Microscopic Study of the Nucleus-Nucleus Interaction on the Basis of the Realistic Effective Interaction. I

Formulation

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We investigate the inter-nucleus complex potential by the many body theory containing the Pauli principle entirely and by the microscopic scattering state complex G-matrix. Our main purpose is to investigate the nature of the imaginary part of the nucleus-nucleus potential as well as the real part of it. In order to obtain the complex inter-nucleus potential by the complex G-matrix, we reformulate and extend the many body theory (CMWP) originally formulated for the calculation of the real inter-nucleus potential by Saraceno et al. And also we show how to treat the density dependence of the G-matrix. To ensure the reliability of CMWP we make a comparison between the numerical results by the CMWP method and the reliable RGM+WKB method. As a result we have found reliability and great facility of CMWP.

§ 1. Introduction

Understandings of the process of nucleus-nucleus scattering have been obtained by many kinds of microscopic studies. In particular, the analyses with the resonating grouping method (RGM) have clarified the basic structure of the inter-nucleus potential. Wada and one of the present authors (H.H.) have succeeded in reproducing differential cross sections of $\alpha$-16O and $\alpha$-40Ca elastic scattering in a wide energy range by RGM with an effective interaction which is fixed on the basis of the reproduction of the level spectra of bound and quasi-bound states and with a phenomenological imaginary potential. They have shown that the equivalent local potential to the RGM non-local potential is almost the same as the optical model potential of Michel et al. in $\alpha$-16O and that of Delbar et al. in $\alpha$-40Ca which are both widely regarded as having been determined uniquely. These studies showed the efficiency of RGM as a many body theory to scattering states.

In terms of the comprehension of scattering processes from the first principle, however, we must say that such a successful investigation by RGM is still insufficient because the use of more realistic effective two-body interactions is indispensable. In general two ingredients are necessary for the microscopic analysis, that is, a many body theory describing the motion of a many body system and a realistic effective two-nucleon interaction. As for the many body theory for the nucleus-nucleus scattering, we can use RGM as a very satisfactory theory as we mentioned above. On the other hand in many investigations including the above-mentioned study of Refs.1) and 2),

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effective two-nucleon interactions are usually constructed for bound state problems, which means they have only real part, and phenomenological Woods-Saxon like functions are assumed to imaginary nucleus-nucleus potentials. In order to investigate the properties of the scattering state from a microscopic point of view it is highly desirable to use a scattering state effective two-nucleon interaction which is composed of consistent real and imaginary parts and to calculate both real and imaginary nucleus-nucleus potentials simultaneously with such an interaction. Such a two-nucleon force is provided by the $G$-matrix theory for the nuclear matter by the use of the local density approximation.

The purpose of this series of papers is twofold. The first is to formulate a many body theory feasible for the calculation of nucleus-nucleus interactions even for heavier system on the basis of a realistic complex effective two-nucleon interaction and the second is to research properties of the calculated complex inter-nucleus potential and to make a comparison of theoretical results with the experimental data.

The many body theory we formulate here is an extended version of the moving wave packet method — from now on we call it canonical moving wave packet method (CMWP) — introduced by Saraceno et al. which was originally formulated for the real inter-nucleus potential calculation. The important characteristic feature of CMWP is that a distance and a relative momentum between nuclei, which are not canonical variables in the original moving wave packet method, are transformed into canonical ones. This transformation results in the existence of the Pauli forbidden region in the phase space of the relative motion which is exactly the same as the situation found in the semiclassical treatment of the RGM ($\text{RGM} + \text{WKB}$). Though, as is mentioned above, it is desirable to use more reliable RGM in our investigation, the calculation of RGM kernels becomes more and more complicated or tedious for heavier systems when the effective interaction has a density dependence. On the other hand in the moving wave packet method various quantities are easily obtained only by the calculation of the diagonal kernels of the complex generator coordinate method. Therefore as far as the numerical results by CMWP are close to those by RGM, we can expect the large flexibility of CMWP to the microscopic research for heavier systems. The effective interaction we use is the complex effective Gauss force (CEG force) by Yamaguchi, Nagata and Matsuda that is made by totally microscopic calculation based on the Brueckner-Hartree-Fock theory and that has no fitting parameters. The imaginary part of CEG expresses the particle-hole excitation (emission of nucleons) in nuclear matter. They well reproduced the cross section and the spin observables of nucleon-nucleus scattering by the folding model with CEG.

Studies similar to ours have been made by Faessler et al. by using scattering state complex $G$-matrix. However, their many body theory for calculating the nucleus-nucleus potential differs from ours in that they use the non-canonical relative distance and momentum and the relative momentum is fixed to its asymptotic value at any relative distance.

In this paper we will formulate the CMWP method for the derivation of the complex inter-nucleus potential, and then to confirm the reliability of CMWP we will compare the complex potentials for $\alpha-\alpha$ system calculated by RGM + WKB and by CMWP using the CEG force. Consideration of the physical meaning of the calculated
inter-nucleus potential and comparison of the theoretical results with the experimental data are performed in the next paper of this series. In § 2 we will make a brief review of original CMWP, extend CMWP so as to treat the complex effective interaction and then give an explanation of CMWP in case of using a density-dependent effective interaction. In § 3 comparison of numerical results by CMWP with those by RGM+WKB is given in $\alpha$-$\alpha$ system. We will discuss some features of CMWP and the calculated potentials in § 4. Finally § 5 is devoted to a summary and concluding remarks.

§ 2. Formulation

2.1. Review and refinement of CMWP, and definition of inter-nucleus potential

We will review and refine the CMWP method for the system in which both target and projectile are spin 0 closed-shell nuclei. First we will explain the CMWP method with the real $G$-matrix. The method to use the complex $G$-matrix is formulated in the next subsection. We adopt a harmonic oscillator basis as a single particle wave function for nucleons in scattering nuclei. A wave function of a nucleus moving with momentum $K$ at location $D$ is assumed to be composed of coherent states of such a basis as

$$\phi(D, K) = \hat{A}\left\{ \varphi_1\left( r_1 - D - \frac{i}{2\hbar \nu A} K \right) \cdots \varphi_A\left( r_A - D - \frac{i}{2\hbar \nu A} K \right) \right\},$$

$$\nu = \frac{m \omega}{2\hbar},$$

where $\omega$ and $A$ are the harmonic oscillator frequency and the mass number, respectively. It must be noted here that $K$ and $D$ are time-dependent parametric vectors. The description by Eq. (2·1) of a nucleus having momentum $K$ at location $D$ is ensured in the sense of the expectation values of the operators of the momentum and the location of center of mass of the nucleus,

$$\langle \phi(D, K) \sum_1^A \tilde{r_i}/A | \phi(D, K) \rangle = D,$$

$$\langle \phi(D, K) \sum_1^A \tilde{p_i}/A | \phi(D, K) \rangle = K.$$

Then the wave function of the system composed of two nuclei which has relative momentum $K$ and relative distance $D$ is given in a form of the Slater determinant as follows:

$$\Psi(D, K) = \hat{A}\left\{ \varphi_1\left( \frac{-A_1}{A_1 + A_2} D - K \right) \varphi_2\left( \frac{A_2}{A_1 + A_2} D, K \right) \right\} \exp\left( \frac{1}{2} Z^2 \right)$$

$$= \phi_{\text{col}} \hat{A}\left\{ \varphi_1^{\text{int}} \varphi_2^{\text{int}} \varphi_{\text{rel}}(R_{\text{rel}}, Z) \right\}$$

$$= |Z\rangle,$$
\[
\phi_{\text{rel}}(R_{\text{rel}}, Z) = \left(\frac{2\nu \mu_A}{\pi}\right)^{3/4} \exp\left[-\nu \mu_A \left(R_{\text{rel}} - \sqrt{\frac{1}{2\nu \mu_A}} Z^2 + \frac{1}{2} Z^2\right)\right],
\]
\[
Z = \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu \mu_A} D + i \sqrt{\frac{1}{2\nu \mu_A}} K \right],
\]
\[
\bar{Z} = \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu \mu_A} D - i \sqrt{\frac{1}{2\nu \mu_A}} K \right],
\]
\[
R_{\text{rel}} = \sum_{i=A_1+1}^{A_1+A_2} \frac{r_i}{A_1} - \frac{A_1}{A_1 + A_2}, \quad \mu_A = \frac{A_1 A_2}{A_1 + A_2}, \tag{2.3}
\]

where \(\phi_G, \phi_{i}^\text{int}\) and \(\phi_{\text{rel}}\) are wave functions with respect to the total center of mass, to the internal degrees of freedom of scattering nuclei, and to the relative motion of the two nuclei, respectively. The normalization of the relative wave function implies,\(^9\)

\[
\int dR \phi_{\text{rel}}(R, Z) \phi_{\text{rel}}(R, Z') = e^{Z' \cdot \bar{Z}},
\]
\[
\int d\mu(Z) \phi_{\text{rel}}(R, Z) \phi_{\text{rel}}(R', Z) = \delta(R - R'),
\]
\[
d\mu(Z) = \frac{1}{\pi} \exp(-Z \cdot \bar{Z}) d(\text{Re}Z) d(\text{Im}Z). \tag{2.4}
\]

With the measure \(d\mu(Z)\), \(\exp(Z' \cdot \bar{Z})\) behaves like a delta function,

\[
\int d\mu(Z) \exp(Z' \cdot \bar{Z}) \omega(Z) = \omega(Z'). \tag{2.5}
\]

Now we adopt the time dependent variational principle\(^10\) to describe the motion of the system. The action \(S\) and the Lagrangian \(\mathcal{L}\) of the system are given by

\[
S = \int \mathcal{L} dt,
\]
\[
\mathcal{L} = \frac{i}{\hbar} \langle \dot{Z} | \hat{H} | Z \rangle - \frac{i}{\hbar} \frac{\partial}{\partial t} \langle Z | Z \rangle
\]
\[
= \frac{i}{\hbar} \left[ \dot{Z} \cdot \frac{\partial}{\partial Z} - \dot{\bar{Z}} \cdot \frac{\partial}{\partial \bar{Z}} \right] \ln \mathcal{H} - \mathcal{N},
\]
\[
\frac{\partial}{\partial t} = \frac{1}{2} \left( \overrightarrow{\partial} - \overleftarrow{\partial} \right), \tag{2.6}
\]

where \(\mathcal{N}\) and \(\mathcal{H}\) represent norm and Hamiltonian kernels, respectively,

\[
\mathcal{N} = \langle Z | Z \rangle, \quad \mathcal{H} = \frac{\langle Z | \hat{H} | Z \rangle}{\langle Z | Z \rangle}. \tag{2.7}
\]

It can be proved that in case of the system composed of the closed-shell nuclei the norm kernel depends only on the scalar product of \(Z\) and \(\bar{Z}\) (Appendix A),

\[
\mathcal{N}(Z, \bar{Z}) = \mathcal{N}(Z \cdot \bar{Z}) = \mathcal{N}(s),
\]
\[
s = Z \cdot \bar{Z}. \tag{2.8}
\]
Then the Lagrangian is rewritten as

\[ \mathcal{L} = -\frac{i\hbar}{2} [\dot{\mathbf{Z}} \cdot \mathbf{Z} - \dot{\mathbf{Z}} \cdot \mathbf{Z}] \frac{\partial}{\partial s} \ln \mathcal{H} - \mathcal{H} \]  

(2.9)

It should be noted that the Lagrangian (2.9) is a singular one. In this case \( \mathcal{L} \) is a function of \( \mathbf{Z}, \dot{\mathbf{Z}}, \mathbf{Z} \) and \( \dot{\mathbf{Z}} \). However, the time evolution of \( \mathbf{Z} \) and \( \dot{\mathbf{Z}} \) is completely determined by that of \( \mathbf{Z} \) and \( \dot{\mathbf{Z}} \), which means the Lagrangian (2.9) contains excessive degrees of freedom (Appendix B). We adopt \( \mathbf{Z} \) and \( \dot{\mathbf{Z}} \) as independent variables and make the following canonical transformation to remove the excessive degrees of freedom:

\[ \mathcal{L} = -\frac{i\hbar}{2} [\dot{\mathbf{Z}} \cdot \mathbf{Z} - \dot{\mathbf{Z}} \cdot \mathbf{Z}] \frac{\partial}{\partial s} \ln \mathcal{H} - \mathcal{H} \]

\[ = \hbar \dot{\mathbf{Z}} \cdot \mathbf{Z} \frac{\partial}{\partial s} \ln \mathcal{H} - \mathcal{H} + \frac{i\hbar}{2} \frac{d}{dt} \int \mathbf{Z} \cdot \mathbf{Z} \frac{\partial^2}{\partial s^2} \ln \mathcal{H}(s) \]

\[ \approx \hbar \dot{\mathbf{Z}} \cdot \mathbf{Z} \frac{\partial}{\partial s} \ln \mathcal{H} - \mathcal{H} , \]  

(2.10)

where the time evolution of \( \mathbf{Z} \) is determined by that of \( \mathbf{Z} \). From the above Lagrangian we can define the generalized momentum conjugate to \( \mathbf{Z} \),

\[ \mathbf{P}_Z = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{Z}}} = i\hbar \dot{\mathbf{Z}} \frac{\partial}{\partial s} \ln \mathcal{H} , \]  

(2.11)

and we get the equations of motion,

\[ \dot{\mathbf{Z}} = \frac{\partial \mathcal{H}}{\partial \mathbf{P}_Z} , \quad \dot{\mathbf{P}}_Z = -\frac{\partial \mathcal{H}}{\partial \mathbf{Z}} . \]  

(2.12)

By \( \mathbf{Z} \) and \( \mathbf{P}_Z \) the special relation is given as follows:

\[ \frac{1}{i\hbar} \mathbf{Z} \cdot \mathbf{P}_Z = s \frac{\partial}{\partial s} \ln \mathcal{H} \geq N_A . \]  

(2.13)

The value \( N_A \) on the right-hand side of inequality (2.13) corresponds to the lowest number of oscillator quanta of Pauli allowed states of RGM (Appendix A). This inequality means that the Pauli forbidden region in the phase space of relative motion appears when the canonical coordinate and momentum are properly defined from the complex generator coordinates. But in the asymptotic region \( |D| \rightarrow \infty \), where the effect of antisymmetrization disappears, the above \( \mathbf{P}_Z \) and \( \mathbf{Z} \) become

\[ \mathbf{Z} \rightarrow \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu \mu_A} D + i\sqrt{\frac{1}{2\nu \mu_A}} \frac{K}{\hbar} \right] , \]

\[ \mathbf{P}_Z \rightarrow \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu \mu_A} D - i\sqrt{\frac{1}{2\nu \mu_A}} \frac{K}{\hbar} \right] , \]  

(2.14)
of which physical interpretation is not transparent. In order to obtain the canonical coordinates and momenta whose physical interpretation is easy, the next canonical transformation has only to be performed, 5)

\[ \mathcal{L} = i\hbar \dot{Z} \cdot \mathbf{\frac{\partial}{\partial s} \ln \mathcal{H}} - \mathcal{H} \]

\[ = i\hbar \dot{\omega} - \frac{i\hbar}{2} \frac{d}{dt} \left[ s \frac{\partial \ln \mathcal{H}}{\partial s} - \ln \mathcal{H} \right] \]

\[ \cong i\hbar \dot{\omega} - \mathcal{H} \]

(2.15)

and

\[ \omega = Z \sqrt{\frac{\partial}{\partial s} \ln \mathcal{H}} , \quad \bar{\omega} = \bar{Z} \sqrt{\frac{\partial}{\partial s} \ln \mathcal{H}} , \]

(2.16)

which means that the physical relative distance \( R \) and momentum \( P \) are defined as

\[ R = D \sqrt{\frac{\partial}{\partial s} \ln \mathcal{H}} , \quad P = K \frac{\partial}{\partial s} \ln \mathcal{H} , \]

(2.17)

and their asymptotic forms \(|D| \to \infty\) are

\[ R \to D , \quad P \to K . \]

(2.18)

It should be noted that though the above definition of the physical relative distance and the relative momentum is not unique, this definition seems to be most natural. The characteristic feature of CMWP is the existence of the Pauli forbidden region in the phase space of the relative motion. In terms of \( \omega \) and \( \bar{\omega} \), Eq. (2.13) is expressed as

\[ \omega \cdot \bar{\omega} = s \frac{\partial}{\partial s} \ln \mathcal{H} \geq N_A \]

(2.19)

or with \( P \) and \( R \),

\[ \nu_\mu_A R^2 + \frac{1}{4 \nu_\mu_A} P^2 \geq N_A . \]

(2.20)

This inequality indicates the existence of some region in the phase space of relative coordinates (spatial and momentum) in which the two nuclei cannot access with each other in the sense of the classical motion. The existence of the Pauli forbidden region in this semi-classical approach is exactly equivalent to that found in the semi-classical treatment of RGM (hereafter, abbreviated as RGM+WKB). The Pauli forbidden region in the phase space originates from the existence of the Pauli
forbidden states in RGM. The potentials obtained by CMWP and RGM+WKB coincide well, as we will show later, and this is largely because of the existence of the Pauli forbidden region which is one of the most important results of the proper treatment of the Pauli principle.

In order to describe the relative motion we will not trace the time evolution of the trajectory in the phase space by the equations of motion, but we use the constants of motion, i.e., the total energy $E$ and the angular momentum $l$. The reason the angular momentum is a constant of motion is that the target and the projectile we consider are both spin 0 nuclei, that is, channel spin is 0. The trajectory is given by the equations,

$$\mathcal{H}(D, K) = E,$$

$$R(D, K) \times P(D, K) = \hbar \sqrt{l(l+1)} e_\perp,$$  \hspace{1cm} (2.21)

where $e_\perp$ is a unit vector perpendicular to both $R$ and $P$. By the above equations parallel and vertical components of $K$ to $D$ are determined at each $|D|$. The internucleus potential determined by the physical distance and the momentum which are calculated by the transformation (2.17) is defined as follows:

$$V_{\text{int}}(R(D, K)) = \mathcal{H}(D, K) - \frac{P^2(D, K)}{2\mu} \frac{\hbar^2 l(l+1)}{2\mu R^2(D, K)},$$

where $\mu$ is a reduced mass and $P_\parallel$ is a parallel component of $P$ to $R$.

2.2. Derivation of complex potential with complex two-nucleon effective interaction

The CMWP method explained above is not applicable for the use of a complex effective two-nucleon force in its original form because the Hamiltonian is assumed to be a real function. So we extend this method so as to be able to use the real and also imaginary parts of the scattering state complex $G$-matrix. As we use the complex two-nucleon effective interaction, the Hamiltonian kernel becomes the complex function of $Z$ and $\bar{Z}$. However, we put the total energy of the system, which is a constant of motion, to be a real value equal to the incident energy. Then we should make $K$ and $D$ to be complex vectors. This means the phase space of the relative motion is extended to the complex space. By this treatment there is no need to change the formulation in the previous subsection. The variables $Z$ and $\bar{Z}$ are redefined as

$$Z = \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu\mu_A} (D_r + iD_i) + i \sqrt{\frac{1}{2\nu\mu_A}} (K_r + iK_i) \right],$$

$$\bar{Z} = \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu\mu_A} (D_r + iD_i) - i \sqrt{\frac{1}{2\nu\mu_A}} (K_r + iK_i) \right],$$

where we extend $D$ and $K$ to be time-dependent complex vectors. The norm and the Hamiltonian kernels are

$$\mathcal{H}(D, K) = \mathcal{H}(D_r + iD_i, K_r + iK_i),$$

$$\mathcal{I}(D, K) = \mathcal{I}(D_r + iD_i, K_r + iK_i).$$
Canonical relative distance \( R \) and momentum \( P \) are modified as

\[
R(D_r+iD_i, K_r+iK_i) = (D_r+iD_i) \sqrt{\frac{\partial}{\partial (Z \cdot \bar{Z})} \ln \mathcal{H}},
\]

\[
P(D_r+iD_i, K_r+iK_i) = (K_r+iK_i) \sqrt{\frac{\partial}{\partial (Z \cdot \bar{Z})} \ln \mathcal{H}}.
\]  

(2.25)

Then in order to get the trajectory of the relative motion of the system we determine numerically \( \text{Im}D, \text{Re}K \) and \( \text{Im}K \) as a function of \( \text{Re}D \) by the following equations:

\[
\text{Re} \mathcal{H}(D_r+iD_i, K_r+iK_i) = E,
\]

\[
\text{Im} \mathcal{H}(D_r+iD_i, K_r+iK_i) = 0,
\]

\[
\text{Re}[R(D_r+iD_i, K_r+iK_i) \times P(D_r+iD_i, K_r+iK_i)] = \hbar \sqrt{l(l+1)} e_\perp,
\]

\[
\text{Im}[R(D_r+iD_i, K_r+iK_i) \times P(D_r+iD_i, K_r+iK_i)] = 0,
\]

\[
\text{Im}R(D_r+iD_i, K_r+iK_i) = 0,
\]

(2.26)

(2.27)

where Eq. (2.26) expresses the constants of motion and Eq. (2.27) means the physical constraint we require. The reason we adopt the equation (2.27) as a constraint is that \( D \) and \( K \) are not canonical variables, which means they are mere parameters having the dimensions of distance and momentum, respectively, but that the canonical variables \( R \) and \( P \) must be interpreted as physical relative distance and momentum. Under this condition we get real relative distance \( R \) and complex relative momentum \( P \). The complex full potential is now given by

\[
\text{Re} V_{\text{full}}^{(l)}(R(D, K)) = \text{Re} \mathcal{H}(D, K) - \frac{P_{\perp r}(D, K) - P_{\perp i}(D, K)}{2\mu} \frac{\hbar^2 l(l+1)}{2\mu R^2(D, K)}
\]

\[
= E - \frac{P_{\perp r}(D, K) - P_{\perp i}(D, K)}{2\mu} - \frac{\hbar^2 l(l+1)}{2\mu R^2(D, K)},
\]

(2.28)

(2.29)

Finally we would like to call the readers' attention: If we put \( D \) and \( K \) to be complex vectors, the relation (2.20) expressing the Pauli forbidden region cannot be satisfied mathematically. However, \( R \) and \( \text{Re}P \) are expected to satisfy the relation (2.20) approximately when the imaginary part of the inter-nucleus potential is weaker enough than the real part of it. But, in fact, it means that the Pauli forbidden region may vary by the coupling to the other channels. This point we will discuss in § 4.

2.3. Structure of Hamiltonian kernel with the scattering state complex G-matrix

In this section we will discuss the treatment of the scattering state complex G-matrix. In this study we use the CEG force by Yamaguchi, Nagata and Matsuda as a scattering state G-matrix. The features in the mathematical form of the CEG force
are not only that force parameters are complex, but also that the dependence on the density distribution of the nucleons is taken into account. Then in the calculation of the Hamiltonian kernel it is important, in particular, how the nucleon density dependence should be treated.

The Hamiltonian operator and kernel are given,

\[
\hat{H} = \hat{T} - \hat{T}_c + \frac{1}{2} \sum_{ij} \hat{v}_{ij} - \varepsilon_1^{\text{int}} - \varepsilon_2^{\text{int}} - \frac{3}{4} \hbar \omega ,
\]

\[
\mathcal{H}(D, K) = \frac{K^2}{2\mu} + CV(D, K) ,
\]

where \( \hat{T} , \hat{T}_c , \hat{v}_{ij} \) and \( \varepsilon^{\text{int}} \) (\( i = 1, 2 \)) denote the kinetic energy operator of each nucleon, kinetic energy operator of the center of mass of the total system, two-nucleon effective interaction and internal energies of scattering nuclei, respectively. The term \( 3/4 \hbar \omega \) is the energy shift caused by the Gaussian form taken to the wave function of the relative motion.

The CEG force is derived based on the Brueckner-Hartree-Fock theory with the local density approximation. As the real and imaginary parts of CEG, which contain no adjustable parameters, are constructed consistently and the folding model with the CEG force well reproduces nucleon-nucleus elastic scattering, it may be said that CEG is one of the most realistic two-nucleon effective interaction for the scattering state problem at present. Though CEG has central, \( L-S \), and tensor parts, in this paper we use only the central part because for the system composed of two closed shell nuclei such as \( a-a \) one the \( L-S \) and the tensor parts make no contribution. The central part of CEG has the following form:

\[
\hat{v}_{ij}^{(c)} = \sum_{\lambda=1}^{3} v_{ij}^{(c)}(1 + \alpha_{i}^{(c)} k_{F(1),2} + \beta_{i}^{(c)} k_{F(1),2}^{2}) \exp\left\{ -\left( \frac{r_i - r_j}{\lambda_i} \right)^2 \right\} , \quad (j=1,4,3,0)
\]

\[
(2·31)
\]

where \( v_{ij}^{(c)} \), \( \alpha_{i}^{(c)} \) and \( \beta_{i}^{(c)} \) are the complex functions of an incident energy and \( k_{F} \) is a Fermi momentum in the local density approximation. With this approximation the relation between the Fermi momentum and the spatial density distribution of nucleons is given by

\[
k_{F(1),2} = \left[ \frac{3\pi^2}{2} \rho \left( \frac{r_i + r_j}{2} \right) \right]^{1/3} ,
\]

\[
(2·32)
\]

where \( \rho(r) \) is a density distribution function of nucleons, and is given by

\[
\rho(r) = \frac{\langle Z | \sum_{i=1}^{A_{1}+A_{2}} \delta(r_i - X_{c} - r) | Z \rangle}{\langle Z | Z \rangle} ,
\]

\[
(2·33)
\]

It must be noted that this density distribution function of nucleons are obtained by fully antisymmetrized wave function \( |Z\rangle \).

When the two-body effective interaction becomes complex and has the dependence on the nucleon density distribution, the real and the imaginary part of the
internal energy of the nuclei become the functions of the relative distance and momentum because the density distribution function in the internal energy kernel also has a distance and momentum dependence,

\[ \epsilon_{I}^{\text{int}} = \frac{1}{2} \sum_{i,j=1}^{l} \frac{\bar{q}_{ij} \phi_{I}(D,K) \phi_{I}}{\phi_{I}^{\dagger} \phi_{I}} . \quad (I=1,2) \]  

As for the treatment of the internal energy of nuclei, there would be two ways of thinking. The one is that the internal energy subtracted from the expectation value of the Hamiltonian should be taken as a constant and fixed to its asymptotic value of infinite relative distance (large \(|D|\)). And the other one is the following: Since the probability flux should not be decreased by the interaction between two nucleons in the same nucleus, the imaginary part of the internal energy term in the interaction kernel should not be incorporated in the imaginary part of the inter-nucleus interaction. So the formulation by the first way in which the change of the imaginary part of the internal energy of the nuclei affects the inter-nucleus interaction is improper. Then in this study we put the internal energy subtracted from the expectation value of the Hamiltonian kernel to be the function of the relative distance and the momentum. But we think that this treatment is still insufficient, because in the calculation where the channels are explicitly specified, at least concerning the imaginary part, the two-nucleon effective interaction between the nucleons in the same nucleus should be close to the bound state real effective interaction and the one between the nucleons in the different nuclei close to the scattering state complex effective interaction. This conjecture suggests that the use of both the bound state real effective interaction and the scattering state complex one is necessary when we research properties of the scattering state inter-nucleus interaction in the channel specified formalism. On this point we will have a detailed discussion in the next paper.

2.4. Structure of the full potential

To see the structure of the full potential we transform the Hamiltonian (2·30) into the following form:

\[ H(D,K) = \frac{P_{\mu}^{2}(R(D,K))}{2\mu} + \frac{\hbar^{2} I(I+1)}{2\mu R^{2}(D,K)} + V_{0\text{dir}}(R(D,K)) + V_{0\text{tot}}(R(D,K)) , \]  

\[ V_{0\text{dir}}(R(D,K)) = \frac{K^{2} - P^{2}}{2\mu} + V_{\text{dir}}(R(D,K)) \]

\[ = \frac{K^{2} - P^{2}}{2\mu} + V_{0}(R(D,K)) + V_{\text{tot}}(R(D,K)) \]

\[ = V_{0}(R(D,K)) + V_{\text{tot}}(R(D,K)) , \]  

where \(V_{0}\) and \(V_{\text{tot}}\) are direct and total exchange potentials, respectively,

\[ V_{0}(R) = \frac{\langle \phi_{1}(D,K) \phi_{2}(D,K) | \sum_{i=1,2}^{l} \bar{q}_{ij} \phi_{1}(D,K) \phi_{2}(D,K) \rangle}{\langle \phi_{1}(D,K) \phi_{2}(D,K) | \phi_{1}(D,K) \phi_{2}(D,K) \rangle} . \]  

The reason \(V_{\text{ex}}\) and \(V_{0}\) have angular momentum dependence is that the trajectories
of $D - K$ differ for each $l$. And also we define the knock-on exchange potential here,

$$V_{K}^{(l)}(R) = -\frac{\langle \phi_{1}(D, K)\phi_{2}(D, K) | \sum_{i \in \{D,K\}} \delta_{ij} P_{ij} | \phi_{2}(D, K)\phi_{1}(D, K) \rangle}{\langle \phi_{1}(D, K)\phi_{2}(D, K) | \phi_{1}(D, K)\phi_{2}(D, K) \rangle},$$

(2.38)

where $P_{ij}$ is the transposition operator of nucleon $i$ and $j$. The important ingredient in the total exchange potential of the CMWP method is the term,

$$\frac{K^2}{2\mu} \frac{P^2}{2\mu} \equiv V_{ex}$$

which is not included in the original (non-canonical) moving wave packet method.

§ 3. Numerical results

In this section we will show the numerical results for $a-a$ elastic scattering by the CMWP method explained in § 2 and also make a comparison with the results obtained by RGM+WKB to verify the efficiency of the CMWP method. In the paragraph below all the energies are measured in the center of mass system.

The most characteristic feature of the CMWP method is the transformation of the parametric relative coordinates $D$ and $K$ into the canonical relative coordinates $R$ and $P$. Figure 1 indicates the effects of this transformation. In Fig. 1 Re$P$ is plotted as functions of $R$ and the Pauli forbidden region which we get by Eq. (2.20) by putting $R$ and $P$ to real variables is also shown. In this figure we also show Re$K$ as a function of $R$ in order to compare with Re$P$. It is clear from Fig. 1 that the transformation pushes out the trajectories of $R - \text{Re}K$, which penetrate into the Pauli forbidden region, to the trajectories of $R - \text{Re}P$ outside of the Pauli forbidden region. We can also find that the effect of the transformation decreases when the incident energy gets higher. This is because the high incident energy results in the high momentum of the relative motion, and the increase of separation of two nuclei in the phase space decreases the antisymmetrization effect.

Next we will compare the real parts of the full potentials by CMWP in Fig. 2(a) and by RGM+WKB in
Fig. 2. (a) Real part of the full potential by CMWP. Numbers in the figure are the incident energy (MeV) in the center of mass system.
(b) Real part of the full potential by RGM+WKB. Numbers in the figure are the incident energy (MeV) in the center of mass system. At $E=10$ MeV and $E=20$ MeV there are no solutions in inner region $|R|\leq 4\text{fm}$ and $|R|\leq 2\text{fm}$, respectively. We do not plot the solution for $E=10$ MeV.

Fig. 2(b). The calculational method by RGM+WKB with the density-dependent effective interaction is given in Ref. 12. In the RGM+WKB calculation in this study we employed the same nucleon density distribution function in the CEG force as the one in the CMWP calculation and the parametric vectors $D$ and $K$ in the density are regarded as the functions of the physical vectors $R$ and $P$. But in this RGM+WKB calculation there are no solutions in the inner region ($R\leq 4\text{fm}$) for $E=10$ MeV and ($R\leq 2\text{fm}$) for $E=20$ MeV. Then for $E=10$ MeV we do not plot the solutions in all of the figures below. In the comparison we performed entirely the same calculations by these two methods using the CEG force. In the inner region ($R\leq 2\text{fm}$) the full potential by CMWP is shallower than the one obtained by RGM+WKB. In spite of this difference in the inner region the coincidence of the potentials for outer region ($R\geq 2\text{fm}$) obtained by these two methods is good. This result indicates the large efficiency of the CMWP method. The feature of the real part of the full potential is as follows: When the incident energy increases, the potential in the inner region ($0\leq |R|\leq 2.5\text{fm}$) becomes shallower and the one in the outer region ($2.5\text{fm}\leq |R|$) becomes deeper.

Figures 3 (a) and (b) show the imaginary parts of the full potentials by CMWP and RGM+WKB with the CEG force, respectively. The features of the imaginary part are as follows: At the incident energy of 20 MeV the potential is of surface absorptive type, and at 40 MeV ~ 60 MeV it shows the volume absorptive nature, and at 100 MeV it becomes surface absorptive again. From another point of view, as the
Fig. 3. (a) Imaginary part of the full potential by CMWP. Numbers in the figure are the incident energy (MeV) in the center of mass system. (b) Imaginary part of the full potential by RGM+WKB. Numbers in the figure are the incident energy (MeV) in the center of mass system. As in Fig. 2 (a), at $E=10$ MeV and $E=20$ MeV there are no solutions in inner region $|R| \leq 4$ fm and $|R| \leq 2$ fm, respectively. We do not plot the solution for $E=10$ MeV.

Fig. 4. (a) Real parts of the direct and knock-on exchange potentials. Numbers in the figure are the incident energy (MeV) in the center of mass system. (b) Real part of the total exchange potential. Numbers in the figure are the incident energy (MeV) in the center of mass system.
incident energy gets higher, in the outer region (3fm≤|R|) the imaginary part of potential becomes deeper, while in the medium region (2fm≤|R|≤3fm) it becomes shallower. We can find that the coincidence of the imaginary parts of full potentials by CMWP and RGM+WKB is also good.

We also investigate the behavior of the direct (double folding) $V_d$, knock-on exchange $V_{ko}$ and the total exchange $V_{ex}$ potentials obtained by CMWP. The real parts of the direct and the knock-on exchange potentials are shown in Fig. 4(a). The characters of these potentials are as follows: The direct potential is weakly attractive in the outer region and is repulsive in the inner region, and its attraction becomes weaker as the incident energy gets higher. The knock-on exchange potential is strongly attractive in all spatial region and the attraction becomes weaker according to the increase of incident energy. We can see the same result is given in Ref. 12), where the similar analysis is performed by RGM+WKB with only the real part of the CEG force. Another character seen in Fig. 4(a) is the incident energy dependence of the direct potential. The energy dependence of $V_d$ is due to the following reasons. The direct potential has a dependence on the parametric relative coordinates $D$ and $K$ because of the dependence on the spatial density distribution of nucleons in the effective two-body interaction, which depends on $D$ and $K$. And also the force parameters of the CEG force are given as functions of the incident energy. Moreover the transformation of $D$ and $K$ into $R$ and $P$ makes a contribution to the energy dependence of $V_d$. The real part of the total exchange potential is shown in Fig. 4(b). It is attractive in the inner region and when the incident energy gets higher, it becomes

![Fig. 5. (a) Imaginary parts of the direct and knock-on exchange potentials. Numbers in the figure are the incident energy (MeV) in the center of mass system. (b) Imaginary part of the total exchange potential. Numbers in the figure are the incident energy (MeV) in the center of mass system.](https://academic.oup.com/ptp/article-abstract/82/1/53/1914515)
closer to the knock-on exchange one. And another feature is the repulsive tail in the low energy region. By the comparison of Fig. 2 and Fig. 4 it is obvious that the real part of the full potential differs from the sum of the direct and knock-on exchange potentials, especially in the low energy region where the contributions of the exchange processes other than the knock-on-exchange are outstanding. Then in the system where the imaginary part of the full potential is weak, it is expected that the theoretical expectation of the quantities of the scattering process by the double folding model differs from the one by the many body theory fully treating the Pauli principle.

The imaginary parts of the direct and the knock-on exchange potentials are shown in Fig. 5(a). We can find that as the incident energy goes up, the direct potential becomes deeper in $(2 fm \leq |R|)$. The knock-on exchange potential has a repulsive (emissive) peak in low energy region, but in high energy region this peak disappears. Figure 5(b) shows the imaginary part of the total exchange potential. The total exchange potential is repulsive almost everywhere and becomes close to the knock-on-exchange potential with the increase of the incident energy.

§ 4. Discussion

4.1. Pauli forbidden region by the complex potential

As already mentioned in § 2.2, the inequality (2.20) expressing the Pauli forbidden region is not satisfied in a purely mathematical sense because $R$ and $P$ are complex vectors, but when the imaginary part of the potential is weak, $R$ and $ReP$ is approximately satisfies (2.20). To elaborate on the above statements, let us consider the following function:

$$f(u) = \min_t \Re \left[ s \frac{\partial}{\partial s} \ln \mathcal{N}(s) \right],$$

where $s$ is any complex number, and $t$ and $u$ are the real and imaginary parts of $s$, respectively. The operator $\min_t$ means to take the minimum value with respect to $t$. The function $f(u)$ indicates the volume of the allowed phase space of the relative motion,

$$\nu \mu_A R^2 + \frac{1}{4 \nu \mu_A} \Re(P^2) \geq f(u).$$

When the imaginary part of $s$ is 0, which means the inter-nucleus potential is real, the function $f(s)$ is equal to the lowest
number of oscillator quanta \( N_A \) of the Pauli allowed state in RGM. If the potential becomes complex, that is, the other channels couple to the elastic channel, the Pauli forbidden region varies, and the \( f(u) \) becomes different from \( N_A \). Figure 6 shows such behavior of \( f(u) \) in case of the \( \alpha-\alpha \) system. In the figure we can find that the Pauli forbidden region shrinks as \( u \) becomes larger. This effect emerges as the variation of the real part of the full potential. However in the actual numerical studies we have done, the magnitude of \( u \) is less than 1.

4.2. Perturbative treatment of extended version of the CMWP method

If the imaginary parts of \( P \) is the quantities of perturbative order (\( |\text{Im} P| \ll |\text{Re} P| \)), the Hamiltonian kernel is written as

\[
\mathcal{H}(\mathbf{R}, P_r, P_i) = \left[ \frac{P_{Ir}^2}{2\mu} + \frac{\hbar^2 I(I+1)}{2\mu R^2} + V^{(0)}_r(\mathbf{R}, P_{Ir}) \right] \\
+ i \left[ \frac{P_{Ir} \cdot P_{iI}}{\mu} + V^{(0)}_i(\mathbf{R}, P_{Ir}, P_{iI}) \right],
\]  

where

\[
V^{(0)}_i(\mathbf{R}, P_{Ir}, P_{iI}) = \frac{\langle Z | \sum \text{Re} (\bar{\theta} \theta) | Z \rangle}{\langle Z | Z \rangle} \frac{K_{Ir}^2 - P_{iI}^2}{2\mu},
\]

\[
V^{(0)}_r(\mathbf{R}, P_{Ir}) = \frac{\langle Z | \sum \text{Im} (\bar{\theta} \theta) | Z \rangle}{\langle Z | Z \rangle} + \frac{\partial}{\partial P_{Ir}} V^{(0)}_r(\mathbf{R}, P_r),
\]

\[
P_{iI} = P_{Ir} + iP_{iI},
\]

\[
\left( Z = \frac{1}{\sqrt{2}} \left[ \sqrt{2\mu \alpha} D(\mathbf{R}, P_{Ir}) + i \sqrt{\frac{1}{2\mu \alpha}} \frac{K(\mathbf{R}, P_{Ir})}{\hbar} \right] \right)
\]

By the fact that the total energy of the system is real, we can find the relation between the imaginary part of the full potential and the imaginary part of the kinetic energy from Eq. (4·3) as follows:

\[
V^{(0)}_i(\mathbf{R}, P_{Ir}, P_{iI}) = \frac{P_{Ir} \cdot P_{iI}}{\mu}.
\]

Then we will find the following relation by eliminating \( P_{iI} \) from Eqs. (4·4) and (4·5),

\[
V^{(0)}_i(\mathbf{R}, P_{Ir}) = F^2 \frac{\langle Z | \sum \text{Im} (\bar{\theta} \theta) | Z \rangle}{\langle Z | Z \rangle},
\]

where \( F \) is the Perey factor,
§ 5. Summary and concluding remarks

In this paper, the first one of the series of this study, we explained the formulation to calculate the complex inter-nucleus potential by the complex G-matrix; the extended formalism of CMWP and the method to take into account the density-dependence of nucleon-nucleon effective interaction. And also we examined the efficiency of the CMWP method by comparing with the results of more realistic RGM + WKB method.

The ingredient of § 2.1 is essentially due to Saraceno et al., and our contributions are on and after § 2.2. In § 2 we showed that even with the complex G-matrix it is able to define the inter-nucleus complex potential to the relative motion which entirely contain the Pauli principle.

The basic idea to treat the complex G-matrix is the extension of the relative distance and momentum to the complex space, which is a natural extension in case of the non-hermitian Hamiltonian operator. The important point is that to contain the Pauli principle completely in the classical description it is not sufficient to antisymmetrize the wave function but moreover it is indispensable to transform the parametric vectors \( D \) and \( K \) to the physical vectors \( R \) and \( P \). This transformation just ensures the coincidence with the RGM + WKB method. This transformation is easily performed and the calculation of the kernels in CMWP is much easier than RGM. Then the good coincidence of CMWP and RGM + WKB indicates the large facility of the CMWP method.

In this paper we proposed the method to treat the density dependence in the complex G-matrix, which is based on the local density approximation as usually used in the analysis of nucleon-nucleus scattering. Though this treatment in the nucleus-nucleus system has not been justified, we expect the efficiency of this method in not so much higher incident energy region. On this point we will make a detailed discussion in the sequel.

In § 3 we showed the numerical results by CMWP with the CEG force. And to investigate the efficiency of CMWP we also performed the RGM + WKB calculation. In that section we found the good coincidence of the results by CMWP and RGM + WKB. Also we found the importance of the total antisymmetrization of the wave function. It is obvious that in the microscopic calculation of the complex potential the sum of only the direct and knock-on exchange potential cannot be used for the inter-nucleus potential as a substitution of the microscopic full potential. It will become clear especially in the weak-absorptive system. The shapes of the real and imaginary parts of the full potential are quite different and also their incident energy dependences differ from each other. We think that the effect of the total antisymmetrization plays an important role in obtaining the microscopic inter-nucleus poten-
More physical consideration of the theoretical results and the comparison of the theoretical calculation with the experimental results will be performed in the next paper of this series, in which we will discuss from the viewpoint of the nucleon-nucleon effective interaction in the nucleus-nucleus system and we will investigate especially the imaginary part of the inter-nucleus potential. What kind of processes can we take into account as an origin of the imaginary part of the inter-nucleus potential in the single channel calculation? And what does such an imaginary part mean?

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Appendix A

--- GCM Norm Kernel and Pauli Forbidden Region ---

By using the harmonic oscillator creation operator $a^\dagger$ as

$$a^\dagger_R = \frac{1}{\sqrt{2}} \left[ \sqrt{2\nu_R} R - \frac{1}{\sqrt{2\nu_R}} \frac{\partial}{\partial R} \right]. \quad (A\cdot1)$$

We can express $\phi_{rel}$ of Eq. (2.3) as follows:

$$\phi_{rel}(R, Z) = \exp(Z \cdot a^\dagger_R) \phi_{rel}(R, Z=0), \quad (A\cdot2)$$

where $\phi_{rel}(R, Z=0)$ is just the harmonic oscillator ground state wave function. From Eq. (A.2) we get

$$\phi_{rel} = \sum_{n_x, n_y, n_z=0}^\infty \phi_{n_x, n_y, n_z}(R) f_{n_x, n_y, n_z}(Z)$$

$$= \sum_{n_l m} \phi_{ln}(R) f_{ln}^m(Z), \quad (A\cdot3)$$

where $\phi_{n_x, n_y, n_z}(R)$ and $\phi_{ln}(R)$ are the harmonic oscillator wave functions in Cartesian and polar coordinate representations, respectively, and

$$f_{n_x, n_y, n_z}(Z) = \frac{Z_x^{n_x} Z_y^{n_y} Z_z^{n_z}}{\sqrt{n_x!} \sqrt{n_y!} \sqrt{n_z!}},$$

$$f_{ln}^m(Z) = (-)^{1/2(n-l)} \left[ \frac{4\pi}{(n+l+1)!!(n-l)!!} \right]^{1/2} (Z \cdot Z)^{1/2(n-l)} Q_{lm}(Z). \quad (A\cdot4)$$

Here $Q_{lm}$ is a solid spherical harmonics and both $f_{n_x, n_y, n_z}(Z)$ and $f_{ln}^m(Z)$ are orthonormalized with the Bargmann measure of Eq. (2.4).
By using the complete basis $f_{lm}^n$ the delta function in the Bargmann space is expanded as
\[ \exp(Z' \cdot Z) = \sum_{nlm} f_{lm}^n(Z') f_{lm}^n(Z). \]

Since the function $f_{lm}^n$ is a homogeneous polynomial of degree $n$, the above expansion means
\[ \sum_{lm} f_{lm}^n(Z') f_{lm}^n(Z) = \frac{1}{n!} (Z \cdot Z')^n. \]

Now we will prove that the complex GCM norm kernel for the system composed of two closed-shell nuclei depends only on the scalar product of $Z$ and $Z'$. For harmonic oscillator operators $a$ and $a'$, there holds a relation
\[ \exp(ia^\dagger H a) F(a^\dagger) \phi_0 = F(\cdot U a') \phi_0, \]
\[ U = e^{iH}, \]
where $\phi_0$ satisfies $a \phi_0 = 0$ and $U$ and $H$ are $3 \times 3$ matrices and when $U$ is unitary, $H$ is hermitian. In case of the closed shell configuration $\phi_1(\phi_2)$ of the harmonic oscillator shell model, we have
\[ \exp(i \sum_{k=1}^{A-1} a_{jk} H a_{jk}) \phi_j = \phi_j \quad (j=1, 2) \]
for any hermitian matrix $H$, where $a_{jk}$ and $a^\dagger_{jk}$ are the harmonic oscillator operators of the internal coordinate $\xi_{jk}$ of $\phi_j$. For $\phi_{\text{rel}}(R, Z)$, we have
\[ \exp(ia_{\text{rel}}^\dagger H a_{\text{rel}}) \phi_{\text{rel}}(R, Z) = \exp(\cdot (U a_{\text{rel}})) \phi_{\text{rel}}(R, Z=0) \]
\[ = \phi_{\text{rel}}(R, U Z). \]

Hence we obtain the relation
\[ \mathcal{K}(Z, Z') = \langle \phi_{\text{rel}}(R, Z) \phi_{\text{rel}}(R, Z') \phi_{\text{rel}}(R, Z') \rangle \]
\[ = \langle T_U (\phi_{\text{rel}}(R, Z) \phi_{\text{rel}}(R, Z')) \rangle \]
\[ = \langle \phi_{\text{rel}}(R, U Z) \phi_1 \phi_2 | \mathcal{A} \{ \phi_{\text{rel}}(R, U Z') \phi_1 \phi_2 \} \rangle \]
\[ = \mathcal{K}(U Z, U Z') \],
\[ T_U = \exp(i \sum a_{ek} H a_{ek}), \]
\[ a_{ek} = \{ a_{\text{rel}}, a_{1k}, a_{2l} \}. \]

This relation means that $\mathcal{K}(Z, Z')$ should contain $Z'$ and $Z$ only in the form of $(Z' \cdot Z)$. 

\[ \int d\mu(Z) f_{n_1 n_2 n_3} f_{n'_1 n'_2 n'_3} (Z) = \delta_{n_2 n'_2} \delta_{n_3 n'_3} \delta_{n_2 n'_2}, \]
\[ \int d\mu(Z) f_{lm}^n(Z) f_{lm}^m(Z) = \delta_{nn'} \delta_{ll'} \delta_{mm'}. \]
Next we will prove that the value $N_A$ in (2·13) is a lowest number of oscillator quanta of the RGM Pauli allowed state. According to Eq. (2·4) the relation between the RGM and the complex GCM norm kernels is

$$\mathcal{N}^{\text{RGM}}(\mathbf{R}, \mathbf{R}') = \langle \delta(\mathbf{R} - \mathbf{a}) \phi_1 \phi_2 | A(\phi_1 \phi_2 \delta(\mathbf{R} - \mathbf{a})) \rangle = \int d\mu(\mathbf{Z}) d\mu(\mathbf{Z}') \phi_{\text{rel}}(\mathbf{R}, \mathbf{Z}) \mathcal{N}(\mathbf{Z}, \mathbf{Z}') \phi_{\text{rel}}(\mathbf{R}', \mathbf{Z}').$$  

(A·13)

When we expand the GCM norm kernel into the following form:

$$\mathcal{N}(\mathbf{Z}, \mathbf{Z}') = \sum_{n=0}^{\infty} \frac{1}{n!} \mu_n (\mathbf{Z}' \cdot \mathbf{Z})^n = \sum_{n=0}^{\infty} \mu_n \sum_{lm} f_{lm}(\mathbf{Z}') f_{lm}^{\dagger}(\mathbf{Z}).$$  

(A·14)

then we get the RGM norm kernel as follows:

$$\mathcal{N}^{\text{RGM}}(\mathbf{R}, \mathbf{R}') = \sum_{n=0}^{\infty} \sum_{lm} \mu_n \phi_{lm}^{\dagger}(\mathbf{R}) \phi_{lm}(\mathbf{R}').$$  

(A·15)

This means that the harmonic oscillator bases are the eigenfunctions of the RGM norm kernel for two closed-shell nuclei system and its eigenvalue is $\mu_n$.

As all the eigenvalues for the GCM norm kernel are non-negative, then the boundary $N_A$ of Pauli forbidden region in CMWP corresponds to the first non-zero eigenvalue $\mu_{N_A}$ because

$$\min \left[ \mathbf{Z} \cdot \mathbf{Z} \frac{\partial}{\partial (\mathbf{Z} \cdot \mathbf{Z})} \ln \mathcal{N}(\mathbf{Z}, \mathbf{Z}) \right] = \lim_{s \to 0} \frac{\partial}{\partial s} \ln \mathcal{N}(s)$$

$$= \lim_{s \to 0} \left[ \left( \sum_{n=N_A}^{\infty} \frac{1}{(n-1)!} \mu_{n}s^n \right) / \left( \sum_{n=N_A}^{\infty} \frac{1}{n!} \mu_{n}s^n \right) \right]$$

$$= N_A. \quad (A·16)$$

Now it is obvious that the value $N_A$ is the lowest number of the harmonic oscillator quanta of the Pauli allowed state in RGM.

**Appendix B**

--- Singular Lagrangian and Equation of Motion ---

The definition of the singularity of Lagrangian is

$$\text{Det} \frac{\delta^2 \mathcal{L}}{\delta q_i \delta \dot{q}_i} = 0,$$  

(B·1)

where $\mathcal{L}$ is assumed to be a function of $\{q_i, \dot{q}_i\}_{i=1,\ldots,n}$, and all $q_i$ and $\dot{q}_i$ are regarded as independent variables. The singularity is a sign of the existence of certain constraints among the canonical coordinates and momenta.\(^{(11)}\) It is obvious that our Lagrangian,

$$\mathcal{L} = \frac{i\hbar}{2} [\mathbf{Z} \cdot \mathbf{Z} - \dot{\mathbf{Z}} \cdot \mathbf{Z}] \frac{\partial}{\partial s} \ln \mathcal{N} - \mathcal{H},$$  

(B·2)
has singularity. The canonical momenta derived by Eq. (B·2) are expressed by \( Z \) and \( \bar{Z} \), which means that there are some constraints among the canonical coordinates and momenta. Saraceno et al. regarded \( \{ Z_i, \bar{Z}_i, \dot{Z}_i, \dot{\bar{Z}}_i \}_{i=1,2,3} \) as the independent variables as is seen in the definition of the Poisson bracket.\(^5\)

Even if the model Lagrangian has singularity, Lagrange's equation of motion gives a precise description of the time evolution of the system. However, Hamilton's equation of motion with "ordinary" Poisson bracket gives the false description of the motion of the system. The term "ordinary" means the following: Let us define the generalized canonical momentum \( \{ P_{Z,i} \} \) and \( \{ P_{\bar{Z},i} \} \) conjugate to the generalized coordinates \( \{ Z_i, \bar{Z}_i \}_{i=1,2,3} \), which are now regarded as the independent variables, by the following equations:

\[
P_{Z,i} = \frac{\partial L}{\partial \dot{Z}_i} = \frac{i\hbar}{2} Z_i \frac{\partial}{\partial s} \ln \mathcal{H}, \quad (i=1, 2, 3)
\]

\[
P_{\bar{Z},i} = \frac{\partial L}{\partial \dot{\bar{Z}}_i} = \frac{i\hbar}{2} \bar{Z}_i \frac{\partial}{\partial s} \ln \mathcal{H}, \quad (i=1, 2, 3)
\] (B·3)

Here it should be noted that the generalized momenta defined here differ from the ones in § 2.1 by factor 2. By these definitions of \( \{ P_{Z,i} \}_{i=1,2,3} \) and \( \{ P_{\bar{Z},i} \}_{i=1,2,3} \), we get the equations of motion by the Poisson bracket,

\[
\{ F, G \}_p = \sum_i \left( \frac{\partial F}{\partial Z_i} \frac{\partial G}{\partial P_{Z,i}} - \frac{\partial F}{\partial P_{Z,i}} \frac{\partial G}{\partial Z_i} + \frac{\partial F}{\partial \bar{Z}_i} \frac{\partial G}{\partial P_{\bar{Z},i}} - \frac{\partial F}{\partial P_{\bar{Z},i}} \frac{\partial G}{\partial \bar{Z}_i} \right),
\]

\[
\dot{Z}_i = \{ Z_i, \mathcal{H} \}_p = -\frac{\partial \mathcal{H}}{\partial P_{Z,i}}, \quad (i=1, 2, 3)
\]

\[
\dot{P}_{Z,i} = \{ P_{Z,i}, \mathcal{H} \}_p = -\frac{\partial \mathcal{H}}{\partial Z_i}, \quad (i=1, 2, 3)
\]

\[
\dot{\bar{Z}}_i = \{ \bar{Z}_i, \mathcal{H} \}_p = -\frac{\partial \mathcal{H}}{\partial P_{\bar{Z},i}}, \quad (i=1, 2, 3)
\]

\[
\dot{P}_{\bar{Z},i} = \{ P_{\bar{Z},i}, \mathcal{H} \}_p = -\frac{\partial \mathcal{H}}{\partial \bar{Z}_i}. \quad (i=1, 2, 3)
\] (B·4)

It is easily seen that the equations concerning to \( Z \) and \( \dot{Z} \) in (B·4) are also different from the equations of motion (2·11) by factor 2 because of the definition of \( \{ P_{Z,i} \}_{i=1,2,3} \) and \( \{ P_{\bar{Z},i} \}_{i=1,2,3} \).

In our model, as already written in § 2.1, the time evolutions of \( \bar{Z} \) and \( \dot{\bar{Z}} \) are completely determined by those of \( Z \) and \( \dot{Z} \) because the equations of motion describing the time evolution of \( Z \) and \( \dot{Z} \) determine both the real and imaginary parts of \( Z \) and \( \dot{Z} \) simultaneously. It means that we need only 6 equations of motion to determine the time evolution of the system. There are, however, 12 equations in Eq. (B·4) in which the 6 equations are concerning to \( Z \) and \( \dot{Z} \) and the remaining 6 equations to \( \bar{Z} \) and \( \dot{\bar{Z}} \). This fact obviously indicates that if we employ Hamilton's equation of motion with the "ordinary" Poisson bracket in case of the singular Lagrangian, we get the false description of the time evolution of the system.
To avoid this fault caused by the redundant degrees of freedom in our Lagrangian, we can use two different methods. The one is to define the Poisson brackeet taking into account the symplectic structure as employed by Saraceno et al., or to use the Dirac bracket which gives the same results as the Poisson bracket with symplectic structure. The other method, which we use in this paper, is to remove the excessive degrees of freedom from the original Lagrangian. The reason we adopt the second method is that we use the constants of motion to determine the trajectory in the phase space of relative motion, and that in the Hamiltonian formalism it is easy to know what is a constant of motion.

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