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# Discrete Hubbard-Stratonovich transformation for fermion lattice models

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We discuss a new functional-integral formulation of interacting fermion systems on a lattice such as the Anderson or Hubbard models: the fermion-fermion interaction is eliminated by introducing auxiliary Ising variables. The resulting model for a $d$-dimensional quantum system is a $(d+1)$-dimensional Ising model with complicated interactions. The new transformation is particularly useful for performing numerical studies of these models using Monte Carlo techniques. We study its convergence properties and compare it with the usual Gaussian formulation for the case of the Hubbard model.

The Hubbard-Stratonovich transformation[1] is based on the identity

$$\exp(\tfrac{1}{2}A^2)=\sqrt{2\pi}\int dx\,\exp(-\tfrac{1}{2}x^2-xA)\ , \tag{1}$$

where $A$ is a quantum-mechanical operator. This transformation allows for the mapping of an interacting fermion problem to a system of noninteracting fermions coupled to a fluctuating external field. It has been widely used in solid-state physics[2-4] to study models which have a two-body interaction of the form

$$H_1=Un_\uparrow n_\downarrow\ , \tag{2}$$

where $n_\sigma$ is the site occupation number of an electron of spin $\sigma$. Models of this type include the Anderson model,[2,5] where the interaction occurs at one impurity site, and the Hubbard model,[4,6] where the interaction occurs at every lattice site. In order to transform the interaction term so that the square of an operator appears, one of the following expressions is used:

$$n_\uparrow n_\downarrow=-\tfrac{1}{2}(n_\uparrow-n_\downarrow)^2+\tfrac{1}{2}(n_\uparrow+n_\downarrow)\ , \tag{3}$$

$$n_\uparrow n_\downarrow=+\tfrac{1}{2}(n_\uparrow+n_\downarrow)^2-\tfrac{1}{2}(n_\uparrow+n_\downarrow)\ , \tag{4}$$

$$n_\uparrow n_\downarrow=\tfrac{1}{4}(n_\uparrow+n_\downarrow)^2-\tfrac{1}{4}(n_\uparrow-n_\downarrow)^2\ . \tag{5}$$

With (3) or (4) one introduces a single auxiliary field, while with (5) two auxiliary fields are introduced. The relative merits of (3)–(5) have been extensively discussed in the literature.[7,8]

Consider a system described by a Hamiltonian

$$H=H_0+H_1\ ,$$

where $H_0$ is bilinear in fermion operators and $H_1$ is given by Eq. (2). In order to use the Hubbard-Stratonovich transformation, one has to use a functional-integral formulation since $H_0$ and $H_1$ do not commute in general. The partition function for the system can be written as

$$Z=\mathrm{Tr}e^{-\beta(H_0+H_1)}=\mathrm{Tr}\prod_{i=1}^{L}e^{-\Delta\tau(H_0+H_1)}$$
$$\cong\mathrm{Tr}\prod_{i=1}^{L}e^{-\Delta\tau H_0}e^{-\Delta\tau H_1}\ . \tag{6}$$

In the last equality, an error of order

$$O(\Delta\tau^2[H_0,H_1]) \tag{7}$$

has been made in breaking up the exponential, which becomes negligible as $\Delta\tau\to 0$. In that limit, Eq. (6) is usually written as

$$Z=\mathrm{Tr}T_\tau\exp\left(-\int_0^\beta d\tau\,(H_{0\tau}+H_{1\tau})\right)\ , \tag{8}$$

where the subscript $\tau$ on the operators means they are subject to time ordering. One can now use Eqs. (1) and (3)–(5) to eliminate the interaction. For example, using the form (3) one obtains

$$Z\propto\int Dx(\tau)\exp\left(-\int_0^\beta d\tau\,x^2(\tau)\right)\mathrm{Tr}T_\tau\exp\left(-\int_0^\beta d\tau[H_{0\tau}+\sqrt{U}x(\tau)n_{\tau\uparrow}-n_{\tau\downarrow}]+\frac{U}{2}(n_{\tau\uparrow}+n_{\tau\downarrow})\right)\ , \tag{9}$$

which describes a system of noninteracting particles moving in a fluctuating real field $x(\tau)$ which couples to the $z$ component of the spin.

The purpose of this paper is to point out that for the class of models where the Hubbard-Stratonovich transformation has been used in solid-state physics there exists another possible transformation. Since the fermion occupation number can only take the values 0 or 1, it is easy to convince oneself that a fluctuating field that takes only two discrete values is sufficient to eliminate the fermion-fermion interaction. Thus we will introduce an Ising variable $\sigma$ which takes the values $+1$ and $-1$. The following identities are easily proved:

$$\exp(-\Delta\tau Un_\uparrow n_\downarrow)=\tfrac{1}{2}\mathrm{Tr}_\sigma\exp[2a\sigma(n_\uparrow-n_\downarrow)-\tfrac{1}{2}U\Delta\tau(n_\uparrow+n_\downarrow)]\ , \tag{10a}$$

$$\exp(-\Delta\tau Un_\uparrow n_\downarrow)=\tfrac{1}{2}\mathrm{Tr}_\sigma\exp[2b\sigma(n_\uparrow+n_\downarrow-1)-\tfrac{1}{2}U\Delta\tau(n_\uparrow+n_\downarrow)]\ , \tag{10b}$$

with

$$\tanh^2=\tanh(\Delta\tau U/4)\ , \tag{11a}$$

$$\tanh^2 b=-\tanh(\Delta\tau U/4)\ . \tag{11b}$$

 

If one wants to work only with real quantities, Eq. (10a) would be used for $U>0$ and Eq. (10b) for $U<0$. One can, of course, also introduce a "two-field" version:

$$\exp(-\Delta\tau U n_\uparrow n_\downarrow)=\tfrac{1}{4}\mathrm{Tr}_{\sigma_1,\sigma_2}\exp[2c\sigma_1(n_\uparrow-n_\downarrow)+2ci\sigma_2(n_\uparrow+n_\downarrow)] \ , \tag{12}$$

with

$$\tanh^2 c=\tanh(\Delta\tau U/8) \ . \tag{13}$$

For example, using (10a), one obtains for the partition function

$$Z=\mathrm{Tr}_{[\sigma(\tau)]}\mathrm{Tr}\,T_\tau\exp\left[-\sum_\tau\Delta\tau[H_{0\tau}+\lambda\sigma(\tau)(n_{\uparrow\tau}-n_{\downarrow\tau})-\tfrac{1}{2}U(n_{\uparrow\tau}+n_{\downarrow\tau})]\right] \ , \tag{14}$$

$$\lambda=\frac{2}{\Delta\tau}\mathrm{arctanh}[\tanh(\Delta\tau U/4)]^{1/2} \ . \tag{15}$$

The parameter $1/\Delta\tau$ plays the role of a high-energy cutoff and is determined by requiring the error given by Eq. (7) to be small. A sufficient condition is that it is larger than all other energy scales of the problem. Equation (14) is defined on a *discrete* time lattice of $L=\beta/\Delta\tau$ points. In the usual Gaussian formulation, $\Delta\tau$ can be reabsorbed in the definition of the fluctuating field and the continuum limit can be formally taken, but $\Delta\tau$ is still implicit in the integration measure. Here, since we work with fixed-length Ising spins, $\Delta\tau$ appears explicitly in the coupling constant.

The fermion degrees of freedom in Eq. (14) can now be eliminated by taking the fermion trace explicitly, and one obtains

$$Z=\mathrm{Tr}_{[\sigma(\tau)]}\exp\left\{\mathrm{Trln}\left[1+T_\tau\exp\left[-\sum_\tau\Delta\tau K[\sigma(\tau)]\right]\right]\right\} \ , \tag{16}$$

where $K$ is a matrix describing the single-particle motion defined by the exponent of Eq. (14). Equation (16) describes a one-dimensional Ising model with complicated multispin interactions. In general, for a $d$-dimensional quantum system this procedure will yield a $(d+1)$-dimensional Ising system.

The trace over Ising spins in Eq. (16) can be evaluated term by term for small systems or using Monte Carlo techniques for large systems. Since the phase space over which the trace is performed is much smaller in the Ising formulation than in the Gaussian one, one can expect any numerical calculation to converge faster.

We apply the transformation to the Hubbard model, defined by the Hamiltonian

$$H=-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}c_{i\sigma}^\dagger c_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}(n_{i\sigma}-\langle n_{i\sigma}\rangle) \tag{17}$$

and choose the chemical potential $\mu=U/2$ so that the band is half full. We consider the case $U>0$ and use the transformation (10a). The averages of any combination of fermion operators can easily be obtained by averaging appropriate combinations of fermion Green's functions. In

TABLE I. Convergence of the Ising functional-integral formulation as function of $\Delta\tau$ for a two-site Hubbard model. $\beta=2$. The number in brackets is the statistical error in the last figure. $\lambda=(1-e^{-\Delta\tau U})^{-1}$.

| $\Delta\tau$ | $E$ | $\langle n_{i\uparrow}n_{i\downarrow}\rangle$ | $\langle S_iS_{i+1}\rangle$ | $\lambda\langle\sigma_i\sigma_{i+1}\rangle$ | $\langle c_{i\sigma}c_{i+1\sigma}^\dagger\rangle$ |
|---|---|---|---|---|---|
| | | $U=2$ | | | |
| 0.5 | −1.663(1) | 0.1354(5) | −0.703(1) | −0.708(9) | −0.4834(3) |
| 0.25 | −1.549(1) | 0.1741(5) | −0.621(1) | −0.619(11) | −0.4743(5) |
| 0.125 | −1.510(3) | 0.1867(4) | −0.594(1) | −0.605(6) | −0.4708(9) |
| 0.0625 | −1.500(1) | 0.1907(5) | −0.585(1) | −0.589(16) | −0.4703(5) |
| Exact | −1.496 | 0.1916 | −0.5825 | −0.5825 | −0.4697 |
| | | $U=4$ | | | |
| 0.5 | −1.696(4) | 0.0580(5) | −0.868(3) | −0.870(7) | −0.482(1) |
| 0.25 | −1.379(6) | 0.1100(5) | −0.750(5) | −0.755(11) | −0.455(1) |
| 0.125 | −1.239(2) | 0.1310(3) | −0.704(2) | −0.703(5) | −0.441(1) |
| 0.0625 | −1.180(3) | 0.1363(5) | −0.681(5) | −0.687(4) | −0.431(1) |
| Exact | −1.177 | 0.1384 | −0.6824 | −0.6824 | −0.4327 |
| | | $U=8$ | | | |
| 0.5 | −1.84(2) | 0.0084(3) | −0.95(2) | −0.95(2) | −0.476(6) |
| 0.25 | −1.29(2) | 0.0381(7) | −0.86(4) | −0.86(5) | −0.398(7) |
| 0.125 | −0.91(2) | 0.059(1) | −0.79(2) | −0.79(20 | −0.346(6) |
| 0.0625 | −0.78(2) | 0.065(2) | −0.74(2) | −0.74(4) | −0.328(9) |
| Exact | −0.7427 | 0.06646 | −0.7350 | −0.7350 | −0.3186 |

TABLE II. Spin-spin correlation function $G(l_x,l_y)$ [Eq. (19)] for a two-dimensional Hubbard model on a $4\times4$ lattice. $U=2$, $\beta=3$, $\Delta\tau=0.25$. Results were obtained from averaging over 500 lattice sweeps. In the Gaussian formulation, the step size was chosen so that the acceptance fraction was 0.5. We also show exact results for $U=0$ for comparison.

| $(l_x,l_y)$ | (0,0) | (0,1) | (0,2) | (1,1) | (1,2) | (2,2) |
|---|---|---|---|---|---|---|
| Ising | 0.638(1) | −0.113(4) | 0.027(5) | 0.024(4) | −0.025(4) | 0.033(4) |
| Gaussian | 0.637(2) | −0.115(9) | 0.024(11) | 0.019(9) | −0.025(8) | 0.031(9) |
| Exact ($U=0$) | 0.5 | −0.0699 | 0 | 0 | −0.0077 | 0 |

addition, there is a direct relation between correlation functions of the Ising spins and fermion spin-spin correlation functions:

$$\langle S_i(\tau)S_j(0)\rangle=(1-e^{-\Delta\tau U})^{-1}\langle\sigma_i(\tau)\sigma_j(0)\rangle\ , \qquad (18)$$

with $S_i=n_{i\uparrow}-n_{i\downarrow}$. (For $\tau=0$, this relation does not hold for $i=j$). For an attractive Hubbard model one would use (10b) and the $\sigma$-$\sigma$ correlations would be related to fermion charge-charge correlations.

We compute the thermodynamic averages using a Monte Carlo method. To compute the fermion determinant at each step, we use the powerful algorithm proposed recently by Blankenbecler, Scalapino, and Sugar,[9] which involves $N^2$ operations per update ($N=$number of spatial sites) and yields an exact determinant.

To assess the convergence of the procedure, we study various quantities as a function of $\Delta\tau$ for the case $N=2$, where exact results are easily obtained. Table I shows results for $\beta=2$ and various values of $\Delta\tau$ for the cases $U=2$, 4, and 8. The results to converge to the exact answers as $\Delta\tau\rightarrow0$. For an accuracy of a few percent, it appears adequate to choose $\Delta\tau U=0.5$. For other temperatures, the errors found are similar. Note that the statistical error in computing spin-spin correlation functions through Eq. (18) is larger than using fermion Green's functions.

We have compared the performance of the Ising formulation with the one based on the Gaussian formulation, Eq. (9). For small systems, the advantage of the Ising formulation is obvious, since one can easily cover a significant fraction of the total phase space. We find that also for large systems the Ising formulation converges more rapidly and yields smaller statistical errors, a factor of 2 or better. As an example, Table II shows results for the spin-spin correlation function

$$G(l_x,l_y)=\frac{1}{N}\sum_{i,j}\langle S_{(i,j)}S_{(i+l_x,j+l_y)}\rangle \qquad (19)$$

in a two-dimensional Hubbard model on a $4\times4$ lattice [$(i,j)$ denote the $(x,y)$ coordinates].

In summary, we have discussed a new transformation for interacting fermion systems on a lattice which maps the models into Ising models in one higher dimension. It should be interesting to explore the effectiveness of various approximate techniques that have been used with the Gaussian formulation when used with the Ising formulation. For example, with use of the Gaussian formulation the Hubbard model is often reduced to a binary-alloy model[4] by restricting the field to take only two values. With the Ising formulation, the mapping to a binary alloy can be obtained directly. As another example, the single-impurity Anderson model has been mapped to an Ising model with $1/R^2$ interactions by choosing a class of important paths in the Gaussian functional integral.[3] We believe that his mapping can be obtained more directly and have a wider range of validity with use of the Ising formulation. We have explored the convergence of the formulation as function of the time-slice size $\Delta\tau$ for the case of the Hubbard model and have shown that it is more convenient than the usual Gaussian formulation for numerical calculations. A detailed Monte Carlo study of the properties of the two-dimensional Hubbard model is in progress.

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