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Exact treatment of the Pauli exclusion operator in nuclear matter calculation

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Abstract

Exact expressions of the Pauli exclusion operator Q in the nuclear matter calculation are presented in detail. Exact formulae are also given for the calculations of the single-particle potential energy and the binding energy per nucleon with the exact Q operator. Numerical calculations of the G matrix in the lowest-order Brueckner theory are carried out to check the reliability of the standard angle-average approximation for the Q operator by employing the Bonn B and C *NN* potentials. It is observed that the exact treatment of the operator Q brings about non-negligible and attractive contributions to the binding energy.

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1. Introduction

It is one of the fundamental and open problems in nuclear structure physics to understand the saturation property of nuclear matter starting from a nucleon–nucleon (*NN*) interaction [1–3]. Because of the presence of strongly repulsive components in the short-range part of the *NN* interaction, the nucleon–nucleon scattering correlation has a predominant importance in the nuclear matter calculation. The Bethe–Goldstone equation has been used for solving a two-nucleon scattering problem in nuclear matter. The influence of the nuclear medium on nucleon–nucleon scattering is taken into account by considering the Pauli exclusion principle and the self-energy effect on scattering nucleons. Therefore the accurate treatment of the Pauli exclusion operator has been one of the essential requirements for the numerical calculation of nuclear matter.

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The Pauli exclusion operator depends, in principle, not only on the magnitudes of the total and relative momenta of scattering two nucleons but also on their angles. This angular dependence leads to couplings among partial waves, which makes numerical computations difficult. The difficulty due to the angular dependence has been avoided by employing the angle-average approximation [4,5]. The angle-average approximation, however, does not necessarily have a quantitative justification, although there have been some studies to assess the reliability of this approximation [6–12].

One of the purposes of this work is to give analytic formulae for the calculation of the nuclear matter binding energy in the exact treatment of the Pauli exclusion operator Q. Furthermore, we want to clarify how the G matrix depends on angular and linear momenta. With analytic expressions of the operator Q and the G matrix we perform numerical calculations to investigate the effect of the exact treatment of the operator Q on the nuclear matter binding energy by solving the Bethe–Goldstone equation.

Very recently Schiller, Müther and Czerski [13,14] reported their calculations of nuclear matter properties using the exact Pauli operator Q. Their results [14] show that the standard angle-average approximation for the operator Q tends to underestimate the binding energy per nucleon at any densities. The exact treatment of the operator Q thus yields a slight increase in the binding energies and leads to a non-negligible shift in the calculated saturation curve. It would be interesting and deserving to examine whether the similar result can be reproduced in an alternative approach to the nuclear matter calculation with the exact Q operator.

The organization of this paper is as follows. In Section 2 we give an exact and analytic expression of the operator Q in angular-momentum-coupling states. Section 3 is devoted to derive formulae which are necessary for the calculation of the single-particle potential energy and the binding energy per nucleon in the exact treatment of the operator Q. We show, in Section 4, numerical results for the calculations with the exact and angle-averaged Q operators by employing the Bonn B and C *NN* potentials [15]. We discuss the effect of the exact treatment of the operator Q and the accuracy of the angle-average approximation at various nuclear matter densities. Conclusions obtained in this study are given in Section 5.

2. Exact expression of the Pauli exclusion operator

The reaction matrix (G matrix) in nuclear matter is defined by the Bethe–Goldstone equation

$$G = v + v\frac{Q}{e}G, \tag{2.1}$$

where v is the two-body *NN* interaction, e gives the starting energy minus the energy of an intermediate two-particle state, and Q stands for the Pauli exclusion operator. The operator Q prevents two particles from scattering into intermediate states with momenta below the Fermi momentum k_{F}, which is written as

$$Q = \frac{1}{2}\sum_{\alpha\beta} |\alpha\beta\rangle\langle\alpha\beta| \Theta(k_\alpha - k_{\mathrm{F}})\Theta(k_\beta - k_{\mathrm{F}}), \tag{2.2}$$

where α is a single-particle state with the momentum $\boldsymbol{k}_\alpha$, the spin projection s_α and the isospin projection τ_α. The state $|\alpha\beta\rangle$ is a normalized and antisymmetrized two-nucleon state, and $\Theta(x)$ the Heaviside step function. In the relative and center-of-mass (c.m.) momentum system the operator Q is written as

$$Q = \frac{1}{2}\sum_{s_\alpha\tau_\alpha s_\beta\tau_\beta}\int K^2 dK\, d\hat{\boldsymbol{K}}\int k^2\, dk\, d\hat{\boldsymbol{k}}\,|\boldsymbol{K}\boldsymbol{k}s_\alpha\tau_\alpha s_\beta\tau_\beta\rangle\{\langle \boldsymbol{K}\boldsymbol{k}s_\alpha\tau_\alpha s_\beta\tau_\beta| - \langle \boldsymbol{K}-\boldsymbol{k}s_\beta\tau_\beta s_\alpha\tau_\alpha|\}\Theta\left(\left|\frac{\boldsymbol{K}}{2}+\boldsymbol{k}\right|-k_{\mathrm{F}}\right)\Theta\left(\left|\frac{\boldsymbol{K}}{2}-\boldsymbol{k}\right|-k_{\mathrm{F}}\right), \tag{2.3}$$

where $\boldsymbol{K}$ and $\boldsymbol{k}$ are the c.m. and relative angular momenta given by $\boldsymbol{K}=\boldsymbol{k}_\alpha+\boldsymbol{k}_\beta$ and $\boldsymbol{k}=(\boldsymbol{k}_\alpha-\boldsymbol{k}_\beta)/2$, respectively.

We consider a partial wave decomposition of the relative state coupled to the angular momentum $\boldsymbol{J}$ with the c.m. momentum $\boldsymbol{K}$ as

$$|\boldsymbol{K}k(lS)\,JMTT_z\rangle = f_{lST}\sum_{m,S_z}\langle lmSS_z|JM\rangle\int d\hat{\boldsymbol{k}}\,Y_{lm}(\hat{\boldsymbol{k}})|\boldsymbol{K}\boldsymbol{k}\rangle|SS_zTT_z\rangle, \tag{2.4}$$

where $\boldsymbol{S}$ is the total spin and $\boldsymbol{l}$ the orbital angular momentum of two-body relative motion. We here have introduced the anti-symmetrization factor defined by $f_{lST}=[1-(-1)^{l+S+T}]/2$. The matrix element of the operator Q between angular-momentum-coupling states becomes

$$\langle \boldsymbol{K}k(l_1S_1)\,J_1M_1T_1T_{z1}|Q|\boldsymbol{K}'k'(l_2S_2)\,J_2M_2T_2T_{z2}\rangle = \delta(\boldsymbol{K}-\boldsymbol{K}')\frac{\delta(k-k')}{k^2}\delta_{S_1S_2}\delta_{T_1T_2}\delta_{T_{z1}T_{z2}}Q(l_1J_1M_1,l_2J_2M_2:S_1T_1kK\theta_K\phi_K), \tag{2.5}$$

where

$$Q(l_1J_1M_1,l_2J_2M_2:STkK\theta_K\phi_K) = f_{l_1ST}f_{l_2ST}\sum_{m_1m_2S_z}\int d\hat{\boldsymbol{k}}\,Y^*_{l_1m_1}(\hat{\boldsymbol{k}})Y_{l_2m_2}(\hat{\boldsymbol{k}})\langle l_1m_1SS_z|J_1M_1\rangle \times\langle l_2m_2SS_z|J_2M_2\rangle\Theta\left(\left|\frac{\boldsymbol{K}}{2}+\boldsymbol{k}\right|-k_{\mathrm{F}}\right)\Theta\left(\left|\frac{\boldsymbol{K}}{2}-\boldsymbol{k}\right|-k_{\mathrm{F}}\right). \tag{2.6}$$

Here θ_K and ϕ_K are the polar angles of $\boldsymbol{K}$. Due to the presence of the step function, the solid angle $\hat{\boldsymbol{k}}$ is restricted in the integration, and therefore l and $\boldsymbol{J}$ are, in general, not conserved in the matrix element of the operator Q, while $\boldsymbol{K}$, k, S, T and T_z are conserved.

If we employ a reference frame, referred to as the K system hereafter, in which $\boldsymbol{K}$ points in the direction of the z axis, the angle between $\boldsymbol{K}$ and $\boldsymbol{k}$ coincides with the

colatitude θ of $\boldsymbol{k}$. In this case the limit on the integration with respect to the angle θ in Eq. (2.6) is given by $-x_0 \leqslant \cos\theta \leqslant x_0$, where

$$x_0 = \begin{cases} 0 & \text{for } k < \sqrt{k_{\rm F}^2 - K^2/4}\,, \\ \dfrac{K^2/4 + k^2 - k_{\rm F}^2}{Kk} & \text{for } \sqrt{k_{\rm F}^2 - K^2/4} < k < k_{\rm F} + K/2, \\ 1 & \text{otherwise.} \end{cases} \tag{2.7}$$

Since the integration with respect to the longitude ϕ of the relative momentum $\boldsymbol{k}$ can be carried out in the K system, the matrix element of the exclusion operator, denoted by Q_0, is written as

$$\begin{aligned} &Q_0(l_1 J_1 M_1, l_2 J_2 M_2 : STkK) \\ &\quad = f_{l_1 ST} f_{l_2 ST} \delta_{M_1 M_2} \sum_L (-1)^{S+M_1} \hat{l}_1 \hat{l}_2 \hat{J}_1 \hat{J}_2 \langle l_1 0 l_2 0 | L 0 \rangle \\ &\qquad \times \langle J_1 - M_1 J_2 M_1 | L 0 \rangle W(l_1 J_1 l_2 J_2 ; SL) \int_0^{x_0} P_L(x)\, dx, \end{aligned} \tag{2.8}$$

where $P_L(x)$ is the Legendre polynomial, and we have used the notation $\hat{l} \equiv \sqrt{2l+1}$. It is clear from the above expression of the operator Q that, in the K system, the projection M is conserved though the magnitude of $\boldsymbol{J}$ is not. It might be useful to show that the matrix element $Q_0(l_1 J_1 M, l_2 J_2 M : STkK)$ satisfies the closure relation

$$\frac{1}{2J_1+1} \sum_M Q_0(l_1 J_1 M, l_2 J_2 M : STkK)\, \delta_{J_1 J_2} = f_{l_1 ST}\, x_0\, \delta_{J_1 J_2} \delta_{l_1 l_2}. \tag{2.9}$$

We next consider the matrix element of the operator Q in an arbitrary reference frame in which the direction of $\boldsymbol{K}$ does not coincide with the z axis. By making rotation of the reference frame through the Euler angles $\alpha = \phi_K, \beta = \theta_K$ and $\gamma = 0$, we obtain a general expression of the matrix element of Q as

$$\begin{aligned} &Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK \theta_K \phi_K) \\ &\quad = \sum_{M'} D^{J_1}_{M_1 M'}(\theta_K, \phi_K, 0)\, D^{J_2 *}_{M_2 M'}(\theta_K, \phi_K, 0)\, Q_0(l_1 J_1 M', l_2 J_2 M' : STkK) \\ &\quad = f_{l_1 ST} f_{l_2 ST} \sum_L (-1)^{S+M_1} \frac{\sqrt{4\pi}\, \hat{l}_1 \hat{l}_2 \hat{J}_1 \hat{J}_2}{\hat{L}} \langle l_1 0 l_2 0 | L 0 \rangle \langle J_1 - M_1 J_2 M_2 | L M \rangle \\ &\qquad \times Y_{LM}(\theta_K, \phi_K) W(l_1 J_1 l_2 J_2 ; SL) \int_0^{x_0} P_L(x)\, dx, \end{aligned} \tag{2.10}$$

where the function $D^J_{MM'}(\alpha, \beta, \gamma)$ is the Wigner D-function [16] of the Euler angles (α, β, γ). In the derivation of Eq. (2.10) we have used the fact that only even integers L are allowed due to the parity conservation. We remark here that the matrix element of the exclusion operator is factorized as

$$\begin{aligned} &Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK \theta_K \phi_K) \\ &\quad = Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK \theta_K \phi_K = 0) \mathrm{e}^{i(M_2 - M_1)\phi_K}. \end{aligned} \tag{2.11}$$

The above expression shows clearly how the matrix element of the operator Q depends on the angle ϕ_K.

By using the recurrence formulae for the Legendre polynomials we obtain an integral formula for an even integer L as

$$\int_0^{x_0} P_L(x)\,dx = \frac{1}{2L+1}\left[P_{L+1}(x_0) - P_{L-1}(x_0)\right]. \tag{2.12}$$

With use of the above relation we may rewrite Eq. (2.10) as

$$\begin{aligned} &Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK\theta_K\phi_K) \\ &\quad = f_{l_1 ST} f_{l_2 ST}\Bigg\{ x_0\,\delta_{l_1 l_2}\delta_{J_1 J_2}\delta_{M_1 M_2} + \sum_{L>0,\,L=\text{even}} (-1)^{S+M_1} \\ &\qquad \times \frac{\sqrt{4\pi}\,\hat{l}_1\hat{l}_2\hat{J}_1\hat{J}_2}{\hat{L}^3}\langle l_1 0 l_2 0|L0\rangle\langle J_1 - M_1 J_2 M_2|LM\rangle \\ &\qquad \times Y_{LM}(\theta_K,\phi_K)\,W(l_1 J_1 l_2 J_2; SL)\left[P_{L+1}(x_0) - P_{L-1}(x_0)\right]\Bigg\}. \end{aligned} \tag{2.13}$$

It might be useful to give another expression of Eq. (2.10) written as

$$\begin{aligned} &Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK\theta_K\phi_K) \\ &\quad = f_{l_1 ST} f_{l_2 ST}\Bigg[x_0\,\delta_{l_1 l_2}\delta_{J_1 J_2}\delta_{M_1 M_2} + \sum_{L>0,\,L=\text{even}} (-1)^{S+M_1} \\ &\qquad \times \frac{\sqrt{4\pi}\,\hat{l}_1\hat{l}_2\hat{J}_1\hat{J}_2}{\hat{L}}\langle l_1 0 l_2 0|L0\rangle\langle J_1 - M_1 J_2 M_2|LM\rangle \\ &\qquad \times Y_{LM}(\theta_K,\phi_K)\,W(l_1 J_1 l_2 J_2; SL)\,\frac{1}{L(L+1)}\left(x_0^2 - 1\right)P'_L(x_0)\Bigg], \end{aligned} \tag{2.14}$$

where $P'_L(x_0)$ is the first derivative of $P_L(x)$ at $x = x_0$. It is easy to see from the above expression of the operator Q that if $x_0 = 1$, the second term on the right-hand side of Eq. (2.14) vanishes. Therefore if $k > k_F + K/2$, in this case $x_0 = 1$ as given in Eq. (2.7), the matrix element of the operator Q conserves l, J and M and becomes unity. We emphasize that Eqs. (2.13) and (2.14) do not include integrals or step functions anymore, and are analytic and general expressions of the matrix element of Q which are valid for any vector $\boldsymbol{K}$.

We discuss here the angle-average approximation for the operator Q, which was first introduced by Brueckner and Gammel [4] and has been adopted in many nuclear matter calculations. The operator Q in the angle-average approximation is defined as an average over the angle of $\boldsymbol{K}$ as

$$\overline{Q}(l_1 J_1 M_1, l_2 J_2 M_2 : STkK) \equiv \frac{1}{4\pi}\int d\hat{\boldsymbol{K}}\,Q(l_1 J_1 M_1, l_2 J_2 M_2 : STkK\theta_K\phi_K). \tag{2.15}$$

In this integration the second term on the right-hand side of Eq. (2.13) or (2.14) vanishes, and we have

$$\overline{Q}(l_1 J_1 M_1, l_2 J_2 M_2 : STkK) = f_{l_1 ST}\, x_0\, \delta_{l_1 l_2}\, \delta_{J_1 J_2}\, \delta_{M_1 M_2}. \tag{2.16}$$

It is obvious that the first term on the right-hand side of Eq. (2.13) or (2.14) gives the angle-averaged Q operator and the second term provides the correction which comes from non-spherical characters of the operator Q.

3. One-body potential and ground-state energy

The G matrix equation in the lowest-order Brueckner theory is given in angular-momentum-coupling states by

$$\begin{aligned}
&\langle k_1 l_1 S J_1 M_1 T | G(\omega, K\theta_K\phi_K) | k_2 l_2 S J_2 M_2 T\rangle \\
&\quad = \langle k_1 l_1 J_1 S T | v | k_2 l_2 J_2 S T\rangle \delta_{J_1 J_2}\delta_{M_1 M_2} + \sum_{l_1' l_2' J_1' J_2' M_1' M_2'} \\
&\qquad \times \int k^2 dk \langle k_1 l_1 J_1 S T | v | k l_1' J_1' S T\rangle \delta_{J_1 J_1'}\delta_{M_1 M_1'} \\
&\qquad \times Q(l_1' J_1' M_1', l_2' J_2' M_2' : STkK\theta_K\phi_K)\, \frac{1}{\omega - T(K,k)} \\
&\qquad \times \langle k l_2' S J_2' M_2' T | G(\omega, K\theta_K\phi_K) | k_2 l_2 S J_2 M_2 T\rangle,
\end{aligned} \tag{3.1}$$

where ω is the starting energy and $T(K,k)$ the kinetic energy defined as

$$T(K,k) = \frac{K^2}{4m} + \frac{k^2}{m} \tag{3.2}$$

with m the nucleon mass. We adopt the conventional QTQ spectra for the intermediate energies in the present work.

The G matrix is generally diagonal in the c.m. momentum $\boldsymbol{K}$, the spin S and the isospin T, but not in the angular momentum $\boldsymbol{l}$ and the coupled angular momentum $\boldsymbol{J}$ of relative states. Corresponding to the factorization of the matrix element of the operator Q as shown in Eq. (2.11), the G matrix is factorized as

$$\begin{aligned}
&\langle k_1 l_1 S J_1 M_1 T | G(\omega, K\theta_K\phi_K) | k_2 l_2 S J_2 M_2 T\rangle \\
&\quad = \langle k_1 l_1 S J_1 M_1 T | G(\omega, K\theta_K\phi_K = 0) | k_2 l_2 S J_2 M_2 T\rangle e^{i(M_2 - M_1)\phi_K}.
\end{aligned} \tag{3.3}$$

This relation expresses explicitly how the G matrix depends on the angle ϕ_K. It is to be noted that the G matrix is not invariant under the rotation about the z axis, but the rotation yields a phase factor as given in Eq. (3.3).

The ground-state energy per nucleon of nuclear matter is given by

$$E/A = \sum_{\lambda} \langle \lambda | t | \lambda\rangle + \frac{1}{2} \sum_{\lambda\mu \leqslant \rho_F} \langle \lambda\mu | G | \lambda\mu\rangle = \frac{3}{5}\left(\frac{\hbar^2}{2m} k_F^2\right) + \frac{3}{2k_F^3}\int_0^{k_F} u(k_\lambda)\, k_\lambda^2 dk_\lambda, \tag{3.4}$$

where t is the one-body kinetic energy, $u(k_\lambda)$ the potential energy of a nucleon in the occupied state $|\lambda\rangle$, and ρ_F the upper most occupied single-particle level (the Fermi

level). Without loss of generality one can choose a reference frame in which the z axis (the quantization axis) coincides with the direction of the momentum $\boldsymbol{k}_\lambda$ as $\boldsymbol{k}_\lambda = (0,0,k_\lambda)$. We call this frame the L system hereafter. The self-consistent potential $u(k_\lambda)$ is written in terms of the G matrix in the L system as

$$u(k_\lambda) = \sum_{\mu \leqslant \rho_F} \langle \lambda\mu|G|\lambda\mu\rangle = \sum_{l_1 J_1 l_2 J_2 S T m_1 m_2 S_z M_1 M_2} \frac{2T+1}{2} \int_0^{k_F} k_\mu^2 dk_\mu \int_{-1}^{1} d\cos\theta_\mu \times \int_0^{2\pi} d\phi_\mu \langle k_{\lambda\mu}(l_1 S) J_1 M_1 T|G(\omega, K\theta_K \phi_K)|k_{\lambda\mu}(l_2 S) J_2 M_2 T\rangle \times \langle l_1 m_1 S S_z|J_1 M_1\rangle \langle l_2 m_2 S S_z|J_2 M_2\rangle Y_{l_1 m_1}(\theta_{\lambda\mu}, \phi_{\lambda\mu}) Y^*_{l_2 m_2}(\theta_{\lambda\mu}, \phi_{\lambda\mu}), \tag{3.5}$$

where ω is the starting energy given by

$$\omega = \langle \lambda|t|\lambda\rangle + u(k_\lambda) + \langle \mu|t|\mu\rangle + u(k_\mu). \tag{3.6}$$

Here the angles (θ_μ, ϕ_μ) and $(\theta_{\lambda\mu}, \phi_{\lambda\mu})$ are the polar angles of $\boldsymbol{k}_\mu$ and $\boldsymbol{k}_{\lambda\mu}$ in the L system, respectively, where $\boldsymbol{k}_{\lambda\mu}$ is the relative momentum defined by $\boldsymbol{k}_{\lambda\mu} = (\boldsymbol{k}_\lambda - \boldsymbol{k}_\mu)/2$.

The integration in Eq. (3.5) is much simplified if we use the G matrix in the K system in which $\phi_K = \theta_K = 0$. Let $\langle k_{\lambda\mu}(l_1 S) J_1 M T|G_0(\omega, K)|k_{\lambda\mu}(l_2 S) J_2 M T\rangle$ be the matrix element of the G matrix in the K system. Rotating the reference frame through the Euler angles $(\alpha = \phi_K, \beta = \theta_K, \gamma = 0)$, the G matrix in the L system is related to that in the K system as

$$\langle k_{\lambda\mu}(l_1 S) J_1 M_1 T|G(\omega, K\theta_k \phi_K)|k_{\lambda\mu}(l_2 S) J_2 M_2 T\rangle = \sum_M D^{J_1}_{M_1 M}(\phi_K, \theta_K, 0) D^{J_2 *}_{M_2 M}(\phi_K, \theta_K, 0) \times \langle k_{\lambda\mu}(l_1 S) J_1 M T|G_0(\omega, K)|k_{\lambda\mu}(l_2 S) J_2 M T\rangle. \tag{3.7}$$

Substituting Eq. (3.7) into (3.5) and carrying out the integration with respect to the angle ϕ_μ we have

$$u(k_\lambda) = \sum_{l_1 J_1 l_2 J_2 M S T} \frac{2\pi(2T+1)}{2} \int_0^{k_F} k_\mu^2 dk_\mu \int_{-1}^{1} d\cos\theta_\mu \times \langle k_{\lambda\mu}(l_1 S) J_1 M T|G_0(\omega, K)|k_{\lambda\mu}(l_2 S) J_2 M T\rangle \times F\big(k_\lambda k_{\lambda\mu} K(l_1 J_1)(l_2 J_2) S T M\big), \tag{3.8}$$

where we have used the facts that $\phi_K = \phi_\mu$ and $\phi_{\lambda\mu} = \phi_\mu + \pi$ in the K system. The coefficient F in Eq. (3.8) is given by

$$F\big(k_\lambda k_{\lambda\mu} K(l_1 J_1)(l_2 J_2) S T M\big) = \sum_{m_1 m_2 S_z M_1 M_2} (-1)^{m_1 - m_2} D^{J_1}_{M_1 M}(0, \theta_K, 0) D^{J_2}_{M_2 M}(0, \theta_K, 0) \langle l_1 m_1 S S_Z|J_1 M_1\rangle \times \langle l_2 m_2 S S_Z|J_2 M_2\rangle Y_{l_1 m_1}(\theta_{\lambda\mu}, 0) Y^*_{l_2 m_2}(\theta_{\lambda\mu}, 0). \tag{3.9}$$

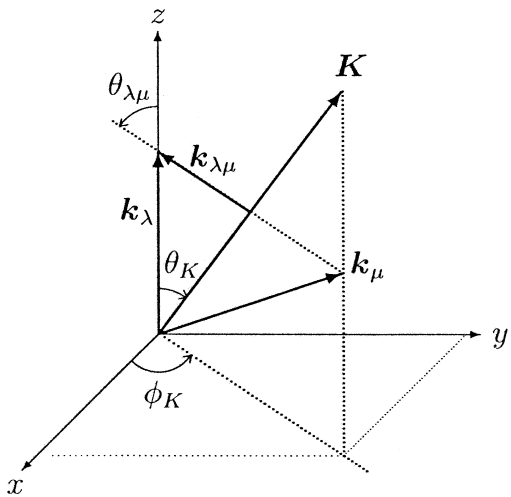

Fig. 1. The relation among relevant momentum vectors.

Using some formulae of the Wigner D-function, the coefficient F becomes

$$F\big(k_\lambda k_{\lambda\mu} K(l_1 J_1)(l_2 J_2) STM\big)$$
$$= \sum_L \frac{1}{4\pi}(-1)^{S+M} \hat{l}_1 \hat{l}_2 \hat{J}_1 \hat{J}_2 W(l_1 J_1 l_2 J_2; SL) \langle J_1 - M J_2 M | L 0\rangle$$
$$\times \langle l_1 0 l_2 0 | L 0\rangle P_L\big(\cos\big(\theta_K + \theta_{\lambda\mu}\big)\big). \tag{3.10}$$

As shown in Fig. 1, $\theta_K + \theta_{\lambda\mu}$ is the angle between the relative momentum $\boldsymbol{k}_{\lambda\mu}$ and the c.m. momentum $\boldsymbol{K}$, which satisfies

$$\cos\big(\theta_K + \theta_{\lambda\mu}\big) = \frac{k_\lambda^2 - k_{\lambda\mu}^2 - K^2/4}{k_{\lambda\mu} K}. \tag{3.11}$$

It is clear from Eq. (3.8) that the single-particle potential $u(k_\lambda)$ is determined by the G matrix in the K system and the F coefficient which is a function of the angle $\theta_K + \theta_{\lambda\mu}$ between $\boldsymbol{k}$ and $\boldsymbol{K}$.

In the angle-average approximation the G matrix in the K system is independent of the quantum number M. Using the following closure relation of the coefficient F

$$\sum_M F\big(k_\lambda k_{\lambda\mu} K(l_1 J_1)(l_2 J_2) STM\big)\delta_{J_1 J_2} = \frac{2J_1 + 1}{4\pi}\delta_{J_1 J_2}\delta_{l_1 l_2}, \tag{3.12}$$

the single-particle potential $u(k_\lambda)$ with the angle-averaged Q operator becomes

$$u(k_\lambda) = \sum_{lJST} \frac{(2T+1)(2J+1)}{4} \int_0^{k_F} k_\mu^2 dk_\mu \int_{-1}^{1} d\cos\theta_\mu$$
$$\times \langle k_{\lambda\mu}(lS) JT | G_0(\omega, K) | k_{\lambda\mu}(lS) JT\rangle. \tag{3.13}$$

This expression of $u(k_\lambda)$ agrees with the usual formula in the angle-average approximation for the operator Q.

4. Numerical calculation

In order to examine the effect of the exact treatment of the Pauli exclusion operator we performed a numerical calculation of the ground-state properties of nuclear matter by adopting the Bonn B and C *NN* potentials [15]. We solved self-consistently the coupled equations (3.1) for the G matrix in the K system where the c.m. momentum $\boldsymbol{K}$ points in the z direction. In the calculation we took into consideration rigorously the contributions of the partial waves of $J \leqslant 6$. Other higher partial waves were taken up to $J = 18$ in the Born approximation. We checked the stability of the calculated result with respect to the number of mesh points in numerical integration. Furthermore we confirmed that the same result was obtained within numerical errors by using two computer codes made independently.

The calculated results of the binding energies per nucleon are presented in Table 1 and shown in Figs. 2 and 3, respectively. From Table 1 it is seen, as a common characteristic of the results for two *NN* potentials, that the exact treatment of the operator Q brings about attractive contributions to the binding energy per nucleon at any nuclear densities, compared with the result in the standard angle-average approximation. Furthermore Table 1 shows that more attractive contributions are obtained at higher densities. It is shown, however, in Figs. 2 and 3, that the saturation densities do not change substantially in the exact treatment of the operator Q from the results in the angle-average approximation.

These observations in the present work are basically the same as those obtained in a very recent study by Schiller, Müther and Czerski [14]. Their results [14] show that the exact treatment of the operator Q brings about, for any *NN* potentials, attractive contributions at any nuclear matter densities. The saturation curves, binding energies versus densities, given by them for the Bonn B and C potentials are almost the same as those in Figs. 2 and 3.

In order to analyse the features of our calculated results in more detail, we introduce an approximate decomposition of partial waves in the exact treatment of the operator Q.

Table 1
Calculated results of the binding energy per nucleon with the exact and angle-averaged Q operators for the Bonn B and C *NN* potentials [15]. The energies are in MeV

k_F [fm^{-1}]	1.2	1.3	1.4	1.5	1.6	1.7	1.8
Bonn B *NN* potential							
Exact	−10.28	−11.72	−12.98	−13.95	−14.47	−14.42	−13.61
Average	−10.18	−11.59	−12.82	−13.75	−14.25	−14.16	−13.32
Difference	−0.10	−0.13	−0.16	−0.20	−0.22	−0.26	−0.29
Bonn C *NN* potential							
Exact	−9.62	−10.82	−11.78	−12.37	−12.46	−11.90	−10.53
Average	−9.52	−10.69	−11.62	−12.18	−12.24	−11.65	−10.24
Difference	−0.10	−0.13	−0.16	−0.19	−0.22	−0.25	−0.29

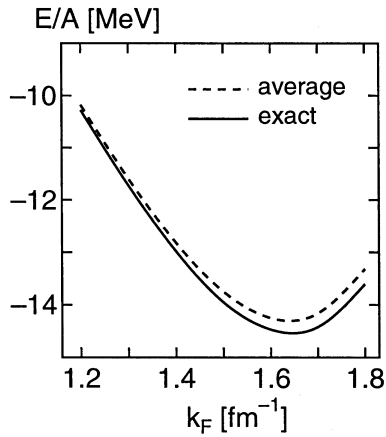

Fig. 2. Calculated binding energies per nucleon as a function of the Fermi momentum k_F for the Bonn B potential.

Since the G matrix in Eq. (3.8) in the K system, $G_0(\omega,K)$, is not diagonal in l and J, as was discussed in Section 3, the partial wave decomposition is not possible in a usual sense in the exact treatment of the operator Q. However, even in this case, we may decompose the contributions to the total potential energy per nucleon into two groups of terms which are diagonal and non-diagonal in l and J. We expect that the partial wave decomposition can be physically meaningful when the magnitudes of the contributions of the lJ-non-diagonal terms are sufficiently small in comparison with the ones of the lJ-diagonal terms. We call the diagonal term in l and J the partial wave contribution of the channel (S,T,l,J). The summation over M is taken in each of the partial wave contributions.

We show in Table 2 the partial wave contributions of the channels with lower l and J, the sum of the lJ-non-diagonal terms and the higher partial wave contributions which

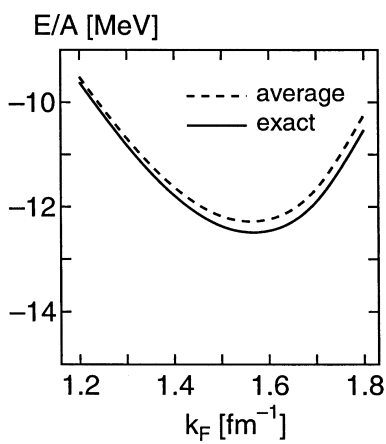

Fig. 3. Calculated binding energies per nucleon as a function of the Fermi momentum k_F for the Bonn C potential.

Table 2
Partial wave contributions to the binding energy per nucleon with the exact and angle-averaged Q operators for the Bonn B *NN* potential [15]. The row of ''non-diag'' means the sum of the lJ-non-diagonal terms. The row of ''higher'' is the sum of contributions of higher partial waves of $7 \leqslant J \leqslant 18$ treated in the Born approximation. The energies are in MeV

k_F[fm^{-1}]	1.2	1.2	1.5	1.5	1.8	1.8
Channel	Exact	Average	Exact	Average	Exact	Average
$^1S_0$	−13.018	−13.019	−20.112	−20.117	−26.749	−26.760
$^1D_2$	−1.419	−1.419	−3.673	−3.671	−7.741	−7.737
$^1G_4$	−0.227	−0.227	−0.708	−0.708	−1.674	−1.674
$^1I_6$	−0.049	−0.049	−0.195	−0.195	−0.540	−0.540
$^3S_1$	−15.638	−15.637	−22.195	−22.210	−28.058	−28.109
$^3D_1$	0.909	0.910	2.300	2.301	4.605	4.607
$^3D_2$	−2.393	−2.393	−5.933	−5.930	−11.813	−11.808
$^3D_3$	0.145	0.147	0.426	0.430	0.920	0.932
$^3G_3$	0.105	0.105	0.365	0.365	0.931	0.931
$^3G_4$	−0.369	−0.369	−1.212	−1.212	−2.957	−2.957
$^3G_5$	0.038	0.038	0.150	0.150	0.418	0.419
$^3I_5$	0.016	0.016	0.072	0.072	0.222	0.222
$^3I_6$	−0.071	−0.071	−0.301	−0.300	−0.873	−0.873
$^1P_1$	2.982	2.989	6.443	6.462	11.944	11.987
$^1F_3$	0.492	0.493	1.320	1.320	2.783	2.784
$^1H_5$	0.104	0.104	0.363	0.363	0.911	0.911
$^3P_0$	−2.552	−2.552	−4.535	−4.536	−6.216	−6.218
$^3P_1$	6.690	6.693	14.980	14.988	28.680	28.702
$^3P_2$	−4.423	−4.415	−10.859	−10.839	−21.637	−21.598
$^3F_2$	−0.305	−0.305	−0.908	−0.908	−2.015	−2.014
$^3F_3$	0.876	0.876	2.486	2.486	5.458	5.458
$^3F_4$	−0.148	−0.148	−0.579	−0.578	−1.661	−1.660
$^3H_4$	−0.040	−0.040	−0.160	−0.160	−0.457	−0.457
$^3H_5$	0.159	0.159	0.590	0.590	1.564	1.564
$^3H_6$	−0.016	−0.016	−0.077	−0.077	−0.250	−0.250
$^3J_6$	−0.007	−0.007	−0.034	−0.034	−0.115	−0.115
Higher	0.044	0.044	0.204	0.204	0.624	0.624
Non-diag	−0.083	0.0	−0.156	0.0	−0.226	0.0
Total	−28.197	−28.094	−41.940	−41.747	−53.921	−53.630

are treated in the Born approximation. The contributions of the lJ-non-diagonal terms are shown to be indeed small in the numerical calculation. The net contributions of the terms non-diagonal in l and J are estimated to be at most 0.4% of the total potential energy. Therefore we may say that the partial wave analysis could be meaningful even in the exact treatment of the operator Q.

We observe from Table 2 that about sixty percent of the difference between the exact and approximate treatments of the operator Q comes from the lJ-non-diagonal terms and the remainder does from the lJ-diagonal terms. We also note that the P waves give the most important and attractive contributions. The S waves give the secondary important and repulsive contributions to the difference. The difference becomes, in general, smaller as l (or J) increases. The reason is that the Born approximation works well in higher partial waves and the G matrix approaches to the bare *NN* potential, which is independent of the operator Q.

Table 3
Single-particle potential energies for various k_λ values at $k_F = 1.40[\mathrm{fm}^{-1}]$ in the exact and angle-average treatments of the operator Q for the Bonn B *NN* potential [15]. The other notations are the same as in Table 1

	$u(k_\lambda)$		
$k_\lambda[\mathrm{fm}^{-1}]$	Exact	Average	Difference
0.047	−87.96	−88.54	0.58
0.237	−87.33	−87.84	0.51
0.533	−84.69	−84.90	0.21
0.867	−79.33	−79.12	−0.21
1.163	−72.69	−72.22	−0.47
1.353	−67.71	−67.22	−0.49

Next we show in Table 3 the single-particle potentials in the exact and angle-average treatments of the operator Q and their differences for the values of k_λ of the mesh points in the Gaussian integration. The differences of the single-particle potential energies in the exact treatment from those in the angle-average approximation are found to be rather small for all the k_λ values. It is remarkable to see that the angle-average approximation leads to an overestimation of the single-particle potential energy for smaller values of k_λ and to an underestimation for larger values of k_λ. This feature is observed at any nuclear matter densities both for the Bonn B and C potentials. We display in Fig. 4 the k_λ dependence of the differences between two $u(k_\lambda)$'s in the exact and angle-average treatments of the operator Q at three nuclear matter densities. As shown in Table 3 and Fig. 4, the differences change the sign at about $k_\lambda = k_F/2$. This fact implies that the angle-average approximation gives the correct result at around $k_\lambda = k_F/2$. Considering larger phase volumes for larger values of k_λ, it is understandable that the angle-average approximation tends to underestimate the binding energy per nucleon.

We may conclude from the present study that the non-spherical character of the operator Q causes a non-negligible and attractive effect on the nuclear matter binding energy per nucleon, which has been disregarded in the standard angle-average approximation for Q. We believe that the analytic expression given explicitly in this paper for the operator Q in the G matrix is useful in making a precise numerical calculation of nuclear matter.

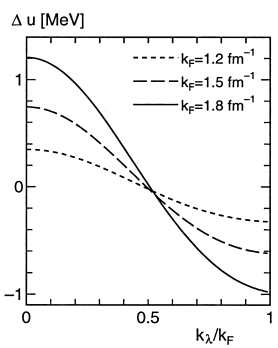

Fig. 4. Differences of $u(k_\lambda)$'s in the exact and angle-average treatments of the operator Q as a function of k_λ / k_F at various nuclear matter densities for the Bonn B potential. The quantity Δu is defined as the difference of $u(k_\lambda)$ with the exact Q from that with the angle-averaged Q.

5. Concluding remarks

We derived an exact and analytic expression of the matrix element of the Pauli exclusion operator in nuclear matter, and gave its relation to that in the angle-average approximation. Furthermore we discussed the breaking of relevant symmetries in the matrix element of the exclusion operator. We presented the rigorous expressions of the single-particle potential energies and the ground-state energy in a form that would be suitable for a precise numerical calculation in the exact treatment of the operator Q.

In order to examine the effect of the exact treatment of the operator Q and assess the reliability of the angle-average approximation for the operator Q we performed numerical calculations of the ground-state properties of nuclear matter for various k_F values by employing the Bonn B and C *NN* potentials. We found that the exact treatment of the operator Q brought about non-negligible and attractive contributions to the nuclear matter binding energy per nucleon. Our calculations also clarified the degree in which the angle-average approximation is reliable quantitatively.

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