A discrete Hubbard-Stratonovich decomposition for general, fermionic two-body interactions

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Abstract

A scheme is presented to decompose the exponential of a two-body operator in a discrete sum over exponentials of one-body operators. This discrete decomposition can be used instead of the Hubbard-Stratonovich transformation in auxiliary-field quantum Monte-Carlo methods. As an illustration, the decomposition is applied to the Hubbard model, where it is equivalent to the discrete Hubbard-Stratonovich transformation introduced by Hirsch, and to the nuclear pairing Hamiltonian.

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In auxiliary-field quantum Monte-Carlo methods (AFQMC), such as the projector, grand-canonical  and shell-model quantum Monte-Carlo methods , the Boltzmann operator , with the Hamiltonian, is decomposed in a sum or integral of exponentials of one-body operators. This sum or integral is then evaluated using Monte-Carlo techniques. For the decomposition, these methods rely on the Hubbard-Stratonovich transformation , which is based on the identity

\[
e^{\beta \hat{\rho}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2}} e^{\sigma \sqrt{2\beta \hat{\rho}}} d\sigma,
\]

where is a one-body operator. In order to avoid problems due to non-commuting operators, one can split up the Boltzmann operator using the Suzuki-Trotter formula . One can discretize the Hubbard-Stratonovich transformation by applying a Gaussian quadrature formula to the integral over . After a Suzuki-Trotter expansion in slices, a three-points quadrature formula leads to an error of the order of . This is of the same order in and as the errors due to the non-commutativity of the squared operators that build up . For some systems one can derive an exact, discrete Hubbard-Stratonovich transform. Hirsch showed how one can write an operator of the form , where is the site occupation number for an electron with spin projection , exactly as a sum of two exponentials of one-body operators . Recently, Gunnarsson and Koch extended this to systems with higher orbital degeneracy .

The aim of this paper is to describe another discrete decomposition scheme, which is exact for a certain class of operators. This decomposition scheme is generalized to any two-body Hamiltonian using the Suzuki-Trotter formula. For the application in AFQMC methods, especially the shell-model Quantum Monte-Carlo method, this new decomposition has the advantage, compared to the discretized Hubbard-Stratonovich transform based on Eq., that it is more accurate and that it leads to low-rank matrices. This leads to faster matrix multiplications and requires less computer memory. AFQMC methods for fermions often have sign problems . Fahy and Hamann showed that these sign problems can be related to the diffusive behavior of states in the Hubbard-Stratonovich transformation. Because our decomposition, in general, is based on exponentials of one-body operators of a completely different type, one can expect different sign properties. Our decomposition is not free of sign problems, but there might be systems where it leads to a sign rule while the Hubbard-Stratonovich transformation does not, or where our decomposition causes significantly less sign problems.

In Section II we introduce a matrix notation for Slater determinants and operators needed for a clear discussion of the decomposition. In Section III a basic lemma is given on which the decomposition is based. In Section IV the exact decomposition for a certain class of operators is presented. We indicate how to apply this decomposition to a general two-body Hamiltonian. In Section V the relation with Hirsch’s decomposition for the Hubbard model is elucidated. Finally, in Section VI the decomposition for the nuclear pairing Hamiltonian is discussed and illustrated with AFQMC-results for an exactly solvable model.
II. A MATRIX NOTATION FOR SLATER DETERMINANTS AND OPERATORS

In order to avoid confusion between matrix representations in the space of single-particle states and the operators themselves in Fock space, we will denote the former with upper case and the latter with lower case characters. Let \{\phi_1, \ldots, \phi_{N_s}\} be a set of basis states for the single-particle space, \(\hat{a}_1, \ldots, \hat{a}_{N_s}\) be the related creation operators and the \(A\)-particle state \(\Psi_M\) the antisymmetrized product of a set of single-particle states \(\sum_{i=1}^{N_s} M_{ij} \phi_i, \ j = 1 \ldots A\) i.e. \(\Psi_M\) is a Slater determinant. Thus in second quantization one can write

\[
|\Psi\rangle = \prod_{j=1}^{A} \left( \sum_{i=1}^{N_s} M_{ij} \hat{a}_i \right) |\rangle. \tag{2}
\]

This defines a matrix representation \(M\) for a Slater determinant \(\Psi_M\). The value of this representation is that one can represent certain operations on the Slater determinant by matrix operations on \(M\). e.g. the overlap between two Slater determinants \(\Psi_M\) and \(\Psi_M'\) is given by \(\langle \Psi_M | \Psi_M' \rangle = \det (M^\dagger M')\). The exponential of a one-body operator acting on \(\Psi_M\) results in a new Slater determinant, \(e^{-\beta h}|\Psi_M\rangle = |\Psi_{M'}\rangle\) (this is a corollary of the Thouless-theorem [9]), whose matrix representation is related to \(M\) by \(M' = e^{-\beta H}M\), where the \(N_s \times N_s\) matrix \(H\) is defined by \(\hat{h} = \sum_{ij} H_{ij} \hat{a}_i^\dagger \hat{a}_j\). Reversely, given a \(N_s \times N_s\) matrix \(Q\), one can consider the operator \(\hat{O}(Q)\), defined by its action on Slater determinants:

\[
\hat{O}(Q) : |\Psi_M\rangle \longrightarrow \hat{O}(Q)|\Psi_M\rangle = |\Psi_{M'}\rangle \quad \text{with} \quad M' = QM. \tag{3}
\]

If \(Q\) is non-singular, \(\hat{O}(Q)\) is the exponential of a one-body operator.

III. A BASIC LEMMA

Lemma: The operation represented by the unit matrix plus a matrix of rank two can be expressed as a sum of one- and two-body operators in the following way:

\[
\hat{O}(1 + \alpha B_1^\dagger B_4 + \beta B_2^\dagger B_3) = 1 + \alpha \hat{b}_1^\dagger \hat{b}_4 + \beta \hat{b}_2^\dagger \hat{b}_3 + \alpha \beta \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3 \hat{b}_4, \tag{4}
\]

where \(B_1, B_2, B_3\) and \(B_4\) are \(1 \times N_s\) row matrices and \(\hat{b}_k = \sum_{j=1}^{N_s} (B_k)_j \hat{a}_j\), \(k = 1, 2, 3, 4\).

Proof: Consider the \(A\)-particle Slater determinant \(\Psi_M\) represented by the matrix \(M\). Consider also a Slater determinant \(\Psi_L\) that has particles in the single-particle states \(\phi_{i_1}, \phi_{i_2}, \ldots, \phi_{i_A}\). The Slater determinants of this type constitute a basis of the \(A\)-particle Hilbert space. The overlap of \(\Psi_L\) with \(\Psi_M\) is given by

\[
\langle \Psi_L | \Psi_M \rangle = \det \left( \tilde{M}_1 \tilde{M}_2 \cdots \tilde{M}_A \right). \tag{5}
\]

The notation \(M_{j}\) denotes the vector that is given by the \(j\)th column of \(M\), the notation \(\hat{B}\) for an \(N\)-element vector \(B\) denotes the \(A\)-element vector \((B_{i_1} B_{i_2} \cdots B_{i_A})\). The operator in Eq.(4) transforms \(\Psi_M\) into \(\Psi_{M'}\) with \(M' = (1 + \alpha B_1^\dagger B_4 + \beta B_2^\dagger B_3)M\). To calculate the overlap of \(\Psi_{M'}\) with \(\Psi_L\), we have to replace every column \(M_{j}\) in Eq.(5):

\[
\tilde{M}_j \rightarrow \tilde{M}'_j = \tilde{M}_j + \alpha_j B_1^\dagger + \beta_j B_2^\dagger, \quad \text{with} \quad \alpha_j = \alpha B_4 M_{j}, \quad \beta_j = \beta B_3 M_{j}. \tag{6}
\]
The overlap is then given by
\[ \langle \Psi_L | \Psi_{M'} \rangle = \det \left( \tilde{M}_1 + \alpha_1 \tilde{B}_1^1 + \beta_1 \tilde{B}_2^1 \cdots \tilde{M}_A + \alpha_A \tilde{B}_1^A + \beta_A \tilde{B}_2^A \right). \tag{7} \]

This determinant can be expanded as the sum of all determinants that are obtained by selecting in every column of Eq. (7) one of the terms \( \tilde{M}_j, \alpha_j \tilde{B}_1^j \text{ or } \beta_j \tilde{B}_2^j \). If in more than one column the term \( \alpha_j \tilde{B}_1^j \) is selected, then the determinant has two linearly dependent columns, so it will vanish. The same holds for the term \( \beta_j \tilde{B}_2^j \). Only four types of determinants remain:

- \( \tilde{M} \) is selected in every column. This determinant is just \( \langle \Psi_L | \Psi_M \rangle \) (see Eq. (3)).
- \( \alpha_j \tilde{B}_1^j \) is selected in column \( j \), \( \tilde{M} \) in all others. These determinants sum up to \( \langle \Psi_L | \alpha \hat{b}_4 \hat{b}_4 | \Psi_M \rangle \) (one particle is moved from state \( b_4 \) to state \( b_1 \)).
- \( \beta_j \tilde{B}_2^j \) is selected in column \( j \), \( \tilde{M} \) in all others. These determinants sum up to \( \langle \Psi_L | \beta \hat{b}_3 \hat{b}_3 | \Psi_M \rangle \) (one particle is moved from state \( b_3 \) to state \( b_2 \)).
- \( \alpha_j \tilde{B}_1^j \) is selected in column \( j \), \( \beta_k \tilde{B}_2^k \) is selected in column \( k \), \( \tilde{M} \) in all others. These determinants sum up to \( \langle \Psi_L | \alpha \beta \hat{b}_4 \hat{b}_4 \hat{b}_4 \hat{b}_4 | \Psi_M \rangle \) (two particles are moved from states \( b_4 \) and \( b_3 \) to states \( b_1 \) and \( b_2 \)).

Taking all these terms together, we find that
\[ \langle \Psi_L | \Psi_{M'} \rangle = \langle \Psi_L | 1 + \alpha \hat{b}_4 \hat{b}_4 + \beta \hat{b}_3 \hat{b}_3 + \alpha \beta \hat{b}_4 \hat{b}_4 \hat{b}_3 \hat{b}_3 \hat{b}_4 | \Psi_M \rangle. \tag{8} \]

This holds for any basis state \( \Psi_L \), so that
\[ \Psi_{M'} = (1 + \alpha \hat{b}_4 \hat{b}_4 + \beta \hat{b}_3 \hat{b}_3 + \alpha \beta \hat{b}_4 \hat{b}_4 \hat{b}_3 \hat{b}_3 \hat{b}_4) \Psi_M. \tag{9} \]

This proves Eq. (8).

End of proof.

IV. A DISCRETE HUBABRD STRATONOVICH DECOMPOSITION

Consider a fermionic two-body operator \( \hat{Q} \) of the form
\[ \hat{q} = \sum_{i,j,k,l=1}^{N_s} Q_{ij} (B_1)_k (B_2)_l \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l. \tag{10} \]

An operator of this form has the special property that
\[ \hat{q}^2 = \lambda \hat{q}, \quad \text{with } \lambda = \sum_{k,l=1}^{N_s} (Q_{kl} - Q_{lk}) (B_1)_k (B_2)_l. \tag{11} \]

Because of this relation, the exponential of \( \hat{q} \) can be written as
\[ e^{-\beta \hat{q}} = 1 + \gamma \hat{q}, \quad \text{with } \begin{cases} \gamma = \frac{e^{-\beta \lambda} - 1}{\lambda} & \text{for } \lambda \neq 0, \\ \gamma = -\beta & \text{if } \lambda = 0. \end{cases} \tag{12} \]
Now we can use the lemma to obtain a discrete decomposition of $e^{-\beta \hat{q}}$ in a sum of exponentials of one-body operators:

$$
e^{-\beta \hat{q}} = \sum_{i,j=1}^{N_s} \frac{1}{2} \sum_{\sigma=-1,+1} |Q_{ij}| \left( 1 + \sigma \chi_{ij} \hat{a}_i^\dagger \hat{b}_1 + \sigma \chi'_{ij} \hat{a}_j^\dagger \hat{b}_2 + \chi_{ij} \chi'_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{b}_2 \hat{b}_1 \right),$$

$$= \sum_{i,j=1}^{N_s} \sum_{\sigma=-1,+1} |Q_{ij}| \left( 1 + \sigma \chi_{ij} A_i^\dagger B_1 + \sigma \chi'_{ij} A_j^\dagger B_2 \right),$$

(13)

with $A_i$ the $1 \times N_s$ row matrix which has a 1 on the $i^{th}$ entry and zeros anywhere else, and

$$\Theta = \sum_{i,j=1}^{N_s} |Q_{ij}|,$$

(14)

$$\chi_{ij} = \sqrt{|\gamma| / \Theta},$$

(15)

$$\chi'_{ij} = \sqrt{|\gamma| / \Theta} \text{sign} (\gamma Q_{ij}),$$

(16)

$$\hat{b}_k = \sum_{l=1}^{N_s} (B_k)_l \hat{a}_l, \quad k = 1, 2.$$  

(17)

This is an exact Hubbard-Stratonovich-like decomposition of the form of Eq.(10). To apply this discrete Hubbard-Stratonovich-like decomposition to the Boltzmann operator $e^{-\beta \hat{v}}$ for a general fermionic two-body operator $\hat{v}$, one has to rewrite $\hat{v}$ as a sum of operators of the form Eq.(10). A trivial way to do this, is given by

$$\hat{v} = \sum_{i,j,k,l=1}^{N_s} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k = \sum_{k,l=1}^{N_s} \hat{q}_{kl}, \quad \text{with} \quad \hat{q}_{kl} = \left( \sum_{i,j=1}^{N_s} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \right) \hat{a}_l \hat{a}_k.$$  

(18)

The Suzuki-Trotter formula can be used to split up the Boltzmann operator into factors with only one operator $\hat{q}_{kl}$ in the exponent. Then each of these factors can be decomposed exactly using the discrete decomposition in Eq.(13). Note that the total decomposition is no longer exact because of the non-commutativity of the operators $\hat{q}_{kl}$. The error will be of the order $\mathcal{O}(\beta^3 / N_t^2)$. It will be much smaller than in case of a decomposition based on a Gaussian discretization of the integral in Eq.(1), because now the error is proportional to the commutators of the operators $\hat{q}_{kl}$ and no longer to a power of $\hat{v}$.

V. RELATION TO HIRSCH’S DECOMPOSITION FOR THE HUBBARD HAMILTONIAN

For the Hubbard model we have to find a decomposition for a Boltzmann operator of the form $e^{-\beta U \hat{n}_\uparrow \hat{n}_\downarrow}$, where $U$ is the interaction strength and $\hat{n}_\sigma = \hat{a}_\sigma^\dagger \hat{a}_\sigma$. $\sigma = \uparrow, \downarrow$ is an index for the spin degree-of-freedom. The exponent has a two-body operator $\hat{n}_\uparrow \hat{n}_\downarrow$, which is an operator of the form of Eq.(11), so we can apply the decomposition given in Eq.(13) and obtain:

$$e^{-\beta U \hat{n}_\uparrow \hat{n}_\downarrow} = \frac{1}{2} \sum_{\sigma=-1,+1} \hat{O} \left( 1 + \sigma \chi_\uparrow N_\uparrow + \sigma \chi_\downarrow N_\downarrow \right),$$

(19)
with \( N_t(N_d) \) the matrix which is zero everywhere except for the diagonal element related to the spin-up (spin-down) site, which is equal to 1. \( \chi \) and \( \chi' \) are given by

\[
\chi^\uparrow = -\chi^\downarrow = \sqrt{1 - e^{-\beta U}} \quad \text{for } \beta U > 0, \tag{20}
\]

or

\[
\chi^\uparrow = \chi^\downarrow = \sqrt{e^{-\beta U} - 1} \quad \text{for } \beta U < 0. \tag{21}
\]

Now one could scale each term in Eq. (19) with an operator of the form \( e^{-\beta \mu (\hat{n}^\uparrow + \hat{n}^\downarrow)} \), because in the canonical ensemble this is just a constant. The matrices in the decomposition now have to be multiplied with the matrix \( 1 + \left( e^{-\beta \mu} - 1 \right) N^\uparrow + \left( e^{-\beta \mu} - 1 \right) N^\downarrow \). In case of the repulsive Hubbard model, the choice \( \mu = -U/2 \) leads to the discrete Hubbard-Stratonovich transform of Hirsch \[6\]. From the computational point of view this particular choice of \( \mu \) has the advantage that the matrix representation for the spin-down part is related to the matrix representation for the spin-up part by a matrix inversion. Then one only has to keep track of the spin-up part in actual AFQMC calculations. Hirsch’s decomposition for the attractive Hubbard model can also be obtained from Eq. (19), with a particular choice for \( \mu \). In this case however, there is no computational advantage in taking any particular value.

VI. APPLICATION TO THE NUCLEAR PAIRING HAMILTONIAN

The Hamiltonian for nuclear pairing in a degenerate shell is given by

\[
\hat{h} = -G \sum_{k,k'=1}^{N_S} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k'} \hat{a}_k. \tag{22}
\]

Here it is assumed that there are \( 2N_S \) degenerate single-particle states. The single-particle energy is shifted to 0 MeV. So there is no one-body part in the Hamiltonian. The states with \( j_z > 0 \) are labeled from 1 to \( N_S \) and \( \bar{k} \) denotes the time-reversed state of state \( k \). The many-body problem for this model can be solved analytically using the seniority scheme \[10\].

Using the Suzuki-Trotter formula, the Boltmann operator for this Hamiltonian can be written as

\[
e^{-\beta \hat{h}} = e^{-\frac{\beta}{2} \hat{q}_1} e^{-\frac{\beta}{2} \hat{q}_2} \ldots e^{-\frac{\beta}{2} \hat{q}_{N_S}} e^{-\frac{\beta}{2} \bar{q}_{N_S}} \ldots e^{-\frac{\beta}{2} \bar{q}_1} e^{-\frac{\beta}{2} \bar{q}_1} + \mathcal{O} \left( \beta^3 \right), \tag{23}
\]

with

\[
\hat{q}_k = -G \left( \sum_{k'=1}^{N_S} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \right) \hat{a}_k. \tag{24}
\]

The error is of the order \( \mathcal{O} (\beta^3) \). It is assumed that \( \beta \) is small. In practice, one has to split \( \beta \) in a number of inverse-temperature slices using the Suzuki-Trotter formula. Then one can apply the procedure that is discussed here to each inverse-temperature slice separately. We have \( \bar{q}_k^2 = -G \bar{q}_k \). So we can find a decomposition of the type given in Eq. (13)

\[
e^{-\frac{\beta}{2} \bar{q}_k} = \sum_{k'=1}^{N_S} \sum_{\sigma=-1,1} \frac{1}{2N_S} \hat{O} \left( 1 + \sigma \chi A_k^\dagger A_k + \sigma \chi A_k^\dagger A_k \right), \tag{25}
\]
where $\chi^2 = N_S \left( e^{2G} - 1 \right)$.

We have applied this decomposition to study a degenerate shell of 20 states ($N_S = 10$), with 10 particles. This could model the valence model space for neutrons in the $fp$ shell in $^{56}\text{Fe}$, if one neglects the energy gap between the $1f_{7/2}$ and the $2p_{3/2}, 2p_{1/2}$ orbitals. For the strength of the interaction we took $G = 20/A \text{ MeV} = 20/56 \text{ MeV}$, as recommended in [11]. We have performed a shell-model quantum Monte-Carlo calculation in the canonical ensemble, following [2], but now using the new decomposition of Eq.(25) instead of the Hubbard-Stratonovich transformation. In order to make the systematic error smaller than the statistical error, the inverse temperature $\beta$ was split into slices of length 0.05 MeV$^{-1}$. We point out that the form $1 + \sigma \chi \hat{A}_{k'} \hat{A}_k + \sigma \chi \hat{A}_{k'} \hat{A}_{\bar{k}}$ can be rewritten as $(1 + \sigma \chi \hat{A}_{k'} \hat{A}_k) (1 + \sigma \chi \hat{A}_{k'} \hat{A}_{\bar{k}})$, such that there is a symmetry between states with $j_z > 0$ and their time-reversed states. This symmetry guarantees that there will be no sign problem for systems with an even number of particles. This sign-rule is analogous to the sign rule for the pairing-plus-quadrupole Hamiltonian decomposed using the Hubbard-Stratonovich transform [12]. In figure 1 we show the internal energy of the system as a function of temperature. In figure 2 we show the corresponding specific heat of the system as a function of temperature. The Monte-Carlo results are in excellent agreement with the analytical results. The peak in the specific-heat curve around a temperature of 0.8 MeV can be associated with the breakup of $J^\pi = 0^+$ pairs. It is straightforward to take into account the different single-particles energies and more general forms of the pairing Hamiltonian:

$$\hat{h} = \sum_{k=1}^{N_S} \epsilon_k (\hat{n}_k + \hat{n}_{\bar{k}}) - \sum_{k,k'=1}^{N_S} G_{k,k'} \hat{a}^\dagger_k \hat{a}^\dagger_{k'} \hat{a}_{k'} \hat{a}_k.$$

Extension to even more general two-body Hamiltonians is possible. Then there can be sign problems at low temperatures.

**VII. CONCLUSION**

We have presented a new type of discrete Hubbard-Stratonovich decomposition for the Boltzmann operator. It is exact for a special class of two-body operators. Applied to the Hubbard Hamiltonian, it leads to Hisrch’s discrete Hubbard-Stratonovich decomposition. The decomposition is well suited for the nuclear pairing Hamiltonian, where it leads to a sign rule for systems with an even number of particles. Quantum Monte-Carlo results based on this decomposition are in excellent agreement with the analytical results for an exactly solvable model.

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FIG. 1. Internal energy versus temperature. Error bars on the Monte-Carlo data are omitted because they are smaller than the symbols marking the data points.

FIG. 2. Specific heat versus temperature. Error bars on the Monte-Carlo data represent 95%-confidence intervals.