Appendix G

Hubbard-Stratonovich transformations

The original Hubbard-Stratonovich transformation converts the exponential of a two-body operator into a sum of exponentials of one-body operators. Each term in the sum depends on an auxiliary field. The models typically simulated have a small number of orbitals per lattice site and density-density Coulomb interactions acting only on site. This simplicity leads to the number of auxiliary fields being at most a few times the number of lattice sites. In these cases, Hirsch's discrete transformation (Hirsch, 1983) is more efficient than the standard continuous transformation. Here, we consider simulations of more complex models and discuss Hubbard-Stratonovich transformations for models with extended-range interactions and more general Coulomb interactions. More specifically, we discuss the use of the continuous Hubbard-Stratonovich transformation when the interactions are long ranged and present a novel discrete Hubbard-Stratonovich transformation for interactions that are not simply products of number operators. In both cases, the auxiliary fields are real. We also mention in passing other Hubbard-Stratonovich transformations used in special applications. These transformations include ones that preserve the SU(2) symmetry (Assaad, 1998) and couple the auxiliary field to fluctuations in the pairing field (Batrouni and Scalettar, 1990).

G.1 Extended interactions

We start by considering the exponentiation of the interaction

$$V = \sum_{ij} V_{ij} n_i n_j, \tag{G.1}$$

where the subscript i represents a combination of electron spin, orbital quantum numbers, and lattice position identifiers. The interactions, described by the elements V_{ij} of a symmetric $N \times N$ matrix, are not restricted to being on site or being between nearest neighbors. We have $n_i^2 = n_i$.

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With $n = (n_1, n_2, \ldots, n_N)^T$ being a N-vector of occupation numbers, the operative Hubbard-Stratonovich transformation is

$$e^{-\frac{1}{2}\Delta\tau n^T V n} = \frac{1}{\sqrt{\Delta\tau \det V}} \int \prod_i \left(\frac{dy_i}{\sqrt{2\pi}}\right) e^{-\frac{1}{2}\Delta\tau y^T V y} e^{-\Delta\tau y^T n}, \tag{G.2}$$

where $y = (y_1, y_2, \ldots, y_N)^T$ is a vector of auxiliary fields. The convergence of this multi-variable Gaussian integral requires V to be positive definite. If it is not, we write

$$e^{-\frac{1}{2}\Delta\tau n^T V n} = e^{\Delta\tau V_0 n^T n - \frac{1}{2}\Delta\tau n^T V n} e^{-\Delta\tau V_0 n^T n} \equiv e^{-\frac{1}{2}\Delta\tau n^T V' n} e^{-\Delta\tau V_0 n^T n}$$

and choose V_0 such that the matrix V' obtained by shifting the diagonal elements of V by $-2V_0$ is positive definite. Since $n^T n = \sum_i n_i = \sum_i c_i^\dagger c_i$, the additional exponential we introduce is that of a one-body interaction. We accommodate it by absorption into another one-body part of the Hamiltonian.

The generalized Hubbard-Stratonovich transformation (G.2) has had the same effect as the simpler transformations in Section 7.1.1, namely, converting the interacting problem into a noninteracting one. We can thus use it in a Monte Carlo simulation, instead of the others. What are the auxiliary fields and how do we sample them?

With V positive definite, a Cholesky factorization (Meyer, 2000) exists such that $V = R^T R$, where R is an upper triangular matrix with positive diagonal elements. Because of the factorization we can write $n^T V n = y^T y$ where $y = Rn$. After generating a vector $\zeta^T = (\zeta_1, \zeta_2, \ldots, \zeta_N)$ of Gaussian random variables of unit variance and zero mean, we then obtain a sample of the vector y by using the back-substitution method to solve the linear system of equations $\zeta = Ry$. Note that we need only N auxiliary fields.

A general two-body interaction can be put into the form

$$V = \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l. \tag{G.3}$$

With the definition of the operator $\rho_{ij} = c_i^\dagger c_j$, and the mapping of the subscript pairs ij and kl to the integers m and n, (G.3) takes the quadratic form

$$V = \sum_{mn} V_{mn} \rho_m \rho_n.$$

After ensuring the V_{mn} are elements of a positive-definite matrix, we sample the auxiliary field y in the same manner as we did for (G.1).

The Gaussian Hubbard-Stratonovich transformation is useful for a variety of applications other than those with long-range interactions. An important way to improve the efficiency in many of these simulations is to subtract background terms

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prior to making the transformation, leading to sampling from a shifted Gaussian (Purwanto and Zhang, 2004).

G.2 General discrete transformations

We ease into the general discrete Hubbard-Stratonovich transformation for interactions that are not simply products of number operators by first revisiting Hirsch's transformation from a perspective different from those that are. The new perspective is an expression of the exponential of the operators as a quadratic function of operators.

With $V_{ij} > 0$ and the relation $n_i^2 = n_i$, Hirsch's transformation for the exponential of each term in the potential energy (G.1) is

$$e^{-\Delta\tau V_{ij} n_i n_j} = \frac{1}{2} \sum_{\sigma=\pm 1} e^{-\sigma \Delta\tau J_{ij}\left(n_i - n_j\right) - \frac{1}{2}\Delta\tau V_{ij}\left(n_i + n_j\right)},$$

with $\cosh(\Delta\tau J_{ij}) = \exp(\frac{1}{2}\Delta\tau V_{ij})$. If expanded as a power series, the left-hand side of this equation becomes

$$e^{-\Delta\tau V_{ij} n_i n_j} = 1 + \lambda_{ij} n_i n_j,$$

where we defined

$$\lambda_{ij} = e^{-\Delta\tau V_{ij}} - 1. \tag{G.4}$$

From these results follows the trivial identity

$$e^{-\Delta\tau V_{ij} n_i n_j} = \tfrac{1}{2} \sum_{\sigma=\pm 1} \left(1 + \sigma\alpha_{ij} n_i + \sigma\beta_{ij} n_j + \alpha_{ij}\beta_{ij} n_i n_j\right) \tag{G.5}$$

if the product of α_{ij} and β_{ij} equals λ_{ij}. Noting that

$$e^{-\sigma \Delta\tau J_{ij}\left(n_i - n_j\right) + \frac{1}{2}\Delta\tau V_{ij}\left(n_i + n_j\right)} \neq 1 + \sigma\alpha_{ij} n_i + \sigma\beta_{ij} n_j + \alpha_{ij}\beta_{ij} n_i n_j$$

unless $\alpha_{ij} = -\beta_{ij}$, we choose[1]

$$\alpha_{ij} = \sqrt{\left|\lambda_{ij}\right|} \quad \text{and} \quad \beta_{ij} = \operatorname{sign}\left(\lambda_{ij}\right)\sqrt{\left|\lambda_{ij}\right|}. \tag{G.6}$$

Next, we comment that because the action of $\exp[-\sigma\Delta\tau J_{ij}\left(n_i - n_j\right) + \frac{1}{2}\Delta\tau V_{ij}\left(n_i + n_j\right)]$ on a Slater determinant produces another one (Appendix F), then so must the action of the operator $1 + \sigma\alpha_{ij} n_i + \sigma\beta_{ij} n_j + \alpha_{ij}\beta_{ij} n_i n_j$. If

$$|\psi_A\rangle = a_1^\dagger a_2^\dagger \cdots a_M^\dagger |0\rangle,$$

[1] If $V_{ij} < 0$, we would take $\alpha_{ij} = \beta_{ij}$.

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where

$$a_j^\dagger = \sum_i c_i^\dagger A_{ij},$$

the consequence of the exponential operators acting on $|\psi_A\rangle$ is $|\psi_{A'}\rangle$, where $A' = \exp(\chi^+)\exp(\chi^-)A$, χ^+ is an $N \times N$ matrix that is null except for its i-th diagonal element equaling $-\Delta\tau(\frac{1}{2}V_{ij} - \sigma J_{ij})$, and χ^- is an $N \times N$ matrix that is null except for its j-th diagonal element equaling $-\Delta\tau(\frac{1}{2}V_{ij} + \sigma J_{ij})$. The effect of $\exp(\chi^-)$ on A is to multiply the j-th row of A by $\exp[-\Delta\tau(\frac{1}{2}V_{ij} + \sigma J_{ij})]$, and the effect of $\exp(\chi^+)$ on this matrix product is to multiply its i-th row by $\exp[-\Delta\tau(\frac{1}{2}V_{ij} - \sigma J_{ij})]$. It is straightforward to show that these matrix-matrix multiplications are equivalent to

$$A' = \left(I + \sigma\alpha_{ij} I_{\bullet i} I_{i\bullet}^T + \sigma\beta_{ij} I_{\bullet j} I_{j\bullet}^T\right) A,$$

where α_{ij} and β_{ij} are as defined by (G.4) and (G.6). For an arbitrary matrix X, $X_{\bullet i}$ is an N-vector formed from the i-th column of X, and $X_{i\bullet}$ is an N-vector formed from its i-th row. In particular, the outer product $I_{\bullet i} I_{i\bullet}^T$ is an $N \times N$ null matrix except for its i-th diagonal element equaling unity. Hence, the two different-looking Hubbard-Stratonovich transformations, one using an exponential of a product of operators and the other using a quadratic polynomial of operators, are equivalent.

We now write the two-body potential energy in still another form,[2]

$$V = \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k = \sum_{kl} q_{kl},$$

with

$$q_{kl} = \left(\sum_{ij} V_{ijkl} c_i^\dagger c_j^\dagger\right) c_l c_k.$$

We can show that

$$q_{kl}^2 = \lambda_{kl} q_{kl},$$

where $\lambda_{kl} = V_{kkll} - V_{klkl}$. Hence

$$e^{-\Delta\tau q_{kl}} = 1 + \gamma_{kl} q_{kl}$$

and

$$\gamma_{kl} = \begin{cases} \frac{e^{-\Delta\tau\lambda_{kl}} - 1}{\lambda_{kl}} & \text{if } \lambda_{kl} \neq 0 \\ -\Delta\tau & \text{if } \lambda_{kl} = 0. \end{cases}$$

[2] The V_{ijkl} here are not necessarily the same as those in (G.3).

$$e^{-\Delta\tau q_{kl}} = \frac{1}{2}\sum_{\sigma=\pm1}\sum_{ij}\frac{\left|V_{ijkl}\right|}{\Lambda_{kl}}\left(1+\sigma\alpha_{kl}c_i^\dagger c_k+\sigma\beta_{kl}c_j^\dagger c_l+\alpha_{kl}\beta_{kl}c_i^\dagger c_j^\dagger c_l c_k\right), \tag{G.7}$$

and choose

$$\Lambda_{kl}=\sum_{ij}\left|V_{ijkl}\right|, \quad \alpha_{kl}=\sqrt{\Lambda_{kl}\left|\gamma_{kl}\right|}, \quad \beta_{kl}=\operatorname{sign}\left(\gamma_{kl}V_{ijkl}\right)\sqrt{\Lambda_{kl}\left|\gamma_{kl}\right|} \tag{G.8}$$

and then ask, Do the σ-dependent operators in (G.7) yield a single Slater determinant $|\psi\rangle_{A'}$ if they act on $|\psi\rangle_A$?

Rombouts et al. (1999a) showed that the answer to this question is yes. More specifically, if $|\psi\rangle_A$ is a Slater determinant defined by the $N\times M$ matrix A, then the operator $I+\alpha c_i^\dagger c_l+\beta c_j^\dagger c_k+\alpha\beta c_i^\dagger c_j^\dagger c_l c_k$ acting on $|\psi_A\rangle$ produces a Slater determinant $|\psi_{A'}\rangle$ defined by the $N\times M$ matrix

$$A'=\left(I+\alpha I_{\bullet i}I_{k\bullet}^T+\beta I_{\bullet j}I_{l\bullet}^T\right)A. \tag{G.9}$$

Equations (G.7) and (G.8) define a discrete Hubbard-Stratonovich transformation for the general two-body interaction (G.2). After the Monte Carlo procedure selects an auxiliary field σ, (G.9) defines a simple procedure for updating the Slater determinant.

We now express this updating in a more familiar form. We start by letting $\Delta=\alpha I_{\bullet i}I_{k\bullet}^T+\beta I_{\bullet j}I_{l\bullet}^T$. If we are interested in the ratio of the overlap integrals of two Slater determinants after and before a proposed change, we have

$$\frac{\langle\psi_L|\,I+\alpha c_i^\dagger c_k+\beta c_j^\dagger c_l+\alpha\beta c_i^\dagger c_j^\dagger c_l c_k\,|\psi_R\rangle}{\langle\psi_L|\,\psi_R\rangle}=\det\left(I+G\Delta\right), \tag{G.10}$$

where $G=R(L^TR)^{-1}L^T$ is the single-particle Green's function matrix (Appendix I). Because of the sparsity of Δ, (G.10) reduces to a determinant of a 2×2 matrix

$$\det\begin{pmatrix}1+\alpha G_{ki} & \beta G_{li}\\ \alpha G_{kj} & 1+\beta G_{lj}\end{pmatrix}=1+\alpha G_{ki}+\beta G_{lj}+\alpha\beta\left(G_{ki}G_{lj}-G_{li}G_{kj}\right),$$

a result we could have obtained from (G.10) by using Wick's theorem. Using the Sherman-Morrison formula (Meyer, 2000; Press et al., 2007)

$$\left(A+c\,d^T\right)^{-1}=A^{-1}-\frac{A^{-1}c\,d^TA^{-1}}{1+d^TA^{-1}c}$$

twice yields an efficient procedure for updating the Green's function: First, we execute

$$B^{-1} \equiv \left(G + \beta I_{\bullet j} I_{l\bullet}^T\right)^{-1} = G^{-1} - \beta \frac{\left[G^{-1}\right]_{\bullet j} \left[G^{-1}\right]_{l\bullet}^T}{1 + \beta \left[G^{-1}\right]_{lj}}$$

and then

$$G' = \left(A + \alpha I_{\bullet i} I_{k\bullet}^T + \beta I_{\bullet j} I_{l\bullet}^T\right)^{-1} = \left(B + \alpha I_{\bullet i} I_{k\bullet}^T\right)^{-1} = B^{-1} - \alpha \frac{\left[B^{-1}\right]_{\bullet i} \left[B^{-1}\right]_{k\bullet}^T}{1 + \alpha \left[B^{-1}\right]_{ki}}.$$