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# Second quantized reduced Bloch equations and the exact solutions for pairing Hamiltonian

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## Abstract

In this article, we present a set of hierarchy Bloch equations for the reduced density operators in either canonical or grand canonical ensembles in the occupation number representation. They provide a convenient tool for studying the equilibrium quantum statistical mechanics for some model systems. As an example of their applications, we solve the equations for the model system with a pairing Hamiltonian. With the aid of its symplectic group symmetry, we obtain the statistical reduced density matrices with different orders. As a special instance for the solutions, we also get the reduced density matrices of the ground state for a superconductor.

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## 1. Introduction

The language of the second quantization is a convenient and ubiquitous tool for studying the quantum many-body systems in modern physics. The quantum statistics

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of the identical many particles is automatically satisfied by the commutation relations of the creation or annihilation operators, and the complicated mathematical manipulation with wavefunctions such as Slater determinants and with matrix elements of operators is significantly simplified. It is no surprise that a familiarity with the related knowledge of the occupation number representation is a must for a serious theorist [1].

In a recent paper, we have developed an equation of motion approach for a direct determination of the reduced density matrices for the statistical ensembles under the framework of equilibrium quantum statistical mechanics [2–5]. We have derived the hierarchy Bloch equations which provide the laws according to which the reduced statistical density operators vary in temperature. We also take the orbital approximation, and solve the equations for the identical fermion systems with two-body interaction in a grand canonical ensemble. We have gained significant new physical insights. We find that the usual Fermi–Dirac statistics for the free fermion gas holds also for the interacting fermions, and that the usual Hartree–Fock equation at zero-temperature can be extended to the case of any finite temperature. The mean force field that every orbital or particle is subject to will be from the contribution of both coherent and incoherent superpositions of the wavefunctions of other orbitals or particles, and is therefore temperature-dependent [6–12]. This opens a way for investigating the interplay between the microscopic structure and macroscopic thermodynamic quantities for molecules and solids [6–13]. In addition, the Fermi–Dirac distribution for interacting particles demonstrates that there exists an effective one-particle description for the interacting many-body system [3,14,15].

In the current paper, we begin the presentation of the scheme for an *exact* solution of the reduced Bloch equations which will be developed in a second quantized form. In quantum many-body theory, the systems are often represented by the model Hamiltonians in an occupation number representation. We study the pairing Hamiltonian, which is a useful model for the study of nuclear structure [16–18], microscopic state of superconductors [19,20], and electronic structure of molecules [21,22]. As we have argued in paper [23], however, the pairing of electrons is a most commonly occurring phenomenon in the formation of the chemical bonds, but not their physical nature. It is a consequence of energy scale principle and Pauli exclusion principle.

We organize this paper as follows. In the next section, starting from the Bloch equation, we deduce a set of hierarchy equations in the occupation number representation for the reduced density operators in the canonical ensemble. The derivation is based on the second quantized form of the contraction operator which is presented in Appendix A. We also extend it to the case of a grand canonical ensemble. In Section 3, we first briefly review the symplectic group symmetry of the pairing Hamiltonian and present the second quantized form of its eigenvectors characterized by the particle number, the weight and the seniority number. Then using the symmetric conditions among  $D^1$ ,  $D^2$  and  $D^3$ , we solve the reduced Bloch equations in the canonical ensemble for the pairing Hamiltonian and obtain its canonical reduced density matrices with different orders. As a special situation, they yield the reduced density matrices of the ground state for superconductors. We conclude our discussion in Section 4.

## 2. Reduced Bloch equations in the occupation number representation

We consider an identical  $N$ -fermion system with a two-body interaction. Its Hamiltonian has the following form:

$$H = \sum_{i=1}^N h(i) + \sum_{i<j}^N v(i, j), \quad (1)$$

where  $h(i)$  and  $v(i, j)$  are one- and two-particle operators, respectively. Assume a generic and complete set of single-particle states  $\{|i\rangle\}$ , which form a single-particle Hilbert space  $V$ . For each  $|i\rangle$ , the corresponding creation or annihilation operators are defined as

$$|i\rangle = a_i^\dagger |0\rangle, \quad a_i |j\rangle = \delta_{ij} |0\rangle. \quad (2)$$

They satisfy the anticommutation relations

$$\begin{aligned} \{a_i, a_j^\dagger\} &= \delta_{ij}, \\ \{a_i, a_j\} &= \{a_i^\dagger, a_j^\dagger\} = 0. \end{aligned} \quad (3)$$

Define an  $N$ -fold antisymmetrized direct product space of the single-particle Hilbert space  $V$  as

$$V^{N\wedge} = V_1 \wedge V_2 \wedge \cdots \wedge V_N. \quad (4)$$

The Fock space  $F$  can be written as

$$F = \sum_{N=0}^{\infty} \oplus V^{N\wedge} \quad (5)$$

and any operator  $T$  on  $F$  can be expressed as the direct sum of the  $N$ -fold tensor  $T^N$

$$T = \sum_{N=0}^{\infty} \oplus T^N. \quad (6)$$

The contraction operator  $L_N^p$ , which defines the  $p$ th-order reduced density matrix as follows [2,24,25]:

$$D^p = L_N^p(D^N), \quad (7)$$

is a superoperator acting on the  $N$ th-order density matrix  $D^N$  which can be regarded as an  $N$ th-order irreducible tensor. It is the extension of usual integral operation in the coordinate space but is independent of any representations. It has following second quantized form:

$$L_N^p(T^N) = \frac{p!}{N!} (\mathcal{A}_-)^{N-p} (T^N), \quad (8)$$

where  $\mathcal{A}_-$  is defined by

$$A_-(T^N) = \sum_i a_i(T^N) a_i^\dagger. \quad (9)$$

See Appendix A for a more detailed explanation.

Equipped with these definitions as well as the Hamiltonian in the occupation number representation

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \quad (10)$$

where  $h_{ij} = \langle i|h|j \rangle$  and  $v_{ijkl} = \langle ij|v|kl \rangle$ , we can now deduce the second quantized reduced Bloch equations [26–33]. For the canonical ensemble, the Bloch equation is [2,4,5]

$$-\frac{\partial}{\partial \beta} D^N = \left( \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \right) D^N, \quad (11)$$

where the  $\beta$  is the inverse of the product of the Boltzmann constant  $k_B$  and the absolute temperature  $T$ . Applying on both sides of above equation with the operator  $L_N^p$  gives

$$-\frac{\partial}{\partial \beta} D^p = \sum_{ij} h_{ij} L_N^p(a_i^\dagger a_j D^N) + \frac{1}{2} \sum_{ijkl} v_{ijkl} L_N^p(a_i^\dagger a_j^\dagger a_l a_k D^N). \quad (12)$$

The evaluation of the first term of the right-hand side of the Eq. (12) results in

$$\frac{N!}{p!} L_N^p(a_i^\dagger a_j D^N) = (N-p) \frac{N!}{(p+1)!} a_j L_N^{p+1}(D^N) a_i^\dagger + \frac{N!}{p!} a_i^\dagger a_j L_N^p(D^N) \quad (13)$$

and the calculation of the second term yields

$$\begin{aligned} \frac{N!}{p!} L_N^p(a_i^\dagger a_j^\dagger a_l a_k D^N) &= \frac{(N-p)(N-p-1)N!}{(p+2)!} a_l a_k L_N^{p+2}(D^N) a_i^\dagger a_j^\dagger \\ &+ \frac{(N-p)N!}{(p+1)!} \{a_j^\dagger a_l a_k L_N^{p+1}(D^N) a_i^\dagger - a_i^\dagger a_l a_k L_N^{p+1}(D^N) a_j^\dagger\} \\ &+ \frac{N!}{p!} a_i^\dagger a_j^\dagger a_l a_k L_N^p(D^N). \end{aligned} \quad (14)$$

Define

$$\hat{v}_{ijkl} = \frac{1}{2} (v_{ijkl} - v_{jikl}), \quad (15)$$

then the set of reduced Bloch equations for the canonical ensemble in the occupation number representation is

$$\begin{aligned} -\frac{\partial}{\partial \beta} D^p &= HD^p + \frac{N-p}{p+1} \left( \sum_{ij} h_{ij} a_j D^{p+1} a_i^\dagger + \sum_{ijkl} \hat{v}_{ijkl} a_j^\dagger a_l a_k D^{p+1} a_i^\dagger \right) \\ &+ \frac{(N-p)(N-p-1)}{2(p+2)(p+1)} \sum_{ijkl} \hat{v}_{ijkl} a_l a_k D^{p+2} a_i^\dagger a_j^\dagger. \end{aligned} \quad (16)$$

For the grand canonical ensemble, whose  $p$ th-order reduced density matrix is defined by [2]

$$D_G^p = \sum_{N=p}^{\infty} \oplus \binom{N}{p} L_N^p [D^N], \quad (17)$$

similar procedure leads to the following equation:

$$\begin{aligned} -\frac{\partial}{\partial \beta} D_G^p &= \bar{H} D_G^p + \sum_{ij} \bar{h}_{ij} a_j D_G^{p+1} a_i^\dagger + \sum_{ijkl} \hat{v}_{ijkl} a_j^\dagger a_l a_k D_G^{p+1} a_i^\dagger \\ &\quad + \frac{1}{2} \sum_{ijkl} \hat{v}_{ijkl} a_l a_k D_G^{p+2} a_i^\dagger a_j^\dagger, \end{aligned} \quad (18)$$

where

$$\bar{h}_{ij} = h_{ij} - \mu \delta_{ij} \quad (19)$$

and

$$\bar{H} = \sum_{ij} \bar{h}_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k. \quad (20)$$

This is a set of second quantized reduced Bloch equations for the reduced density matrices in the grand canonical ensemble.

### 3. Reduced density matrices with different orders for pairing Hamiltonian

#### 3.1. The pairing Hamiltonian and its eigenvalues and eigenstates

Prior to solve the reduced Bloch equations in the case of the canonical ensemble for a pairing Hamiltonian, we need to review its eigenvalue problem as well as related symmetry properties which is discussed in details in paper [34].

Label a set of  $2\lambda$  spin-orbitals  $|\psi_i\rangle$  ( $\dim V = 2\lambda = r$ ) as

$$1, \dots, i, \dots, \lambda, 1', \dots, i', \dots, \lambda',$$

where  $i' = i + \lambda$ , and  $|i'\rangle$  represents the pairing of a single-particle state  $|i\rangle$ . The pairing Hamiltonian is defined as [34–37]

$$H = \epsilon N - G Q_+ Q_- = \epsilon \sum_{i=1}^r a_i^\dagger a_i - G \sum_{i,j=1}^{\lambda} a_i^\dagger a_{i'}^\dagger a_j a_j, \quad (21)$$

where

$$Q_+ = \sum_{i=1}^{\lambda} b_i^\dagger, \quad b_i^\dagger = a_i^\dagger a_{i'}^\dagger$$

and

$$Q_- = \sum_{i=1}^{\lambda} b_i, \quad b_i = a_{i'} a_i, \quad (22)$$

are called the quasi-spin operators. They are the generators of the Lie algebra for the quasi-spin group  $SU^Q(2)$ . The second term of the Hamiltonian indicates that the interaction is only for the pairing states of the particles, and is therefore called the pairing force. The matrix element of the interaction is represented by a constant  $G$ . When  $G > 0$ , the interaction is repulsive; when  $G < 0$ , the interaction is attractive.

Since the pairing Hamiltonian Eq. (21) exhibits a symplectic symmetry, its  $N$ -particle eigenstates should be the basis vectors of the irreducible representation space of the symplectic group, and can be characterized by its weight [38]. For the symplectic group  $Sp(2\lambda)$  and its corresponding Lie algebra  $C_\lambda$ , the weight is the eigenvalue for the generator

$$S_{ii} = a_i^\dagger a_i - a_i a_i^\dagger, \quad i = 1, 2, \dots, \lambda,$$

which is the difference of occupation numbers between the pairing spin orbitals  $|i\rangle$  and  $|i'\rangle$ , with the value being 1, 0, or  $-1$ . They can be grouped together as a vector

$$(\vec{S}) = (s_1, s_2, \dots, s_\lambda).$$

Furthermore, every irreducible representation can be characterized by the maximal weight. For the symplectic group  $Sp(2\lambda)$ , this maximal weight takes the form of  $(1^v 0^{\lambda-v})$ , where the number  $v$  is called the seniority number and the irreducible representation of the symplectic group can be written as  $\langle 1^v \rangle$ . However, there is a possibility that the same weight might still correspond to the different basis vectors. To completely distinguish all the basis vectors of an irreducible representation space for the symplectic group, we therefore need to classify the  $N$ -particle eigenstates according to the following group chain:

$$Sp(2\lambda) \supset Sp(2\lambda - 2) \supset \dots \supset Sp(2). \quad (23)$$

This means that each basis vector will further be characterized by a group of  $\lambda$  seniority numbers

$$(\vec{V}) = (v_1 \ v_2 \ \dots \ v_\lambda).$$

Thus, the eigenvectors of the pairing Hamiltonian will be completely identified by the particle number  $N$ , the weight  $(\vec{S})$ , and seniority number  $(\vec{V})$ :  $|N, (\vec{S}), (\vec{V})\rangle$ . They belong to the irreducible representation spaces  $\langle 1^{v_1} \rangle, \langle 1^{v_2} \rangle, \dots$ , and  $\langle 1^{v_\lambda} \rangle$  of the group  $Sp(2), Sp(4), \dots$ , and  $Sp(2\lambda)$ , respectively, and satisfy the eigenequation

$$S_{ii}|N, (\vec{S}), (\vec{V})\rangle = s_i|N, (\vec{S}), (\vec{V})\rangle, \quad (s_i = 1, 0, -1). \quad (24)$$

The branching rule of  $V^{N\wedge}$  under the group chain (23) of  $Sp_p(2\lambda)$  is

$$[1^N] \rightarrow \langle 1^N \rangle + \langle 1^{N-2} \rangle + \dots + \langle 1 \rangle \text{ or } \langle 0 \rangle$$

for  $N \leq \lambda$ , or

$$[1^N] \rightarrow \langle 1^{2\lambda-N} \rangle + \langle 1^{2\lambda-N-2} \rangle + \dots + \langle 1 \rangle \text{ or } \langle 0 \rangle \quad (25)$$

for  $N > \lambda$ . The dimension of the irreducible space  $\langle 1^v \rangle$  is given by

$$\dim\langle 1^v \rangle = \binom{2\lambda}{v} - \binom{2\lambda}{v-2}. \quad (26)$$

The analytical expression for the basis vectors can be constructed as the following form [34]:

$$|N, (\vec{S}), (\vec{V})\rangle = |N, (1^v), W\rangle = \sqrt{\frac{(\lambda - v - m)!}{m!(\lambda - v)!}} Q_+^m g_{k_1}^\dagger \cdots g_{k_y}^\dagger a_{j_1}^\dagger \cdots a_{j_x}^\dagger |0\rangle, \quad (27)$$

where

$$g_k^\dagger = \frac{1}{\sqrt{(k - v_k + 2)(k - v_k + 1)}} \left[ \sum_{i=1}^{k-1} b_i^\dagger - (k - v_k + 1)b_k^\dagger \right] \quad (28)$$

and

$$m = \frac{1}{2}(N - v).$$

In Eq. (27), the  $k_i$  is the positive number which gives the difference of two consecutive seniority numbers in the  $(\vec{V})$  which is two:  $v_k - v_{k-1} = 2$ ; the  $j_i$  means the same thing but its value equals one:  $v_{|j|} - v_{|j|-1} = 1$ . The sign of  $j_i$  is decided by the sign of  $s_{|j|}$ : if  $s_{|j|} = 1, j > 0$ ; while if  $s_{|j|} = -1, j < 0$ . In other words,  $\pm k_1, \dots, \pm k_y$  are the pairing numbers in the corresponding symplectic table  $W$ , while  $j_1, \dots, j_x$  are the unpairing numbers appearing in the table, which captures all the features of the basis vectors (27) classified according to the group chain (23) [34,39,40].

The actions of the quasi-spin operators  $Q_+$  or  $Q_-$  on the eigenvectors are

$$Q_+ |N, (\vec{S}), (\vec{V})\rangle = \frac{1}{2} \sqrt{(N - v + 2)(r - N - v)} |N + 2, (\vec{S}), (\vec{V})\rangle, \quad (29)$$

or

$$Q_- |N, (\vec{S}), (\vec{V})\rangle = \frac{1}{2} \sqrt{(N - v)(r - N - v + 2)} |N - 2, (\vec{S}), (\vec{V})\rangle, \quad (30)$$

respectively. Therefore, we can get the analytic expression for the energy eigenvalue as follows:

$$E(v) = N\epsilon - \frac{G}{4}(N - v)(r - N - v + 2). \quad (31)$$

### 3.2. The exact solutions of reduced Bloch equation

We are now in a position to solve the reduced Bloch Eq. (16) for the pairing Hamiltonian (21). For the case of  $p = 1$ , the set of hierarchy equations can be written as

$$\begin{aligned} -\frac{\partial}{\partial \beta} D^1 &= N\epsilon D^1 - \frac{1}{2}(N - 1)G \sum_i a_r^\dagger Q_- D^2 a_i^\dagger + \frac{1}{2}(N - 1)G \sum_i a_i^\dagger Q_- D^2 a_r^\dagger \\ &\quad - \frac{(N - 1)(N - 2)}{6} G Q_- D^3 Q_+. \end{aligned} \quad (32)$$

Since the pairing Hamiltonian is invariant under the symplectic group  $Sp(2\lambda)$ , the density matrix describing the states of the system can be characterized by its irreducible representations as follows:

$$D^N(\beta) = \sum_{\nu} e^{-\beta E(\nu)} \bar{D}^N(\nu), \tag{33}$$

where

$$\bar{D}^N(\nu) \equiv \frac{1}{\dim\langle 1^{\nu} \rangle} \sum_{W \in \langle 1^{\nu} \rangle} |N, \langle 1^{\nu} \rangle, W\rangle \langle N, \langle 1^{\nu} \rangle, W|, \tag{34}$$

is the density matrix associated with the irreducible representation  $1^{(\nu)}$  or subgroup  $Sp(2\nu)$  and is normalized

$$\text{Tr} \bar{D}^N(\nu) = 1 \quad (\nu = N, N - 2, \dots, 1 \text{ or } 0). \tag{35}$$

In addition

$$\sum_{\nu} e^{-\beta E(\nu)} = Z(\beta, V, N). \tag{36}$$

For the same reason, the  $p$ th-order reduced density matrix of  $N$ th-order density matrix can be written as

$$D^p(\beta) = \sum_{\nu, \nu'} \omega_p(\nu, \nu', \beta) \bar{D}^p(\nu'), \tag{37}$$

where

$$\bar{D}^p(\nu') \equiv \sum_{W \in \langle 1^{\nu'} \rangle} |p, \langle 1^{\nu'} \rangle, W\rangle \langle p, \langle 1^{\nu'} \rangle, W| \quad (\nu' = p, p - 2, \dots, 1 \text{ or } 0) \tag{38}$$

and

$$\text{Tr} D^p(\beta) = Z(\beta, V, N). \tag{39}$$

The thermal probability coefficients  $\omega_p(\nu, \nu', \beta)$  are to be decided.

According to the branching rule (25) and dimension formula (26), the one-particle Hilbert space  $V$  (denoted as  $\langle 1 \rangle$ ) is irreducible and its dimension is  $r$ . Thus

$$D^1(\beta) = \sum_{\nu} \omega_1(\nu, 1, \beta) \bar{D}^1(1). \tag{40}$$

The two-particle Hilbert Space  $V^{2\wedge}$  comprises two irreducible subspaces  $\langle 0 \rangle$  and  $\langle 1^2 \rangle$  of  $Sp(2\lambda)$ . Their dimensions are 1 and  $\binom{r}{2} - 1$ , respectively. Therefore

$$D^2(\beta) = \sum_{\nu} \omega_2(\nu, 0, \beta) \bar{D}^2(0) + \sum_{\nu} \omega_2(\nu, 2, \beta) \bar{D}^2(2). \tag{41}$$

The three-particle Hilbert space  $V^{3\wedge}$  also includes two irreducible subspaces  $\langle 1 \rangle$  and  $\langle 1^3 \rangle$  of  $Sp(2\lambda)$  with dimensions being  $r$  and  $\binom{r}{3} - \binom{r}{1}$ , respectively. Thus

$$D^3(\beta) = \sum_{\nu} \omega_3(\nu, 1, \beta) \bar{D}^3(1) + \sum_{\nu} \omega_3(\nu, 3, \beta) \bar{D}^3(3). \tag{42}$$



The substitution of the expressions (40)–(42) into Eq. (32) then leads to an equation that the above five coefficients satisfy. Together with three trace conditions (39) of  $D^1$ ,  $D^2$ , and  $D^3$  as well as the  $N$ -representability conditions among  $D^1$ ,  $D^2$ , and  $D^3$  as shown below

$$D^2(\beta) = L_3^2[D^3(\beta)] = \sum_v \omega_3(v, 1, \beta)L_3^2[\bar{D}^3(1)] + \sum_v \omega_3(v, 3, \beta)L_3^2[\bar{D}^3(3)] \quad (43)$$

and

$$D^1(\beta) = L_3^1[D^3(\beta)] = \sum_v \omega_3(v, 1, \beta)L_3^1[\bar{D}^3(1)] + \sum_v \omega_3(v, 3, \beta)L_3^1[\bar{D}^3(3)], \quad (44)$$

it seems that we can completely determine the reduced density matrices for the pairing Hamiltonian. However, due to the complexity of the  $N$ -representability, it is often replaced by other conditions. Here, we choose the symmetry conditions among  $D^1$ ,  $D^2$ , and  $D^3$ .

Suppose

$$L_3^2[\bar{D}^3(1)] = a_1\bar{D}^2(0) + b_1\bar{D}^2(2). \quad (45)$$

From the relation

$$Q_+Q_- = \lambda \binom{N}{2} \Gamma_2^N(|g\rangle\langle g|), \quad (46)$$

where

$$|g\rangle = \frac{1}{\sqrt{\lambda}}Q_+|0\rangle, \quad (47)$$

is a geminal, and  $\Gamma_2^N$  is an expansion operator from the second-order tensor to the  $N$ th-order one (see [24,39] or Appendix A), we get

$$a_1 = \text{Tr}[|g\rangle\langle g|L_3^2(\bar{D}^3(1))] = \frac{1}{3}(r-2). \quad (48)$$

But

$$\text{Tr}L_3^2[\bar{D}^3(1)] = a_1 + b_1\frac{1}{2}(r+1)(r-2) = r, \quad (49)$$

we therefore have

$$b_1 = \frac{4}{3(r-2)}. \quad (50)$$

In the same manner, we assume

$$L_3^2[\bar{D}^3(3)] = a_2\bar{D}^2(0) + b_2\bar{D}^2(2) \quad (51)$$

and obtain

$$a_2 = 0, \quad b_2 = \frac{r(r-4)}{3(r-2)}. \quad (52)$$

The insertion of Eqs. (45) and (51) into Eq. (43) yields

$$D^2(\beta) = \sum_{\nu} \omega_3(\nu, 1, \beta) \frac{r-2}{3} \bar{D}^2(0) + \sum_{\nu} \left[ \omega_3(\nu, 1, \beta) \frac{4}{3(r-2)} + \omega_3(\nu, 3, \beta) \frac{r(r-4)}{3(r-2)} \right] \bar{D}^2(2). \quad (53)$$

Similarly

$$\begin{aligned} L_3^1(\bar{D}^3(1)) &= \bar{D}^1(1), \\ L_3^1(\bar{D}^3(3)) &= \frac{1}{6}(r+1)(r-4)\bar{D}^1(1), \end{aligned} \quad (54)$$

and we get the expression for  $D^1(\beta)$

$$D^1(\beta) = \sum_{\nu} \left[ \omega_3(\nu, 1, \beta) + \omega_3(\nu, 3, \beta) \frac{1}{6}(r+1)(r-4) \right] \bar{D}^1(1). \quad (55)$$

Therefore, with the aid of symmetry conditions, we have expressed the thermal probability coefficients of  $D^1(\beta)$  and  $D^2(\beta)$  by those of  $D^3(\beta)$ .

Now we can calculate three terms of the right-hand side of Eq. (32) as follows:

$$\sum_i a_i^\dagger Q_- D^2(\beta) a_i^\dagger = \sum_{\nu} \omega_3(\nu, 1, \beta) \frac{r-2}{3} \sum_{i=1}^{\lambda} |i'\rangle \langle i'|, \quad (56)$$

$$\sum_i a_i^\dagger Q_- D^2(\beta) a_i^\dagger = - \sum_{\nu} \omega_3(\nu, 1, \beta) \frac{r-2}{3} \sum_{i=1}^{\lambda} |i\rangle \langle i|, \quad (57)$$

$$Q_- D^3(\beta) Q_+ = \sum_{\nu} \omega_3(\nu, 1, \beta) \frac{r-2}{2} \sum_{i=1}^r |i\rangle \langle i|. \quad (58)$$

Assume

$$\begin{aligned} \omega_3(\nu, 1, \beta) &= e^{-\beta E(\nu)} \omega_3(\nu, 1), \\ \omega_3(\nu, 3, \beta) &= e^{-\beta E(\nu)} \omega_3(\nu, 3), \end{aligned} \quad (59)$$

as can be seen from Eqs. (33) and (37). Then from the trace condition of  $D^3(\beta)$

$$\begin{aligned} \text{Tr} D^3(\beta) &= \sum_{\nu} \exp(-\beta E(\nu)) \left[ \omega_3(\nu, 1)r + \omega_3(\nu, 3) \frac{r}{6}(r+1)(r-4) \right] \\ &= \sum_{\nu} e^{-\beta E(\nu)}, \end{aligned} \quad (60)$$

we get

$$\omega_3(\nu, 1)r + \omega_3(\nu, 3) \frac{r}{6}(r+1)(r-4) = 1. \quad (61)$$

Furthermore, the substitution of (56)–(58) into Eq. (32) gives

$$\sum_v e^{-\beta E(v)} \left[ -\frac{G}{4}(N-v)(r-N-v+2) + \omega_3(v, 1)G \frac{N(N-1)r(r-2)}{12} \right] = 0. \quad (62)$$

This leads to

$$-\frac{G}{4}(N-v)(r-N-v+2) + \omega_3(v, 1)G \frac{N(N-1)r(r-2)}{12} = 0. \quad (63)$$

Hence

$$\omega_3(v, 1) = \frac{3(N-v)(r-N-v+2)}{N(N-1)r(r-2)} \quad (64)$$

and

$$\omega_3(v, 3) = \frac{6}{r(r-4)(r+1)} \left[ 1 - \frac{3(N-v)(r-N-v+2)}{N(N-1)(r-2)} \right]. \quad (65)$$

Finally, we obtain the first-order, the second-order, and the third-order reduced density matrices of  $N$ -particle systems governed by the pairing Hamiltonian at any finite temperature as shown below:

$$D^1(\beta) = \frac{1}{r} \sum_{i=1}^r |i\rangle\langle i| Z(\beta, V, N), \quad (66)$$

$$\begin{aligned} D^2(\beta) &= \sum_v e^{-\beta E(v)} \frac{(N-v)(r-N-v+2)}{N(N-1)r} \bar{D}^2(0) \\ &+ \sum_v e^{-\beta E(v)} \left\{ \frac{4(N-v)(r-N-v+2)}{N(N-1)r(r-2)^2} + \frac{2}{(r-2)(r+1)} \right. \\ &\times \left. \left[ 1 - \frac{3(N-v)(r-N-v+2)}{N(N-1)(r-2)} \right] \right\} \bar{D}^2(2), \end{aligned} \quad (67)$$

and

$$\begin{aligned} D^3(\beta) &= \sum_v e^{-\beta E(v)} \frac{3(N-v)(r-N-v+2)}{N(N-1)r(r-2)} \bar{D}^3(1) + \sum_v e^{-\beta E(v)} \frac{6}{r(r-4)(r+1)} \\ &\times \left[ 1 - \frac{3(N-v)(r-N-v+2)}{N(N-1)(r-2)} \right] \bar{D}^3(3), \end{aligned} \quad (68)$$

where  $r$  is the dimension of one-particle Hilbert space  $V$ , and  $Z(\beta, V, N)$  is the partition function. The eigenvalue  $E(v)$  is given by Eq. (31), and the reduced density matrix  $\bar{D}(v)$  is defined in Eq. (37). The density matrices shown above decide the microscopic states of the system, from which we can calculate the thermodynamic properties.

#### 4. Conclusions

We have derived the second quantized form of the reduced Bloch equations for both the canonical and grand canonical ensembles. The deduction is based on the occupation number representation of the contraction operator, and results in the sets of hierarchy equations which are in a similar spirit to the ones we described in papers [2,3]. The equations obtained provide a direct route for *exactly* solving the reduced density matrices for the systems represented by the model Hamiltonian in the occupation number representation. They therefore open an avenue for investigating the microscopic structures of these systems and their relations to the equilibrium thermodynamic properties.

As an example for an exact solution of the reduced Bloch equations, we have obtained the reduced density matrices of the pairing Hamiltonian with different orders as shown in Eqs. (66)–(68). One very interesting conclusion we can make is that these reduced density matrices can yield the projection of the ground state of superconductors in the  $N$ -particle space  $V^N$ . This is the case when  $G < 0$  and  $N$  is an even number, and the ground state of the pairing Hamiltonian (21) is an antisymmetrized extreme geminal power (AEGP) function  $|N, (0^2), (0^2)\rangle$ . Therefore, if we choose  $E(0)$  as the energy zero point and let  $v = 0$  and  $\beta \rightarrow \infty$  in Eqs. (66)–(68), we can obtain the reduced density matrices of the ground state for the superconductors as follows:

$$D^1(T=0) = \frac{1}{r} \sum_{i=1}^r |i\rangle\langle i| = \frac{1}{r} I_1,$$

$$D^2(T=0) = \frac{r-N+2}{r(N-1)} \bar{D}^2(0) + \frac{2(N-2)}{r(r-2)(N-1)} \bar{D}^2(2)$$

$$= \frac{r-N}{(r-2)(N-1)} |g\rangle\langle g| + \frac{2r(N-2)}{(r-2)(N-1)} D^1 \wedge D^1,$$

and

$$D^3(T=0) = \frac{3(r-N+2)}{(N-1)r(r-2)} \bar{D}^3(1) + \frac{6(N-4)}{r(r-2)(r-4)(N-1)} \bar{D}^3(3)$$

$$= \frac{9(r-N)}{r(r-2)(r-4)(N-1)} |g\rangle\langle g| \wedge D^1$$

$$+ \frac{6r^2(N-4)}{(r-2)(r-4)(N-1)} D^1 \wedge D^1 \wedge D^1, \quad (69)$$

where  $|g\rangle$  is given by Eq. (47). These results are identical to Coleman's [41].

There are many other interesting physical systems often modelled in an approximate way by the Hamiltonians with a second quantized form such as the Heisenberg model, the Hubbard model, and the Haldane–Shastry model [42–47]. We thereby expect that the ideas and methodologies we have discussed in this paper might be further explored, and that the fundamental equation (16) or (18) we have derived will find wide applications in the study of their microscopic states as well as their interplay with macroscopic thermodynamic properties.

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**Appendix A. Second quantized form of contraction and expansion operators**

Consider an antisymmetrized  $N$ -particle state ket  $|i_1 i_2 \dots i_N\rangle$  composed of the single-particle states defined in Section 2. It is easy to see that the action of an annihilation operator  $a_j$  on this state ket is

$$a_j|i_1 i_2 \dots i_N\rangle = \sum_{k=1}^N (-1)^{N-k} \delta_{ji_k} |i_1 i_2 \dots \hat{i}_k \dots i_N\rangle, \tag{A.1}$$

where the superscript  $\hat{\phantom{x}}$  indicates that the state  $|i_k\rangle$  is destroyed. The conjugate of Eq. (A.1) is

$$\langle i_1 i_2 \dots i_N | a_j^\dagger = \sum_{k=1}^N (-1)^{N-k} \delta_{ji_k} \langle i_1 i_2 \dots \hat{i}_k \dots i_N |. \tag{A.2}$$

The combination of Eqs. (A.1) and (A.2) therefore yields

$$\sum_i a_i |i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N | a_i^\dagger = \sum_{k,k'} (-1)^{k+k'} \delta_{i_k j_{k'}} |i_1 i_2 \dots \hat{i}_k \dots i_N\rangle \langle j_1 j_2 \dots \hat{j}_{k'} \dots j_N|. \tag{A.3}$$

On the other hand, the state ket  $|i_1 i_2 \dots i_N\rangle$  can be expanded as a determinant as follows:

$$|i_1 i_2 \dots i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{k=1}^N (-1)^{k-1} |i_1 i_2 \dots \hat{i}_k \dots i_N\rangle |i_k\rangle_{(N)}. \tag{A.4}$$

Thus, the action of contraction operator  $L_N^{N-1}$  on the basis operator  $|i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N |$  is

$$L_N^{N-1}(|i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N |) = \frac{1}{N} \sum_{k,k'} (-1)^{k+k'} \delta_{i_k j_{k'}} |i_1 i_2 \dots \hat{i}_k \dots i_N\rangle \langle j_1 j_2 \dots \hat{j}_{k'} \dots j_N|. \tag{A.5}$$

The comparison of Eqs. (A.3) and (A.5) leads to

$$L_N^{N-1}(|i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N |) = \frac{1}{N} \sum_i a_i |i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N | a_i^\dagger. \tag{A.6}$$

Furthermore, since any  $N$ th-order tensor operator  $T^N$  can be expressed as a linear combination of the basis operators  $\{|i_1 i_2 \dots i_N\rangle \langle j_1 j_2 \dots j_N | \}$ , we finally get

$$L_N^{N-1}(T^N) = \frac{1}{N} \sum_i a_i(T^N) a_i^\dagger \quad (\text{A.7})$$

$$= \frac{1}{N} A_-(T^N), \quad (\text{A.8})$$

which is the second quantized form for the contraction operator.

The expansion operator  $\Gamma_p^N$  is the reverse operation of the contraction operator  $L_N^p$  and transforms a  $p$ th-order tensor to an  $N$ th-order one ( $p \leq N$ ) [24]

$$\Gamma_p^N(T^p) = A_N[T^p \otimes I^{N-p}]A_N, \quad (\text{A.9})$$

where  $A_N$  is the antisymmetrized operator for  $N$  particles. Since the expansion operator  $\Gamma_p^N$  is the adjoint mapping of the contraction operators  $L_N^p$  [24]

$$\langle \Gamma_p^N(T^p), T^N \rangle = \langle T^p, L_N^p(T^N) \rangle, \quad (\text{A.10})$$

we can also obtain its second quantized form as follows:

$$\Gamma_{N-1}^N(T^{N-1}) = \frac{1}{N} \sum_i a_i^\dagger(T^{N-1}) a_i. \quad (\text{A.11})$$

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