method

Lippmann-Schwinger Equation for the Two-Body Bound System

The Lippmann-Schwinger equation is derived from the time independent Schrödinger equation. The time independent Schrödinger equation has the following form.

$$\hat{H}\Psi = E\Psi \tag{1}$$

But, $\hat{H}$ have kinetic energy $\hat{H}_0$ and potential energy $\hat{V}$ operators. So, Eq.(1) becomes

$$(\hat{H}_0 + \hat{V})\left|\Psi\right\rangle = E\left|\Psi\right\rangle \tag{2}$$

The Eq. (2) can be written as follows. It is Lippmann-Schwinger equation in ket form.

$$\left|\Psi\right\rangle = \frac{1}{E - \hat{H}_0}\left|\Psi\right\rangle \tag{3}$$

By multiplying Eq. (3) with $\langle p\ell m|$ from left and operating $\hat{p}^2$ on to Ψ gets

$$\left\langle p\ell m\middle|\Psi\right\rangle = \frac{1}{E - \frac{p^2}{2m}}\left\langle p\ell m\middle|\hat{V}\middle|\Psi\right\rangle \tag{4}$$

By inserting the completeness relation $\sum_{\ell' m'}\int p'^2\, dp'\left|p'\ell' m'\right\rangle\left\langle p'\ell' m'\right| = 1$ into Eq.(4),

$$\left\langle plm\middle|\Psi\right\rangle = \frac{1}{E - \frac{p^2}{2m}}\sum_{\ell' m'}\int p'^2 dp'\left\langle p\ell m\middle|V\middle|p'\ell' m'\right\rangle\left\langle p'\ell' m'\middle|\Psi\right\rangle \tag{5}$$

Since the local potential is consider, Eq. (5) becomes

$$\Psi_{\ell m}(p) = \frac{1}{E - \frac{p^2}{2m}}\sum_{\ell' m'}\int p'^2 dp'\, V_{\ell\ell' mm'}(p, p')\delta_{\ell\ell'}\delta_{mm'}\Psi_{\ell' m'}(p') \tag{6}$$

Since the potential is spherically symmetric, the index m can be dropped. It becomes

$$\Psi_\ell(p) = \frac{1}{E - \frac{p^2}{2m}} \int_0^\infty p'^2 dp' \, V_\ell(p, p') \Psi_\ell(p') \tag{7}$$

The integral term in Eq. (7) can be transform into discrete form as follows:

$$\Psi_\ell(p_i) = \frac{1}{E - \frac{P_j^2}{2m}} \sum_{j=1}^{N} p_j^2 w_j \; V_\ell(p_i, p_j) \Psi_\ell(p_j) \tag{8}$$

The calculation of potential matrix element is presented in next section. The FORTRAN 90 code is written using Eq. (8) to find the deuteron binding energy. Malfliet-Tjon potential is used in this calculation. In writing numerical code, the potential is written as a function. Then Gauss points, Gauss weights and momentum range are prepared to use Gauss-Legendre integration method. Iterative method is used to find the binding energy of deuteron.

Calculation of Potential Matrix Element

Yukawa type Malfliet-Tjon potential has the following form

$$V(r) = V_A \frac{e^{-\mu_A r}}{r} + V_R \frac{e^{-\mu_R r}}{r}$$

Where, V_A, V_R = depth parameter and μ_A, μ_R = range parameter

The potential matrix element is

$$V_\ell(p, p') = \langle p \ell m | V | p' \ell m \rangle \tag{9}$$

When the normalized equation is used, it becomes

$$V_\ell(p, p') = \frac{1}{2\ell + 1} \sum_{m=-\ell}^{\ell} \langle p \ell m | V | p' \ell m \rangle \tag{10}$$

By inserting the completeness relation into Eq. (10),

$$V_\ell(p, p') = \frac{1}{2\ell + 1} \sum_{m=-\ell}^{\ell} \int d\vec{p}'' \int d\vec{p}''' \langle p \ell m | \vec{p}'' \rangle \langle \vec{p}'' | V | \vec{p}''' \rangle \langle \vec{p}''' | p' \ell m \rangle \tag{11}$$

The Eq.(11) can be written as

$$V_\ell(p, p') = \frac{1}{2\ell + 1} \sum_{m=-\ell}^{\ell} \int p''^2 dp'' d\hat{p}'' \int p'''^2 dp''' d\hat{p}''' \; Y_{\ell m}^*(\hat{p}'') \frac{\delta(p'' - p)}{p'' p}$$

$$\times Y_{\ell m}(\hat{p}''') \frac{\delta(p''' - p')}{p''' p'} \langle p'' | V | p''' \rangle \tag{12}$$

After solving Eq.(12), it becomes

$$V_\ell(p, p') = \frac{1}{4\pi} \int d\hat{p} \int d\hat{p}' \, P_\ell(\hat{p}, \hat{p}') \langle p | V | p' \rangle \tag{13}$$

The Malfliet-Tjon potential which is expressed in coordinate space is used in this calculation. So this potential can be transformed into momentum space by using the completeness relation $\int d\vec{r}\,|\vec{r}\rangle\langle\vec{r}| = 1$.

$$\langle p|V|p'\rangle = \int d\vec{r} \int d\vec{r}' \langle\vec{p}|\vec{r}\rangle\langle\vec{r}|V|r'\rangle\langle r'|p'\rangle \tag{14}$$

For the local potential, it can be written as

$$\langle p|V|p'\rangle = \frac{1}{(2\pi)^3} \int d\vec{r}\, e^{i(\vec{p}'-\vec{p}).\vec{r}}\ V(r) \tag{15}$$

So, the potential matrix element is as follows:

$$\langle p|V|p'\rangle = \frac{4\pi}{(2\pi)^3} \int d\vec{r} \sum_{\ell m} i^{\ell}\, Y^{*}_{\ell m}(\hat{q}) Y_{\ell m}(\hat{r}) j_{\ell}(qr) V(r) \tag{16}$$

For $\ell = 0$, Eq. (16) becomes

$$\langle p|V|p'\rangle = \left[\frac{V_A}{2\pi^2} \frac{1}{\mu_A^2 + p^2 + p'^2 - 2pp'\cos\theta} + \frac{V_R}{2\pi^2} \frac{1}{\mu_R^2 + p^2 + p'^2 - 2pp'\cos\theta} \right] \tag{17}$$

Substituting Eq. (17) in Eq. (13) gets

$$V_{\ell}(p,p') = \frac{1}{4\pi} \frac{1}{2\pi^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \int_{-1}^{1} d\cos\theta \int_{-1}^{1} d\cos\theta'\, P_{\ell}(\cos\theta)$$

$$\times \left[\frac{V_A}{\mu_A^2 + p^2 + p'^2 - 2pp'\cos\theta} + \frac{V_R}{\mu_R^2 + p^2 + p'^2 - 2pp'\cos\theta} \right] \tag{18}$$

For ℓ = 0, $P_0(x) = 1$ and let $\cos\theta = x$. Eq. (18) becomes

$$V_{\ell}(p,p') = \frac{V_A}{2\pi} \frac{1}{pp'} \ell n \left[\frac{\mu_A^2 + (p+p')^2}{\mu_A^2 + (p-p')^2} \right] + \frac{V_R}{2\pi} \frac{1}{pp'} \ell n \left[\frac{\mu_R^2 + (p+p')^2}{\mu_R^2 + (p-p')^2} \right] \tag{19}$$

A numerical code for the potential is written as a function using Eq.(19). In writing numerical code, the values of potential depth parameters (V_A and V_R) and range parameters (μ_A and μ_R) are used.

Calculations by Using Without Partial Wave Decomposition Method

Lippmann-Schwinger Equation for the Two-Body Bound System

Lippmann-Schwinger equation in ket form is

$$|\Psi\rangle = \frac{1}{E - \hat{H}_0} \hat{V} |\Psi\rangle \tag{20}$$

Multiplying Eq.(20) with $\langle\vec{p}|$ from left gets

$$\langle\vec{p}|\Psi\rangle = \langle\vec{p}| \frac{\hat{V}}{E - \hat{H}_0} |\Psi\rangle \tag{21}$$

After operating with $\hat{P}^2$ on to $|\Psi\rangle$, Eq.(21) becomes

$$\langle\vec{p}|\Psi\rangle = \frac{1}{E-\frac{P^2}{2m}}\langle\vec{p}|\hat{V}|\Psi\rangle \tag{22}$$

The completeness relation is inserted in Eq.(22) as follows,

$$\langle\vec{p}|\Psi\rangle = \frac{1}{E-\frac{P^2}{2m}}\int d\vec{p}'\langle\vec{p}|\hat{V}|\vec{p}'\rangle\langle\vec{p}'|\Psi\rangle \tag{23}$$

In Eq.(23) $\vec{p}$ has magnitude p and direction x. $\vec{p}'$ has magnitude p' and direction x'. Therefore it can be written as

$$\Psi(p,x) = \frac{1}{E-\frac{P^2}{2m}}\int d\vec{p}'V(p,p',y)\Psi(p',x') \tag{24}$$

To find out the relations between x, x' and y, the momentum $\vec{p}$ and $\vec{p}'$ are considered in the Cartesian diagram.

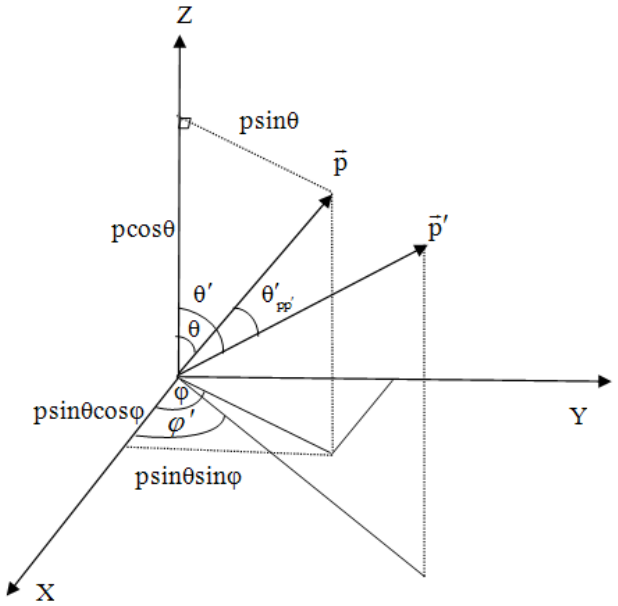

Figure 1 The momenta and in the Cartesian co-ordinate system

From the figure $\vec{p}$ $\vec{p}'$

$$\vec{p} = p\sin\theta\cos\varphi\,\hat{x} + p\sin\theta\sin\varphi\,\hat{y} + p\cos\theta\,\hat{z} \tag{25}$$

$$\vec{p} = p'\sin\theta'\cos\varphi'\,\hat{x} + p'\sin\theta'\sin\varphi'\,\hat{y} + p'\cos\theta'\,\hat{z} \tag{26}$$

We take scalar product of and and then

$$\cos\theta_{pp'} = \cos\theta\cos\theta' + \sin\theta\sin\theta' + \cos(\varphi-\varphi') \tag{27}$$

Let $\cos\theta = x,\ \cos\theta' = x',\ \cos\theta_{pp'} = y$

Eq.(27) can be written as

$$y = xx' + \sqrt{1-x^2}\sqrt{1-x'^2}\cos(\varphi - \varphi') \tag{28}$$

The arbitrary azimuthal angle for momentum $\vec{p}$ is chosen to be zero.

$$y = xx' + \sqrt{1-x^2}\sqrt{1-x'^2}\cos\varphi' \tag{29}$$

Substituting Eq.(29) in Eq.(24) obtains

$$\Psi(p,x) = \frac{1}{E - \frac{P^2}{2m}} \int_0^\infty p'^2 dp' \int_{-1}^{1} dx' \int_0^{2\pi} d\varphi' V\left(p,p',xx' + \sqrt{1-x^2}\sqrt{1-x'^2}\cos\varphi'\right) \Psi(p',x') \tag{30}$$

The integral term in Eq. (30) can be transform into discrete form as follows:

$$\Psi(p_i,x_\ell) = \frac{1}{E - \frac{P_j^2}{2m}} \sum_{j=1}^{N_p} p_j^2 w_j \sum_{k=1}^{N_x} w_k \ V(p_i,x_\ell,p_j,x_k)\Psi(p_j,x_k) \tag{31}$$

The calculation of potential matrix element is presented in next section. We write a FORTRAN 90 code using Eq.(31) to find the deuteron binding energy. Malfliet-Tjon III potential is used in this calculation. In writing numerical code, the potential is written as a function.

Calculation of Potential Matrix Element

The potential matrix element can be written as

$$V(p,p',y) = \langle \vec{p}|V|\vec{p}'\rangle \tag{32}$$

The Malfliet-Tjon potential is expressed in coordinate space. So, it will be transformed into momentum space by using the completeness relation $\int d\vec{p}'|\vec{p}'\rangle\langle\vec{p}'| = 1$.

$$V(p,p',y) = \int d\vec{r}\int d\vec{r}'\langle\vec{p}|\vec{r}\rangle\langle\vec{r}|V|\vec{r}'\rangle\langle\vec{r}'|\vec{p}'\rangle \tag{33}$$

It can be written as

$$V(p,p',y) = \frac{1}{(2\pi)^3}\int d\vec{r}\int d\vec{r}' e^{i(\vec{p}'-\vec{p}).\vec{r}} V(r)\delta(\vec{r}'-\vec{r}) \tag{34}$$

By using the delta function properties, Eq. (34) becomes

$$V(p,p',y) = \frac{1}{8\pi^3}\int_0^\infty r^2 dr \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi\, e^{i(\vec{p}'-\vec{p}).\vec{r}} V(r) \tag{35}$$

After inserting the Malfliet-Tjon potential in Eq.(35), it can be written in the form

$$V(p,p',y) = \frac{V_A}{2\pi^2}\frac{1}{\mu_A^2 + (p'-p)^2} + \frac{V_R}{2\pi^2}\frac{1}{\mu_R^2 + (p'-p)^2} \tag{36}$$

By defining as

$$V(p,x,p',x') = \int_0^{2\pi} d\varphi' \, V\left(p,p', xx' + \sqrt{1-x^2}\sqrt{1-x'^2}\cos\varphi'\right) \tag{37}$$

By substituting Eq.(36) in Eq.(37)

$$V(p,x,p',x') = \int_0^{2\pi} d\varphi' \frac{V_A}{2\pi^2} \frac{1}{\mu_A^2 + (p'-p)^2} + \int_0^{2\pi} d\varphi' \frac{V_R}{2\pi^2} \frac{1}{\mu_R^2 + (p'-p)^2} \tag{38}$$

Solving Eq (38) obtains

$$V(p,x,p',x') = \frac{V_A}{\pi} \frac{1}{\sqrt{\left(\mu_A^2 + p'^2 + p^2 - 2pp'xx'\right)^2 - \left(-2pp'\sqrt{1-x^2}\sqrt{1-x'^2}\right)^2}} + \frac{V_R}{\pi} \frac{1}{\sqrt{\left(\mu_R^2 + p'^2 + p^2 - 2pp'xx'\right)^2 - \left(-2pp'\sqrt{1-x^2}\sqrt{1-x'^2}\right)^2}} \tag{39}$$

The numerical code is written as a function using Eq.(39). In writing numerical code, the potential parameters shown in Table 1 are used.

Calculation of Eigen Value by Using Iterative Method

Let φ_i be the set of the possible state kets.

$$\varphi_i = \varphi_1 + \varphi_2 + \varphi_3 + ... + \varphi_n \tag{40}$$

$|\Psi\rangle$ is the total wave function of all state kets and which can be written as

$$|\Psi\rangle = \sum_{i=1}^{n} c_i \varphi_i \tag{41}$$

K be the square matrix and has the following property

$$K\varphi_i = \lambda_i \varphi_i \tag{42}$$

$$K|\Psi\rangle = \sum_{i=1}^{n} \lambda_i c_i \varphi_i \tag{43}$$

$$K^j|\Psi\rangle = \lambda_1^j c_1 \varphi_1 + \lambda_2^j c_2 \varphi_2 + ... + \lambda_n^j c_n \varphi_n \tag{44}$$

It is assumed that,

$$|\lambda_1| > |\lambda_2| > |\lambda_3| > ..... > |\lambda_n|$$

Eq.(44) becomes

$$K^j|\Psi\rangle = \lambda_1^j\left(c_1\varphi_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^j c_2\varphi_2 + \ldots\ldots + \left(\frac{\lambda_n}{\lambda_1}\right)^j c_n\varphi_n\right) \tag{45}$$

If j becomes large, all terms in the bracket approach to zero expect the first term. So Eq.(45) becomes

$$K^j|\Psi\rangle = \lambda_1^j c_1\varphi_1 \tag{46}$$

For $(j+1)^{th}$ iteration,

$$K^{j+1}|\Psi\rangle = \lambda_1^{j+1} c_1\varphi_1 \tag{47}$$

By taking the ratio of Eq.(46) and (47),

$$\frac{K^{j+1}|\Psi\rangle}{K^j|\Psi\rangle} = \frac{\lambda_1^{j+1} c_1\varphi_1}{\lambda_1^j c_1\varphi_1} = \lambda_1 \tag{48}$$

In this way the largest eigenvalue λ_1 is obtained. In order to apply the iterative method for partial wave decomposition, the Eq.(7) is rewritten again and let Kernel be K(E).

$$\Psi_\ell(p) = \frac{1}{E - \frac{P^2}{2m}} \int_0^\infty p'^2 dp' V_\ell(p,p')\Psi_\ell(p')$$

$$K(E) = \frac{1}{E - \frac{P^2}{2m}} \int_0^\infty p'^2 dp' V_\ell(p,p') \tag{49}$$

Therefore, it can be written as

$$|\Psi\rangle = K(E)|\Psi\rangle \tag{50}$$

Arbitrary value η which is the function of E is introduced into Eq.(50).

$$\eta|\Psi\rangle = K(E)|\Psi\rangle \tag{51}$$

When η becomes 1, Eq. (51) is equal to Eq.(50). Since the true energy eigenvalue E is not known, we start with an estimated energy and determine the corresponding eigenvalue η. Then the energy E is varied such that η approaches the value 1.

Technique of Energy Search Program

Now to search the binding energy, the natures of η and E are needed to know. The arbitrary energy is initialized using Eq.(7) for the calculation with partial wave decomposition method. The arbitrary input energy E_1 and E_2 are introduced. The E_1 and E_2 are upper bound and lower bound absolute value of energy. The input energy is define as $E = (E_1+E_2)/2$. If the value of η is less than 1, we set E_2 should be E and E_1 is kept. If η is greater than 1, we set E_1 should be E and E_2 is kept. Then, the η value is searched by iteration. According to this procedure, the gap between E_1 and E_2 is narrower and narrower and η approaches to 1. In this way, the value of

η converges to 1 and the corresponding energy is obtained. It is true energy for the deuteron. This procedure is written in program code. For the calculation without partial wave decomposition method, Eq.(30) is used to calculate the deuteron binding energy. The parameter set for Yukawa type Malfliet-Tjon III potential is shown in Table 1. The discretization parameters which converge the deuteron binding energy by changing the number of grid points are shown in Table 2 and Table 3.

Table 1 The parameter set for Yukawa type Malfliet-Tjon III potential

V_A (MeV fm)	μ_A (fm^{-1})	V_R (MeV fm)	μ_R (fm^{-1})
- 626.822	1.55	1438.317	3.11

Table 2 The discretization parameters for partial wave decomposition

P_0 (fm^{-1})	p_{max} (fm^{-1})	p_{cut} (fm^{-1})	N_1	N_2	BE (MeV)
0.00	5.0	60.0	20	20	2.2283

Table 3 The discretization parameters for without partial wave decomposition

P_0 (fm^{-1})	p_{mid} (fm^{-1})	p_{max} (fm^{-1})	N_p	N_x	BE (MeV)
0.00	3.0	30.0	26	14	2.2335

Results

According to the numerical result, it is found that the binding energy of deuteron is 2.2283 MeV by using with partial wave decomposition method and 2.2335 MeV by using without partial wave decomposition method. Our calculated results are compared with the experimental result and the results calculated by other theoretical groups. Comparison of deuteron binding energies is shown in Table 4.

Table 4 Comparison of deuteron binding energies

Potential Types	Binding Energy (MeV)
Nijmegen I	2.2245
Nijmegen II	2.2245
Nijmegen 93	2.2245
CD-Bonn	2.2245
Malfliet-Tjon III	2.2300
Malfliet-Tjon IV	2.2300
Experimental result	2.2245
Malfliet-Tjon III (Our result using with partial wave decomposition method)	2.2283
Malfliet-Tjon III (Our result using without partial wave decomposition method)	2.2335

Discussion

Our calculated deuteron binding energy by using with partial wave decomposition method is 2.2283 MeV and it is about 4 keV greater than the experimental result and the results calculated by Nijmegen and CD-Bonn groups. This could be the fact that the potentials (Nijmegen I, Nijmegen II, Nijmegen 93 and CD-Bonn) which are used by theoretical groups are realistic potentials. These potentials are fitted to the experimental data and considered including spin and isospin. But the Malfliet-Tjon III potential which is used in this calculation is a phenomenological potential. This potential can be adjusted the parameter set. Our calculated result is in good agreement in two decimal places with the results calculated by Malfliet-Tjon group using Malfliet-Tjon type III and IV potentials. In this calculation spin and isospin are not considered. Only for S-state ($\ell = 0$) is calculated. Our calculated deuteron binding energy by using without partial wave decomposition method is 2.2335 MeV and it is about 9 keV greater than the experimental result and the results calculated by Nijmegen and CD-Bonn groups. Our calculated result is in good agreement in two decimal places with the results calculated by Malfliet-Tjon group. Our results calculated by using two methods are slightly different. This will be the fact that higher partial waves are needed to consider in the calculation by using partial wave decomposition method. But the deuteron binding is directly calculated and no need to consider partial waves in the calculation by using without partial wave decomposition method.

Conclusion

The two-body problem which is the simplest and one can understand the nucleon-nucleon interaction. Two-body forces are basic to study three-body and many-body problems. The Lippmann-Schwinger equation is used in the calculations of two-body bound state and scattering process. At low energies in the MeV and the few tenth of MeV region very few angular momenta contribute to the nucleon-nucleon (N-N) scattering process. Consequently a description using angular momentum decomposition is an adequate tool for carrying out scattering calculations. However, at intermediate energies, energies of a few hundred MeV and higher energies very many angular momenta contribute to the scattering amplitude. In these energy domains those individual contributions to the scattering amplitude for a fixed high angular momentum oscillate strongly in angle. The without angular momentum decomposition method is suitable for the studying of high energy N-N interaction.

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