Discrete Hubbard-Stratonovich transformations for systems with orbital degeneracy

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A discrete Hubbard-Stratonovich transformation is presented for systems with an orbital degeneracy \( N \) and a Hubbard Coulomb interaction without multiplet effects. An exact transformation is obtained by introducing an external field which takes \( N + 1 \) values. Alternative approximate transformations are presented, where the field takes fewer values, for instance two values corresponding to an Ising spin.

Systems with orbital degeneracy have recently attracted much interest. For instance, in systems with colossal magnetoresistance, like the manganites, the degenerate 3\( d \) orbital plays a major role. Another example is the alkali-doped C\(_{60}\) compounds, A\(_3\)C\(_{60}\) (A = K, Rb), where the partly filled \( t_{1u} \) orbital has a three-fold degeneracy. Other well-known examples are the 3\( d \) metals.

Quantum Monte Carlo, auxiliary field methods are popular methods for treating strongly correlated systems. In this approach a Hubbard-Stratonovich transformation is used to convert the many-body problem into a one-body problem, at the cost of introducing a fluctuating auxiliary field. A substantial simplification was introduced by Hirsch, who showed that for a system without orbital degeneracy the field only needs to take two values and that it can be described by an Ising spin. This method can be generalized to a system with the orbital degeneracy \( N \) by introducing an Ising spin for each pair of orbitals. This leads, however, to a large number \( 2N(2N−1)/2 \) of Ising spins for each site. This approach is very general, and can, for instance, handle the case when multiplet effects are considered. In many cases, however, we are interested in models which only have a Hubbard Coulomb interaction \( U \), without any multiplet effects. This simplifies the problem substantially, since the Coulomb energy then only depends on the total number of electrons on a given site, and not on the precise occupancy of the different levels. It is then natural to focus on the occupation number operator \( n \) for a given site. To calculate the partition function, we would then like to find an expression of the type

\[
e^{-U\Delta\tau n(n-1)/2} = \sum_{k=1}^{N+1} w_k e^{-x_k n} = \sum_{k=1}^{N+1} w_k z_k^n,
\]

where \( n = 0, 1, \ldots; 2N \) corresponding to the possible occupancies of a given site. \( \Delta\tau \) is the step length in \( \tau \) introduced in the Trotter procedure and \( z_k = \exp(-x_k) \). Because there are \( 2N+1 \) conditions, it should be possible to satisfy these conditions exactly by letting \( k \) run over \( N + 1 \) values, since there are then \( 2N + 2 \) parameters. Below we find that this is indeed the case. For \( U < 0 \), i.e., an attractive interaction, \( w_k \) is real and positive and \( x_k \) is real. For \( U > 0 \) the \( x_k \)'s are complex, but come in pairs of complex conjugates.

This problem can be solved analytically by rewriting the identity used by Hubbard

\[
e^{un(n-1)/2} = \int_{-\infty}^{\infty} e^{-\pi x^2 + (u/(\sqrt{2\pi}x-u/2))^2} dx,
\]

as

\[
e^{un(n-1)/2} = \int w(z) z^n dz,
\]

where the weight function \( w(z) \) is defined appropriately and \( u = -U\Delta\tau \). Since the integral now contains a polynomial of a maximum power \( 2N \), the integral can be replaced by a discrete sum of the type in Eq. (1) by using the theory of Gaussian integration and orthogonal polynomials. The transformation (1) is then exact for \( 0 \leq n \leq 2N + 1 \). Below we rework this procedure in such a way that it can be generalized to a more useful form.

We introduce a polynomial

\[
P(z) = \Pi_{k=1}^{N+1} (z - z_k) = \sum_{n=0}^{N+1} \alpha_n z^{N+1-n},
\]

where \( \alpha_0 = 1 \). We also define

\[
B(n) = e^{-U\Delta\tau n(n-1)/2}.
\]

which is the left hand side of Eq. (1). From Eq. (1) together with \( P(z_k) = 0 \) we then obtain

\[
\sum_{m=1}^{N+1} A_{n,m} \alpha_m = C_n \quad n = 1, \ldots, K,
\]

where \( K = N + 1 \) for the moment, \( A_{n,m} = B(N+n-m) \) and \( C_n = -B(N+n) \). The solution of Eq. (1) gives \( \alpha_m \).
These coefficients define $P(z)$ from which we obtain the roots $z_k$. The first $N + 1$ equations in Eq. (1) then form a set of linear equations in $w_k$, which is solved. This approach exactly reproduces the result of the Gaussian method mentioned above. Finally we transform from $z_k$ to $x_k$ by using $x_k = -\ln(z_k)$. Since $B(n)$ is real, the coefficients $\alpha_m$ are also real. The roots $z_k$ of the polynomial $P(z)$ are then real or come in pairs of complex conjugates. The same is true for $x_k$. For $U < 0$ $w_k$ is positive and $x_k$ is real, while for $U > 0$ $w_k$ and $x_k$ in general come in pairs of complex conjugates. In the following we consider a positive (repulsive) $U$.

By using $K = N + 1$ in Eq. (5) we really impose a physically irrelevant condition, since it means that Eq. (5) is satisfied for the occupancy $n = 2N + 1$, which never occurs in the problem. We therefore relax this condition and use $K = N$, thereby satisfying Eq. (5) exactly for $n = 0, \ldots, 2N$. Thus we put $A_{N+1,m} = \delta_{N+1,m}$. The value of $C_{N+1,m} \equiv \alpha_{N+1}$ can then be used to impose some additional condition on the transformation in Eq. (5), as is discussed below.

To use these results in a Monte Carlo approach, we introduce

$$p_k = \frac{|w_k|}{\sum_j |w_j|} \quad \text{and} \quad y_k = \frac{w_k}{|w_k|} \sum_j |w_j|,$$

where $p_k \geq 0$ and $\sum_k p_k = 1$. If $w_k$ are real and positive $y_k = 1$, since $\sum_j w_j = 1$. This leads to

$$B(n) = e^{-U \Delta \tau n(n-1)/2} = \sum_{k=1}^{N+1} p_k y_k e^{-x_k n}.$$

We now use a probability interpretation and choose the term $y_k e^{-x_k n}$ with the probability $p_k$. We introduce the relative standard deviation

$$\sigma(n)^2 = \frac{\sum_{k=1}^{N+1} p_k y_k e^{-x_k n}}{B(n)} - 1^2.$$

The free parameter $\alpha_{N+1}$ can now be used to minimize $\sigma(n)$. For instance, for a half-filled systems with a large value of $U$, most sites have the occupancy $N$. It should then be useful to minimize $\sigma(N)$. Fig. 1 shows $\sigma(n)$ as a function of $\alpha_{N+1}$ for $N = 3$. It illustrates that it is possible to obtain $\sigma(n = 3) = 0$ and at the same time to also obtain rather small values for $n = 2$ and $n = 4$. If the system instead is close to some other integer filling $n$, we can choose $\alpha_{N+1}$ so that the corresponding $\sigma(n)$ is small.

Since we are often interested in a system at or close to some integer occupancy $n_0$, it is also convenient to introduce

$$e^{-U \Delta \tau [(n-1) - n_0]} = \sum_{k=1}^{N+1} \tilde{w}_k e^{-x_k (n-n_0)},$$

TABLE I. Values of $\tilde{w}_k$ and $x_k$ (Eqs. (11,12)) and $\sigma(n)$ (Eq. (10)) for $N = 1$ and $n_0 = N$ as a function of $\Delta \tau U$. $\bar{w}_2 = \tilde{w}_1$ and $x_2 = x_1^*$. The first lines were obtained by using $K = N + 1$ and the following results by using $K = N$ and minimizing $\sigma(1)(\equiv 0)$.

| $\Delta \tau U$ | $\tilde{w}_1$ | $x_1$ | $\sigma(0)$ | $\sigma(1)$ | $\sigma(2)$ |
|-----------------|--------------|------|-------------|-------------|-------------|
| 0.1             | 0.5+i.0781   | 0.10-i.3097 | 0.501 | 0.156 | 0.156 |
| 0.2             | 0.5+i.1089   | 0.20-i.4290 | 0.701 | 0.212 | 0.212 |
| 0.4             | 0.5+i.1499   | 0.40-i.5823 | 1.194 | 0.300 | 0.300 |
| 0.1             | 0.5          | 0.05-i.31360 | 0.324 | 0.000 | 0.324 |
| 0.2             | 0.5          | 0.1-i.43980 | 0.471 | 0.000 | 0.471 |
| 0.4             | 0.5          | 0.2-i.61160 | 0.701 | 0.000 | 0.701 |

where $\tilde{w}_k$ is related to $w_k$ and $x_k$ by a simple transformation

$$\tilde{w}_k = w_k e^{Un_0(n_0-1)}/e^{-x_k n_0 - \Delta \tau}.$$

This result is identical to a result obtained by Hirsch, but presented in a different form. For $N = 2$ we obtain
\[ \tilde{w}_{1,2} = a; \quad x_{1,2} = 1.5U\Delta \tau \pm i \cos^{-1}(2\beta - 1) \]
\[ \tilde{w}_3 = 1 - 2a; \quad x_3 = 1.5U\Delta \tau \]  
(14)

with \( \beta = (\gamma - 1)/(\gamma - 4) \), \( \gamma = \exp(-0.5U\Delta \tau) \) and \( a = (\gamma - 1)/(2\beta - 2)/2 \). We observe that the \( \tilde{w}'s \) are all real in these cases.

For \( N = 3 \) we have not found a simple analytical expression for \( \tilde{w}_k \) and \( x_k \). Therefore numerical results are given in Table II for \( n_0 = N \). The corresponding values of \( \sigma(n) \) are given in Table III.

**TABLE II.** Values of \( \tilde{w}_k \) and \( x_k \) for \( N = 3 \) as a function of \( \Delta \tau U \) obtained by minimizing \( \sigma(N) \). (\( x_2 = x_1^* \) and \( x_4 = x_3^* \)).

| \( \Delta \tau U \) | \( \tilde{w}_1 \) | \( \tilde{w}_3 \) | \( x_1 \) | \( x_3 \) |
|----------------|-----------------|-----------------|-------------|-------------|
| 0.05           | 0.45154         | 0.04846         | 0.12504     | 0.1916385   |
| 0.1            | 0.44890         | 0.05110         | 0.2542883   | 0.2572002   |
| 0.2            | 0.44345         | 0.05655         | 0.5131561   | 0.5199334   |
| 0.4            | 0.43284         | 0.06796         | 1.142465    | 1.1433776   |

So far we have only considered exact transformations of Eq. (1), which requires a field with \( 3 \) values. The table shows that if \( U \Delta \tau = 0.4 \) the largest error is just 0.04, which occurs for \( n = 1 \) and \( n = 3 \). Such an error means that we are effectively using a Hamiltonian where \( U \) depends on \( n \) and has an error of about 4% for \( n = 1 \) and \( n = 3 \), but is almost exact for other values of \( n \). It should therefore be possible to treat \( N = 2 \) with just a single Ising spin, as for \( N = 1 \), although the field in the \( N = 2 \) is complex in contrast to the real field in one of the Hirsch \( N = 1 \) transformations. Table IV shows results for \( N = 3 \) and just two values of the field. In this case the errors are larger than in the \( N = 2 \) case, but the larger errors happen for the configurations with \( n = 0 \) and \( n = 6 \), which should be rare for large values of \( U \).

**TABLE III.** Values of \( \sigma(n) \) for \( N = 3 \) as a function of \( \Delta \tau U \) obtained by minimizing \( \sigma(N) \) and corresponding to the \( \tilde{w}_k \)'s and \( x_k \)'s in Table II.

| \( \Delta \tau U \) | \( \sigma(0) \) | \( \sigma(1) \) | \( \sigma(2) \) | \( \sigma(3) \) | \( \sigma(4) \) | \( \sigma(5) \) | \( \sigma(6) \) |
|----------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 0.05           | 0.75         | 0.47         | 0.23         | \( \cdot 0.000 \) | 0.23         | 0.47         | 0.75         |
| 0.1            | 1.21         | 0.70         | 0.32         | \( \cdot 0.000 \) | 0.32         | 0.70         | 1.21         |
| 0.2            | 2.25         | 1.11         | 0.47         | \( \cdot 0.000 \) | 0.47         | 1.11         | 2.25         |
| 0.4            | 5.97         | 1.99         | 0.70         | \( \cdot 0.000 \) | 0.70         | 1.99         | 5.97         |

In Table IV we show results for \( N = 2 \) using a field with just two values. The table shows that if \( U \Delta \tau \) is not too large, the errors \( \Delta \) are small. For instance, for \( U \Delta \tau = 0.4 \) the largest error is just 0.04, which occurs for \( n = 1 \) and \( n = 3 \). Such an error means that we are effectively using a Hamiltonian where \( U \) depends on \( n \) and has an error of about 4% for \( n = 1 \) and \( n = 3 \), but is almost exact for other values of \( n \). It should therefore be possible to treat \( N = 2 \) with just a single Ising spin, as for \( N = 1 \), although the field in the \( N = 2 \) is complex in contrast to the real field in one of the Hirsch \( N = 1 \) transformations. Table V shows results for \( N = 3 \) and just two values of the field. In this case the errors are larger than in the \( N = 2 \) case, but the larger errors happen for the configurations with \( n = 0 \) and \( n = 6 \), which should be rare for large values of \( U \).

**TABLE IV.** Values of \( \tilde{w}, x, \Delta \) and \( \sigma \) for \( N = 2 \) as a function of \( \Delta \tau U \) obtained by the expression in Eq. (11) using just two values of the field. \( \Delta(n) \) and \( \sigma(n) \) are symmetric around \( n = 2 \).

| \( \Delta \tau U \) | \( \tilde{w}_1 \) | \( x_1 \) | \( \Delta(0) \) | \( \Delta(1) \) | \( \Delta(2) \) | \( \sigma(0) \) | \( \sigma(1) \) | \( \sigma(2) \) |
|----------------|--------------|----------|--------------|--------------|--------------|--------------|--------------|--------------|
| 0.05           | 0.5         | 0.75     | 0.000       | 0.0000       | 0.04         | 0.22         | 0.0          |
| 0.1            | 0.5         | 0.15     | 0.000       | 0.0000       | 0.00         | 0.22         | 0.0          |
| 0.2            | 0.5         | 0.3      | 0.000       | 0.0000       | 0.00         | 0.22         | 0.0          |
| 0.4            | 0.5         | 0.6      | 0.000       | 0.0000       | 0.00         | 0.22         | 0.0          |

In the same spirit we can require that \( \tilde{w}_k \) and \( x_k \) are all real. It is still possible to obtain parameters so that Eq. (11) is rather well satisfied. For an equal number of spin up and spin down electrons, even away from half-filling, the spin up and spin determinants are then equal and real and their product is positive definite. Thus the determinants do not cause a sign problem in this case. For a repulsive \( U \) some of the \( w_k \) must, however, be negative. The sign problem then enters in a different form. It would be interesting to test whether or not this sign problem is less serious than in other formulations, where it enters via the determinants.

To summarize, we have presented an exact discrete Hubbard-Stratonovich transformation for a system with the orbital degeneracy \( N \) using a field which takes \( N + 1 \) complex values. The sign problem in the traditional Quantum Monte Carlo treatment is therefore converted into a phase problem. The standard deviation of the transformation has been minimized. It will be interesting to see how this influences the sampling efficiency. Ana-
lytical formulas for the fields were provided for \(N = 1\) and \(N = 2\) and numerical results for \(N = 3\). Alternative approximate transformations were presented, where the number of values of the field is smaller than \(N + 1\). For instance, it was found that for \(N = 2\) and \(N = 3\) and for \(\Delta \tau U\) not too large, a rather accurate transformation can be obtained with a field which only takes two values, corresponding to an Ising spin.

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