Appendix I

Zero-temperature determinant method

While the zero-temperature determinant algorithm projects to the ground state from a trial state, it does so in a way different from that of the power methods discussed in Chapter 10. It focuses on (7.1) for a large but fixed value of β and is a procedure to estimate expectation values

$$\langle A\rangle = \frac{\langle\psi_L|\, e^{-(\beta-\tau)H} A e^{-\tau H}\, |\psi_R\rangle}{\langle\psi_L|\, e^{-(\beta-\tau)H} e^{-\tau H}\, |\psi_R\rangle}. \tag{I.1}$$

Usually, $\tau = \frac{1}{2}\beta$. One may also calculate

$$\langle A\rangle = \frac{\int_{\beta/2-\tau_1}^{\beta/2+\tau_1} d\tau\, \langle\psi_L|\, e^{-(\beta-\tau)H} A e^{-\tau H}\, |\psi_R\rangle}{\int_{\beta/2-\tau_1}^{\beta/2+\tau_1} d\tau\, \langle\psi_L|\, e^{-(\beta-\tau)H} e^{-\tau H}\, |\psi_R\rangle},$$

that is, average the expectation values over a small interval around $\frac{1}{2}\beta$ to reduce the variance. It is also possible to extend the integration so it ranges from 0 to β. Our purposes are served if we take $\tau = \frac{1}{2}\beta$.

The simulations are done for N_σ fixed. Almost always, $|\psi_L\rangle = |\psi_R\rangle$. These states are usually chosen to be a superposition of basis states for fixed N^σ, for example, the noninteracting or the Hartree-Fock solution for the system being simulated.

Finite-sized systems of electrons display shell effects caused by degenerate states being separated by energy gaps. For *closed shells*, electrons occupy all states below some gap and hence are in a nondegenerate state. In this case, the $|\psi_L\rangle$ and $|\psi_R\rangle$ are often adequately chosen to be the noninteracting state. For *open shells*, not all states below the gap are occupied, and hence the state is degenerate. In this case it is better to choose $|\psi_L\rangle$ and $|\psi_R\rangle$ as a symmetry-adapted linear combination $\sum_\phi c_\phi|\phi\rangle$ of the noninteracting degenerate states. Then, even if $|\psi_L\rangle = |\psi_R\rangle$, we need the expectation values of operators between a $|\phi'\rangle$ and $|\phi\rangle$ that differ. In the following, we assume that the $|\psi_L\rangle = |\psi_L^\uparrow\rangle|\psi_L^\downarrow\rangle$ and $|\psi_R\rangle = |\psi_R^\uparrow\rangle|\psi_R^\downarrow\rangle$ are represented by

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single but different Slater determinants defined by $N_\sigma \times N$ and $N \times N_\sigma$ matrices Φ_L^σ and Φ_R^σ. For example,

$$\begin{aligned}\left|\psi_R^\sigma\right\rangle = & \left(\Phi_{11}c_{1\sigma}^\dagger + \Phi_{21}c_{2\sigma}^\dagger + \cdots + \Phi_{N1}c_{N\sigma}^\dagger\right) \\ & \left(\Phi_{12}c_{1\sigma}^\dagger + \Phi_{22}c_{2\sigma}^\dagger + \cdots + \Phi_{N2}c_{N\sigma}^\dagger\right) \\ & \cdots \\ & \left(\Phi_{1N_\sigma}c_{1\sigma}^\dagger + \Phi_{2N_\sigma}c_{2\sigma}^\dagger + \cdots + \Phi_{NN_\sigma}c_{N\sigma}^\dagger\right)|0\rangle\,,\end{aligned}$$

where

$$\Phi_R^\sigma = \begin{pmatrix} \Phi_{11} & \Phi_{12} & \cdots & \Phi_{1N_\sigma} \\ \Phi_{21} & \Phi_{22} & \cdots & \Phi_{2N_\sigma} \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_{N1} & \Phi_{N2} & \cdots & \Phi_{NN_\sigma} \end{pmatrix}.$$

As is standard, we express the denominator of (I.1) as a path-integral (7.1), make the Trotter approximation and the Hubbard-Stratonovich transformation (7.9), and then recycle the analysis of Section 7.1.2 to find

$$w_C = \prod_\sigma \det\left[\Phi_L^\sigma B^\sigma(\beta,0)\Phi_R^\sigma\right].$$

With the definitions

$$L^\sigma(\tau) = \Phi_L^\sigma B^\sigma(\beta,\tau), \quad R^\sigma(\tau) = B^\sigma(\tau,0)\Phi_R^\sigma,$$

we can show that

$$\mathcal{R}^\sigma = \det\left[I + \Delta^\sigma R^\sigma (L^\sigma R^\sigma)^{-1} L^\sigma\right] = \det\left[I + \Delta^\sigma (I - G^\sigma)\right],$$

which reduces to (7.43). In zero-temperature fixed N^σ calculations, L^σ and R^σ are $N^\sigma \times N$ and $N \times N^\sigma$ rectangular matrices. We still update the Green's function matrix by (7.45).

For the measurement of the equal-time Green's function, an analysis similar to that in Section 7.2.2 yields the formula[1]

$$G_{ij}^\sigma(\tau,\tau) = \delta_{ji} - \left\langle c_{j\sigma}^\dagger(\tau)\, c_{i\sigma}(\tau)\right\rangle = \delta_{ji} - \left[R^\sigma (L^\sigma R^\sigma)^{-1} L^\sigma\right]_{ji}. \tag{I.2}$$

Here, in contrast to the finite-temperature algorithm, τ should be interpreted not as an imaginary time, but rather as a Trotter index. For "equal time" measurements nothing changes, while unequal-time measurements are unphysical. If we move from one Trotter step to a later one, we can use relations such as

[1] Note the transposition of the indices.

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$$L^\sigma(\tau') = L^\sigma(\tau)B^\sigma(\tau',\tau)^{-1}, \quad R^\sigma(\tau') = B^\sigma(\tau',\tau)R^\sigma(\tau).$$

At any Trotter index, the Green's function matrix is primarily composed of two strings of B^σ matrices, one whose number of factors is decreasing from the left and another whose number of factors is increasing from the right as imaginary time advances. Creating and storing the sequences of partial matrix products (and their factorizations) accelerates the simulation. We can store the partial products for each spin σ as indicated in the following equation:

$$\begin{array}{lcl}
L^\sigma(\beta) = P_L^\sigma & \rightarrow & L^\sigma(\beta) = P_L^\sigma, \\
L^\sigma(\beta - \Delta\tau) & \rightarrow & L^\sigma(\beta - \Delta\tau), \\
\quad\vdots & & \quad\vdots \\
L^\sigma(\tau + \Delta\tau) & \rightarrow & L^\sigma(\tau + \Delta\tau), \\
L^\sigma(\tau) & \rightarrow & R^\sigma(\tau + \Delta\tau), \\
R^\sigma(\tau) & \rightarrow & R^\sigma(\tau), \\
\quad\vdots & & \quad\vdots \\
R^\sigma(\Delta\tau) & \rightarrow & R^\sigma(\Delta\tau), \\
R^\sigma(0) = P_R^\sigma & \rightarrow & R^\sigma(0) = P_R^\sigma.
\end{array}$$

The partial products generated in the computation of $L^\sigma(\tau)$ and $R^\sigma(\tau)$ are stored. To move from time τ to time $\tau + \Delta\tau$ we need the factors $L^\sigma(\tau + \Delta\tau)$ and $R^\sigma(\tau + \Delta\tau)$. The left factor $L^\sigma(\tau + \Delta\tau)$ is already available. The right factor $R^\sigma(\tau + \Delta\tau) = B^\sigma(\tau + \Delta\tau, \tau)R^\sigma(\tau)$ is easily computed. $R(\tau)$ may be stored in lieu of $L^\sigma(\tau)$, which is no longer needed. With this storage scheme, we can create the matrix needing inversion just with a few matrix multiplications. The cost of repeatedly stabilizing the matrix inversion becomes minor. Storing partial products in this manner has the added advantage of reducing the accumulation of round-off errors. Instead of storing the partial products for each Trotter index, doing the storage every so many steps is still advantageous. For example, in the above we replace $\Delta\tau \rightarrow m\Delta\tau$.

The matrix factorization procedure for doing the matrix inversion is a bit different. Using the factored forms

$$L^\sigma(\tau) = V_L^\sigma D_L^\sigma U_L^\sigma, \quad R^\sigma(\tau) = U_R^\sigma D_R^\sigma V_R^\sigma$$

in the expression for the Green's function

$$G^\sigma(\tau,\tau) = I - R^\sigma(\tau)\left[L^\sigma(\tau)R^\sigma(\tau)\right]^{-1}L^\sigma(\tau) \tag{I.3}$$

we find that

$$\begin{aligned}
G^\sigma &= I - \left(U_R^\sigma D_R^\sigma V_R^\sigma\right)\left[\left(V_L^\sigma D_L^\sigma U_L^\sigma\right)\left(U_R^\sigma D_R^\sigma V_R^\sigma\right)\right]^{-1}\left(V_L^\sigma D_L^\sigma U_L^\sigma\right) \\
&= I - U_R^\sigma\left(U_L^\sigma U_R^\sigma\right)^{-1}U_L^\sigma.
\end{aligned} \tag{I.4}$$

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Algorithm 50 Modified Gram-Schmidt method: matrix column orthonormalization.

Input: $M \times N$ matrix U.
  for $k = 1$ to N **do**
    $d = 0$;
    for $i = 1$ to M **do**
      $d \leftarrow d + U(i,k)U(i,k)$;
    end for
    $d \leftarrow \sqrt{d}$;
    for $i = 1$ to M **do**
      $U(i,k) \leftarrow U(i,k)/d$;
    end for
    for $j = k + 1$ to N **do**
      $v = 0$;
      for $i = 1$ to N **do**
        $v \leftarrow v + U(i,k)U(i,j)$;
      end for
      for $i = 1$ to M **do**
        $U(i,j) \leftarrow U(i,j) - vU(i,k)$;
      end for
    end for
  end for
  return the column-orthonormalized matrix U.

The U_L^σ and U_R^σ are $N^\sigma \times N$ and $N \times N^\sigma$ rectangular matrices, while the D_L^σ, V_L^σ, D_L^σ, and V_L^σ matrices are $N^\sigma \times N^\sigma$. The Green's function, however, depends only on the rectangular U_L^σ and U_R^σ matrices, so we can stabilize the calculation (Algorithm 50) just by orthonormalizing the rows of L^σ and columns of R^σ. Sugiyama and Koonin (1986) and Sorella et al. (1989) were among the first to note the importance of matrix column orthonormalization.

The zero-temperature algorithm is an elegant complement to the finite-temperature one. Unfortunately, it too has a sign problem. The more recent lattice fixed-node, constrained-path, and constrained-phase methods (Chapter 11) are useful in taming it.

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