Diagonalization of High-order Second Quantization Form

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ABSTRACT

In this letter, by introducing high order tensor representation, the method to diagonalizing second quantization quadratic form is generalized to any orders operators. By some simple calculation and comparison to classic exact diagonalization, this new technique can be verified since has the same result. Moreover, this procedure could also be applied to some analytical computation, which may give some useful information in many-body interacting systems.

KEYWORDS

Many body operators, second quantization, tensor rank decomposition, Hubbard model, diagonalization.

INTRODUCTION

Generally speaking, when considering many-body systems, the most direct and straight forward method is exact diagonalization. Even it always faces computational difficulty since the dimensions of Hamiltonian increase

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exponentially with number of particles. In many cases, one may use mean-field approximation then the multi-particle operators will become single body one. Bogoliubov [1] illustrated that a bunch of quadratic forms in creation and annihilation operators can be diagonalized, and Xiao [2] showed the necessary conditions and sufficient conditions for diagonalization. Apparently, this method is independent of basis choosing, or in other word, there is already a default chosen basis. However, in case of operators including higher orders terms, people used to create a series of trial basis. Once the unsolved operator acting on the basis, the related matrix is generated. In this letter, as a generalization of second order method, higher-order terms will be treated as higher-order tensors, which are equivalent to higher-degree forms. If we diagonalize the tensor, the operators will be solved, just like the quadratic cases. Finally, some simple examples are showed to check the validity of the new method.

**OPERATOR EXPANSION AND TENSOR REPRESENTATION**

Landau asserted [3] that an operator for a many body system can be expanded by the number of interacting particles:

\[
\hat{F} = \sum_i H_i^{(1)} + \sum_{i<j} F_{ij}^{(2)} + \sum_{i<j<k} F_{ijk}^{(3)} + \cdots
\]

where \(H_i^{(1)}\) is single body operator, such as kinetic energy; \(F_{ij}^{(2)}\), \(F_{ijk}^{(3)}\) are operators involving two body and three body interaction respectively. Usually this equation cannot have terms with orders greater than number of particles, \(N\), in the system.

In second quantization language, the above equation is written as:

\[
\hat{F} = \sum_i F_{ij}^{(1)} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} F_{ijkl}^{(2)} a_i^\dagger a_i^\dagger a_j a_j + \cdots
\]

But more generally, and in practice, we may meet operators beyond this scope, such as BCS mean field Hamiltonian. Thus, we set \(\psi^\dagger = (a_1^\dagger, a_2^\dagger, ..., a_D^\dagger, a_1, ..., a_D)\), the operator \(\hat{F}\) will be in this form:
\[ \hat{P} = \sum_{\alpha} \hat{P}^{(\alpha)} = \hat{P}^{(1)} + \hat{P}^{(2)} + \hat{P}^{(3)} + \ldots \]  

(2)

where \( \hat{P}^{(\alpha)} = \frac{1}{2a} F_{i_1 i_2 \ldots i_{2a}} \psi_{i_1}^{\dagger} \psi_{i_2}^{\dagger} \ldots \psi_{i_{\alpha}}^{\dagger} \psi_{i_{\alpha+1}} \ldots \psi_{i_{2a}} \). For example,

\[ F^{(1)} = \frac{1}{2} F_{ij} \psi_i^{\dagger} \psi_j = \frac{1}{2} A_{ij}^{++} a_i^{\dagger} a_j + \frac{1}{2} A_{ij}^{++} a_i^{\dagger} a_j + \frac{1}{2} A_{ij}^{--} a_i a_j + \frac{1}{2} \xi A_{ij}^{+-} a_i^{\dagger} a_j \]

is the well known quadratic form representing single body operators. Here \( \xi = 1 \) for boson and \( \xi = -1 \) for fermion.

Similarly,

\[ \hat{P}^{(2)} = \frac{1}{4} F_{ijkl} \psi_i^{\dagger} \psi_j^{\dagger} \psi_k \psi_l = \frac{1}{4} (A_{ijkl}^{1122} a_i^{\dagger} a_j^{\dagger} a_k a_l + A_{ijkl}^{1121} a_i^{\dagger} a_j^{\dagger} a_k a_l + A_{ijkl}^{1211} a_i^{\dagger} a_j a_k^{\dagger} a_l + A_{ijkl}^{1222} a_i^{\dagger} a_j a_k^{\dagger} a_l + A_{ijkl}^{2111} a_i a_j^{\dagger} a_k a_l + A_{ijkl}^{2122} a_i a_j^{\dagger} a_k a_l + A_{ijkl}^{2121} a_i a_j a_k^{\dagger} a_l + A_{ijkl}^{2222} a_i a_j a_k a_l) \]

(3)

We use the convention that repeated indices means summation; indices in \( F, \psi \) are 2D dimensional and indices in \( A, a \) are D dimensional.

Note that we use upper indices to represent which block in \( F \) (1 = +, 2 = − when in the first two indices and 1 = −, 2 = + when in the last two indices. \( A_{ijkl}^{1111} = A_{ijkl}^{++--} \)) and the lower indices are the real indices in block tensors.

It is not hard to prove that tensor \( F_{ijkl} \) must satisfy these properties:

i. \( F_{ijkl} = (F_{lkji})^\ast \) Hermiticity.

A direct result: \( A_{ijkl}^{\alpha\beta\gamma\delta} = (A_{lkji}^{\alpha\beta\gamma\delta})^\ast \) and \( A_{ijkl}^{\delta\gamma\beta\alpha} = (A_{lijk}^{\delta\gamma\beta\alpha})^\ast \). where \( \alpha \neq \delta \) and \( \beta \neq \gamma \);

ii. \( F_{ijkl} = (F_{lkji})^\ast \) Internal symmetry for each particle.

\( A_{ijkl}^{\alpha\beta\gamma\delta} = (A_{lkji}^{\alpha\beta\gamma\delta})^\ast \) and \( A_{ijkl}^{\alpha\beta\gamma\delta} = \xi A_{lkji}^{\delta\gamma\beta\alpha} \) when \( \alpha \neq \delta \), \( A_{ijkl}^{\alpha\beta\gamma\delta} = \xi A_{ijkl}^{\delta\gamma\beta\alpha} \) when \( \beta \neq \gamma \);
Since the difficulty in reading a high order tensor, we prefer to write it in matrix form. Combine the indices $ij$ and $lk$, or in Wolfram language, Flatten[F,{1,2},{4,3}]. Four-order tensor $F_{ijkl}$ in block matrix form is:

$$F^{(2)} = \begin{pmatrix}
A_{1111}^{11} & A_{1121}^{12} & A_{1112}^{12} & A_{1122}^{12} \\
A_{1211}^{12} & A_{1221}^{12} & A_{1212}^{12} & A_{1222}^{12} \\
A_{2111}^{21} & A_{2121}^{21} & A_{2112}^{21} & A_{2122}^{21} \\
A_{2211}^{22} & A_{2221}^{22} & A_{2212}^{22} & A_{2222}^{22}
\end{pmatrix}$$  \hspace{1em} (4)

By applying properties i, ii, we know there are maximally 4 independent block tensors.

The above illustration can be easily broadened to $2N$ case.

It is nice to change indices arrangement:

$$\tilde{F}^{(\alpha)} = \frac{1}{2\alpha} F_{i_1i_2...i_\alpha j_1j_2...j_\alpha} \psi_1^\dagger \psi_2^\dagger ... \psi_{i_\alpha}^\dagger \psi_{j_\alpha} ... \psi_{j_2} \psi_{j_1} .$$

Therefore, the two properties can be comprehended:

I. $F_{i_1i_2...i_\alpha j_1j_2...j_\alpha} = F^{*}_{j_1j_2...j_\alpha i_1i_2...i_\alpha}$ Hermiticity;

II. We call $s_\mu$ the exchange operation on $F$ that switching $i_\mu$ and $j_\mu$, $\mu \in [1, \alpha] \cap \mathbb{Z}$.

$$s_{\mu_1}s_{\mu_2}...s_{\mu_\alpha}F = s_{\nu_1}s_{\nu_2}...s_{\nu_\alpha}F^*$$, $\{\mu_1, \mu_2, ... \mu_\alpha\} \cap \{\nu_1, \nu_2, ... \nu_\alpha\} = [1, \alpha] \cap \mathbb{Z}$, and $\{\mu_1, \mu_2, ... \mu_\alpha\} \cap \{\nu_1, \nu_2, ... \nu_\alpha\} = \emptyset$. This simply means that transpose on some $ij$ pairs for $F$ is just the transpose on the remaining $ij$ pairs on $F^*$.

Additionally, if we want read tensor $\tilde{F}^{(\alpha)}$ in matrix, we combine the first $2\alpha$ indices and the last $2\alpha$ indices. Flatten[F,{1,2,3,..,\alpha},{\alpha+1,\alpha+2,..,2\alpha}]. It is just a symbolic representation.

**DIAGONALIZATION METHOD**

$F_{ijkl}$ is a four-order tensor, by [3], it can be decomposed in vectors’ tensor-product:
\[ F^{(2)} = \sum_r \lambda_i \sigma_i^{(1)} \sigma_i^{(2)} \sigma_i^{(3)} \sigma_i^{(4)}, \] where \( r \) is rank of the tensor. Since the Hermiticity it should obey, \( \sigma_i^{(1)} = \sigma_i^{(4)^*} \), \( \sigma_i^{(2)} = \sigma_i^{(3)^*} \). We conclude that \( U^\dagger V^\dagger \hat{F}^{(2)} V U = \Lambda \), \( \hat{F}^{(2)} = U V \Lambda V^\dagger U^\dagger \), where \( \Lambda \) is a diagonal four-order tensor and \( U, V \) are two different unitary matrix.

Let us first consider fermionic case. Ignoring coefficient \( \frac{1}{4} \), the above equation in index form:

\[ U^\dagger_i V^\dagger_j F_{ijkl} V_{kk'} U_{ll'} = \Lambda_{ii'} \delta_{jj'} \delta_{kk'} \delta_{ll'} \]  

(5)

By unitarity for \( U \) and \( V \), \( F_{ijkl} V_{kk'} U_{ll'} = U_{ii'} V_{jj'} \Lambda_{ii'} \delta_{jj'} \delta_{kk'} \delta_{ll'} \). A unitary matrix could be a combination of column vectors, thus,

\[ F_{ijkl} \beta_k \alpha_l = \lambda \alpha_i \beta_j = \lambda \delta_{il} \delta_{jk} \beta_k \alpha_l \]  

(6)

Here, \( \lambda \) is the diagonal element related to the \( i \)-th column vector in \( V \) and \( j \)-th column vector in \( U \). This is the eigenequation for a four-order Hermitian tensor.

In addition, we can also manipulate (5):

\[ V^\dagger_{jj'} F_{ijkl} V_{kk'} = U^\dagger_{ii'} \Lambda_{ii'} \delta_{jj'} \delta_{kk'} U^\dagger_{ll'} \]  

(7)

\[ U^\dagger_{ii'} F_{ijkl} U_{ll'} = V^\dagger_{jj'} \Lambda_{ii'} \delta_{jj'} \delta_{kk'} V_{kk'} \]  

(8)

If take complex conjugate on one equation then plug in another, we get:

\[ \begin{cases} F^*_{mjk}\alpha_i^* \alpha_i = \lambda^2 \alpha_m \alpha_n^* = \lambda^2 \delta_{im} \delta_{jn} \alpha_i \alpha_i^* \\ F^*_{lmnl} \beta_j^* \beta_k = \lambda^2 \beta_m \beta_n^* = \lambda^2 \delta_{jm} \delta_{kn} \beta_j \beta_k^* \end{cases} \]  

(9)
Different form (6), these two equations directly give eigenvectors for \(U\) and \(V\) separately.

In matrix notation, (6) is equivalent to:

\[
\det \begin{pmatrix}
A^{1111} - \lambda I_{n\times n} & A^{1121} & A^{1112} & A^{1122} \\
A^{1211} & A^{1221} - \lambda I_{n\times n} & A^{1212} & A^{1222} \\
A^{2111} & A^{2121} & A^{2112} - \lambda I_{n\times n} & A^{2122} \\
A^{2211} & A^{2221} & A^{2212} & A^{2222} - \lambda I_{n\times n}
\end{pmatrix} = 0 \quad (6')
\]

And (9) are:

\[
\begin{pmatrix}
A^{1111} & A^{1121} & A^{1211} & A^{1221} \\
A^{1112} & A^{1122} & A^{1212} & A^{1222} \\
A^{2111} & A^{2121} & A^{2211} & A^{2221} \\
A^{2112} & A^{2122} & A^{2212} & A^{2222}
\end{pmatrix}
\begin{pmatrix}
A^{1111\dagger} & A^{1121\dagger} & A^{1211\dagger} & A^{1221\dagger} \\
A^{1112\dagger} & A^{1122\dagger} & A^{1212\dagger} & A^{1222\dagger} \\
A^{2111\dagger} & A^{2121\dagger} & A^{2211\dagger} & A^{2221\dagger} \\
A^{2112\dagger} & A^{2122\dagger} & A^{2212\dagger} & A^{2222\dagger}
\end{pmatrix}
- \lambda^2 I = 0 \quad (9')
\]

When considering bosons, by analogous way as fermion, one can obtain \(U^\dagger V^\dagger \eta^{\otimes 2} \hat{\rho}^{(2)} V U = \Lambda\) — symplectic property for bosons—then we arrive eigenfunction:

\[
F_{ijkl} \beta_k \alpha_i = \lambda \eta_{ii} \eta_{jk} \beta_k \alpha_i \quad (10)
\]

\[
\begin{aligned}
(F_{mjk} F_{ijkl}^\dagger \alpha_i \alpha_i^\dagger = \lambda^2 \eta_{lm} \eta_{ln} \alpha_i \alpha_i^\dagger \\
(F_{lmnk} F_{ijkl}^\dagger \beta_j \beta_k^\dagger = \lambda^2 \eta_{jm} \eta_{kn} \beta_j \beta_k^\dagger
\end{aligned}
\]

\[
(11)
\]

where \(\eta = \begin{pmatrix} I_{n\times n} & 0 \\ 0 & -I_{n\times n} \end{pmatrix}\).
In matrix representation,

\[
\det \begin{pmatrix}
A_{1111}^{1111} - \lambda I_{n \times n} & A_{1121}^{1121} & A_{1112}^{1112} & A_{1122}^{1122} \\
A_{1211}^{1211} & A_{1221}^{1221} + \lambda I_{n \times n} & A_{1212}^{1212} & A_{1222}^{1222} \\
A_{2111}^{2111} & A_{2211}^{2121} & A_{2112}^{2112} + \lambda I_{n \times n} & A_{2122}^{2122} \\
A_{2211}^{2221} & A_{2221}^{2221} & A_{2212}^{2212} & A_{2222}^{2222} - \lambda I_{n \times n}
\end{pmatrix} = 0 \quad (10')
\]

If we set \( \kappa = \begin{pmatrix} I_{n \times n} & 0 & 0 & 0 \\ 0 & -I_{n \times n} & 0 & 0 \\ 0 & 0 & -I_{n \times n} & 0 \\ 0 & 0 & 0 & I_{n \times n} \end{pmatrix} \), the above equation is \( \det(F - \lambda \kappa) = 0 \).

One may impose more constraint on Hamiltonian, \( F_{ijkl} = F_{jilk} \) symmetry between two particles, we only need to solve (6). Apparently most common systems do have this property. And it can be generalized to many particles matrix case. Just like I and II in section 2, if we see consider \( i_\mu \) and \( j_\mu \) as a whole, then \( S_{1,2,\ldots,\alpha}[F] = F \). \( S_{1,2,\ldots,\alpha} \) are symmetry group elements. This means every permutation of \( i_1j_1, i_2j_2, \ldots, i_\alpha j_\alpha \) pair does not change tensor \( \hat{F}^{(\alpha)} \).

Additionally, if we want read tensor \( \hat{F}^{(\alpha)} \) in matrix, we combine the first \( 2\alpha \) indices and the last \( 2\alpha \) indices, Flatten\([F,\{1,2,3,\ldots,\alpha\},\{\alpha+1,\alpha+2,\ldots,2\alpha\}\]).

**EXAMPLES**

Next, we will show some simple example to illustrate the effectiveness of diagonalization procedure.

**Two Sites Hubbard Model**

Hubbard Models:

\[
H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \text{h. c.} + \frac{u}{2} \sum_{i,\sigma} c_{i\sigma}^+ c_{i\sigma}^+ c_{i\sigma} c_{i\sigma} \quad (12)
\]
Here, \( t_{ij} \) is hopping integral and \( u \) is Coulomb interaction centered at one site; \( c_{i\sigma}^\dagger \) create an electron with spin \( \sigma \) at site \( i \) and \( -\sigma \) means opposite spin.

The question is, kinetic terms are second order, how to write them in forth order form? We have to use a trick. Every single body operator \( \hat{t} \) is equivalent to a two-body operator \( T = \frac{1}{2}(\hat{t} \otimes I + I \otimes \hat{t}) \), thus the electron kinetic terms are rewritten as:

\[
T = -\frac{1}{2} \sum_{i,j,\sigma,\sigma'} t_{ij} (c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{j\sigma'} c_{j\sigma} + c_{i\sigma'}^\dagger c_{i\sigma}^\dagger c_{j\sigma} c_{j\sigma'} + h.c.)
\]

(13)

In two sites case, \( i, j \) can only be 1 and 2, we expand the Hamiltonian (expelling all illegal terms):

\[
H = -\frac{t}{2} (c_{1\uparrow}^\dagger c_{1\uparrow} c_{2\downarrow} + c_{1\downarrow}^\dagger c_{1\downarrow} c_{2\uparrow} + c_{1\uparrow}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{1\downarrow}^\dagger c_{1\uparrow} + c_{2\uparrow}^\dagger c_{2\uparrow} c_{1\downarrow} + c_{2\downarrow}^\dagger c_{2\downarrow} c_{1\uparrow} + c_{2\uparrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{2\downarrow}^\dagger c_{2\uparrow} + c_{2+1}\downarrow c_{1\downarrow} c_{2\uparrow} + c_{2-1}\uparrow c_{1\uparrow} c_{2\downarrow} + c_{2+1}\uparrow c_{1\uparrow}^\dagger c_{2\downarrow} + c_{2-1}\downarrow c_{1\downarrow}^\dagger c_{2\uparrow}) + \frac{u}{2} (c_{1\uparrow}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{1\downarrow} c_{1\uparrow} + c_{2\uparrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow})
\]

(14)

Apparently, this Hamiltonian is just one block in (4), and we do not need to write them all. In matrix notation:

\[
H = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{u}{2} & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{u}{2} & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{u}{2} & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & -\frac{t}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{t}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]
It is easy to diagonalize for the eigenvalues: \(0, u \frac{1}{2}(u - \sqrt{16t^2 + u^2}), \frac{1}{2}(u + \sqrt{16t^2 + u^2})\).

Moreover, eigenvector can also be directly read, Eigenvector for \(u\):
\[-\frac{1}{\sqrt{2}}(c_{1+}c_{1-} - c_{2+}c_{2-})|0\rangle\), Eigenvector for \(\frac{1}{2}(u - \sqrt{16t^2 + u^2})\) \(\mathcal{N}_3\left((4tc_{1+}c_{1-} + (u + \sqrt{16t^2 + u^2})c_{1+}c_{2-} + (u + \sqrt{16t^2 + u^2})c_{2+}c_{1-} + 4tc_{2+}c_{2-})\right)|0\rangle\), Eigenvector for \(\frac{1}{2}(u + \sqrt{16t^2 + u^2})\) \(\mathcal{N}_4\left(4tc_{1+}c_{1-} + (u - \sqrt{16t^2 + u^2})c_{1+}c_{2-} + (u - \sqrt{16t^2 + u^2})c_{2+}c_{1-} + 4tc_{2+}c_{2-}\right)|0\rangle\); here \(|0\rangle\) is vacuum state and \(\mathcal{N}\) are normalization factors.

**General Hubbard Model**

Fourier transform on (12) and (13):

\[
H(k) = -\sum_{k,k',\sigma,\sigma'}t_{k}c_{k\sigma}^\dagger c_{k'\sigma'}c_{k'\sigma'}c_{k\sigma} + \frac{u}{2N}\sum_{k,q,\sigma}c_{k\sigma}^\dagger c_{k+q,\sigma}c_{k+q,-\sigma}c_{k,-\sigma}c_{k\sigma}
\]

(16)

where \(t_{k} = \sum_{i,j} t_{ij} e^{ik(r_{j}-r_{i})}\) is kinetic factor in momentum space.

With a direct choice of basis,

\[\psi^\dagger = \left(c_{k+,k+}^\dagger, c_{k+,k-}^\dagger, c_{k+,k'+}^\dagger, c_{k+,q,+}^\dagger, c_{k+,q,-}^\dagger, c_{k'-q,+}^\dagger, c_{k'-q,-}^\dagger, c_{k+q,-}^\dagger, c_{k'q,-}^\dagger\right),\]

if only considering nearest neighbor hopping, the energy eigenvalue can be computed (reading appendix for details):

\[0, -t_{k}, \pm \frac{u}{2N}, \pm \frac{1}{4}\left(-2t_{k} + \frac{u}{N} \pm \sqrt{\left(\frac{u}{N} + 2t_{k}\right)^2 - 8t_{k}u/N + u^2/N^2}\right).\]

We are interested in the last two eigenvalues, and it has similar dispersion relation with the result solved by traditional method in [5].

**Exchange Interaction**

Electrons exchange interaction is written as:
\[ H = \frac{1}{2} \sum_{ij} J_{ij} \left( c_{i+}^+ c_{j+}^+ c_{i+} c_{j+} + c_{i-}^+ c_{j-}^+ c_{i-} c_{j-} + c_{i+}^+ c_{j-}^+ c_{i-} c_{j+} + c_{i-}^+ c_{j+}^+ c_{i+} c_{j-} + h.c \right) \]  

(17)

Similarly, in momentum space:

\[ H(k) = \sum_{k,k',q,\sigma} \frac{j_q}{N} \left( c_{k+q,+}^+ c_{k',-q,+}^+ c_{k,+} c_{k',+} + c_{k+q,-}^+ c_{k'-q,-}^+ c_{k,-} c_{k'-+}^+ + c_{k+q,+}^+ c_{k'-q,-}^+ c_{k,-} c_{k'+,-} + c_{k+q,-}^+ c_{k'-q,+}^+ c_{k,+} c_{k'+,-} \right) \]  

(18)

and \( j_q = \sum_{ij} J_{ij} e^{ik(r_j-r_i)} \), \( j = j_0 = \sum_{i,j} J_{ij} \). Its eigenvalues are:

\[ 0, \pm j / N, \pm j_q / N, \pm \frac{j}{2N} \sqrt{\frac{j^2}{2} + j^2} \]

In long wave limit approximation, \( |q \cdot \delta| \to 0 \), since

\[ \sqrt{1 + \cos x} \sim \sqrt{2} - \frac{x^2}{2\sqrt{2}} + O[x]^3 \]

the dispersion relation is quadratic in low energy case, similar to the result in ferromagnetic linear spin wave method.

**SUMMARY**

In this letter, we introduce another method for diagonalizing higher order second-quantization terms and show the equivalence to classical methods. This new diagonalization procedure gives us a new vision for many body quantum system or quantum fields.

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Appendix

1. Mathematica Codes

Generating real space one dimensional Hubbard chain Hamiltonian.

```
In[1]:= num = 2;
Out[1]= 2

In[2]:= h = SparseArray[
{SparseArray[{{i_, i_} :> 1}, {num, num}], SparseArray[{{i_, i_} :> 1}, {num, num}], SparseArray[{{i_, i_} :> 1}, {num, num}]}, {num, num}];

In[3]:= Flatten[h, {{1, 2}, {3, 4}, {5, 6}, {7, 8}}]
Out[3]= 2

In[4]:= Flatten[h, {{1, 2}, {4, 3}}] // MatrixForm
```

Generating one dimensional Hubbard model Hamiltonian in reciprocal lattice

```
In[5]:= num = 2;
Out[5]= 2

In[6]:= h = SparseArray[
{SparseArray[{{i_, i_} :> 1}, {num, num}], SparseArray[{{i_, i_} :> 1}, {num, num}], SparseArray[{{i_, i_} :> 1}, {num, num}]}, {num, num}];

In[7]:= Flatten[h, {{1, 2}, {3, 4}, {5, 6}}]
Out[7]= 2

In[8]:= Flatten[h, {{1, 2}, {4, 3}}] // MatrixForm
```

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2. Matrix Elements Choice for Analytical Solution

In 4.2 and 4.3, we computed energy eigenvalue for Hubbard and exchange interaction Hamiltonian. We provide how to build up a matrix for 4-order tensor.

Hubbard model:

We should show Hermiticity, internal symmetry in matrix.

\[
H(k) = -\sum_{kk'} \frac{t_{kk'}}{2} \left( c_{k+}^\dagger c_{k'+}^\dagger c_{k'+} c_{k+} + c_{k+}^\dagger c_{k'+}^\dagger c_{k'-} c_{k+} + c_{k-}^\dagger c_{k'+}^\dagger c_{k'+} c_{k-} + c_{k-}^\dagger c_{k'+}^\dagger c_{k'-} c_{k-} \right)
\]

\[
+ \frac{u}{4N} \sum_{kk',qq'} \left( c_{k+}^\dagger c_{k'-}^\dagger c_{k'+} c_{k-} + c_{k-}^\dagger c_{k'+}^\dagger c_{k'+} c_{k-} + c_{k-}^\dagger c_{k'-}^\dagger c_{k'+} c_{k'-} \right)
\]

Then non-zero matrix elements are:

\[
\{1,4,4,1\} \rightarrow -tk/2 + u/4/n, \{1,4,8,5\} \rightarrow u/2/n, \{1,8,4,5\} \rightarrow u/4/n, \{1,3,3,1\} \rightarrow -tk, \{2,3,3,2\} \rightarrow -tk/2 + u/4/n, \{2,3,7,6\} \rightarrow u/2/n, \{2,7,3,6\} \rightarrow u/4/n, \{2,4,4,2\} \rightarrow -tk/2, \{3,2,2,3\} \rightarrow -tk/2 + u/4/n, \{3,2,6,7\} \rightarrow u/8/n, \{3,1,1,3\} \rightarrow -tk/2, \{4,1,1,4\} \rightarrow -
\]
Exchange interaction:

\[
H(k) = j/4 \left( \sum_{k} \left( c_{k}^\dagger c_{k + k'}^\dagger + c_{k + k'} + c_{k'}^\dagger c_{k'}^\dagger + c_{k - k'} + c_{k - k'}^\dagger \right) \right)
\]

Non-zero elements are:

\[
\{1,3,5,7\} \rightarrow jq/n,\{1,4,6,7\} \rightarrow jq/n,\{1,1,3,3\} \rightarrow jq/n,\{1,2,4,3\} \rightarrow jq/n,\{1,3,1,3\} \rightarrow jq/n,\{1,4,2,3\} \rightarrow jq/n,\{2,3,5,8\} \rightarrow jq/n,\{2,4,6,8\} \rightarrow jq/n,\{2,2,4,4\} \rightarrow jq/n,\{2,1,3,4\} \rightarrow jq/n,\{2,3,1,4\} \rightarrow jq/n,\{2,4,2,4\} \rightarrow jq/n,\{3,1,7,5\} \rightarrow jq/n,\{3,2,8,5\} \rightarrow jq/n,\{3,7,1,5\} \rightarrow jq/n,\{3,8,2,5\} \rightarrow jq/n,\{3,3,1,1\} \rightarrow jq/n,\{3,4,2,1\} \rightarrow jq/n,\{3,1,3,1\} \rightarrow jq/n,\{3,2,4,1\} \rightarrow jq/n,\{4,2,8,6\} \rightarrow jq/n,\{4,1,7,6\} \rightarrow jq/n,\{4,8,2,6\} \rightarrow jq/n,\{4,7,1,6\} \rightarrow jq/n,\{4,4,2,2\} \rightarrow u/8/n\]
>j/n/2,{4,3,1,2}->j/n/2,{4,1,3,2}->j/n/2,{4,2,4,2}->j/n/2,{5,7,1,3}-
>jq/n/4,{5,8,2,3}->jq/n/4,{5,1,7,3}->jq/n/2,{5,2,8,3}->jq/n/2,{6,8,2,4}-
>jq/n/4,{6,7,1,4}->jq/n/4,{6,2,8,4}->jq/n/2,{6,1,7,4}->jq/n/2,{7,5,3,1}-
>jq/n/4,{7,6,4,1}->jq/n/4,{8,5,3,2}->jq/n/4,{8,6,4,2}->jq/n/4