Appendix F

Thouless's theorem

In this appendix, we prove *Thouless's theorem* (Thouless, 1961; Blaizot and Ripka, 1986). It says that if the state $|\phi\rangle$ is the Slater determinant $|\phi\rangle = a^\dagger_{N_\sigma} \cdots a^\dagger_2 a^\dagger_1 |0\rangle$, where $a^\dagger_i = \sum_j c^\dagger_j \Phi_{ji}$ is defined by the $N \times N^\sigma$ matrix Φ, then the propagation of this state $e^{-\Delta\tau c^\dagger M c} |\phi\rangle$ via a noninteracting Fermion Hamiltonian is to a new Slater determinant $|\phi'\rangle$, where $|\phi'\rangle = b^\dagger_{N_\sigma} \cdots b^\dagger_2 b^\dagger_1 |0\rangle$, and $b^\dagger_i = \sum_j c^\dagger_j \Phi'_{ji}$ is defined by the $N \times N^\sigma$ matrix $\Phi' = \exp(-\Delta\tau M)\Phi$. In other words, it says that if the Hamiltonian is noninteracting, a state of noninteracting Fermions evolves into another state of noninteracting Fermions and tells us how to compute the new state via the multiplication of two matrices.

This theorem underlies implicitly or explicitly many Fermion algorithms. Our use of the Hubbard-Stratonovich transformation replaces the exponential of the Hamiltonian of a system of interacting Fermions by the exponential of a Hamiltonian of Fermions that interact only with imaginary-time-dependent auxiliary fields. With this transformation, we were able to reduce the many-body formalism to numerical methods whose core computations are matrix-matrix multiplications. The role of the theorem is most apparent in the constrained path and phase algorithms (Chapter 11) where the projection to the ground state is cast as an open-ended imaginary-time propagation where each discrete imaginary-time step evolves one Slater determinant into another. It is implicit in the finite-temperature determinant method (Chapter 7). There, building the algorithm upon a generalization of the partition function of noninteracting Fermions was most natural. Our language was that of imaginary-time propagators, and our proof of the determinant form of basic single-particle propagators evoked the theorem. While we developed the zero-temperature determinant method by analogy to the finite-temperature one, we could have developed it from the point of view of the constrained path and phase ones by simply capping the length of the projection.

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In fact, the code for any one of these four methods can be easily converted to one of the other three.

The proof of the theorem is simple and mainly uses the anticommutation relation $\{c_i, c_j^\dagger\} = \delta_{ij}$. To evaluate $e^{-\Delta\tau c^\dagger Mc}|\phi\rangle$, we commute $e^{-\Delta\tau c^\dagger Mc}$ and $a_{N_\sigma}^\dagger$,

$$e^{-\Delta\tau c^\dagger Mc} a_{N_\sigma}^\dagger = \left[\sum_{ij} Mc_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{jN_\sigma}\right] e^{-\Delta\tau c^\dagger Mc},$$

so

$$e^{-\Delta\tau c^\dagger Mc} a_{N_\sigma}^\dagger \cdots a_2^\dagger a_1^\dagger |0\rangle = \left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{jN_\sigma}\right] e^{-\Delta\tau c^\dagger Mc} a_{N_\sigma-1}^\dagger \cdots a_2^\dagger a_1^\dagger |0\rangle .$$

Repeating this process until the operator exponential acts on the vacuum state yields

$$\begin{aligned} e^{-\Delta\tau c^\dagger Mc} a_{N_\sigma}^\dagger \cdots a_2^\dagger a_1^\dagger |0\rangle = &\left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{jN_\sigma}\right] \left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{j,N_\sigma-1}\right] \\ &\cdots \left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{j1}\right] e^{-\Delta\tau c^\dagger Mc} |0\rangle . \end{aligned}$$

Next, we note that $e^{-\Delta\tau c^\dagger Mc}|0\rangle = \left[I - \Delta\tau c^\dagger Mc + \frac{1}{2}\left(\Delta\tau c^\dagger Mc\right)^2 + \cdots\right]|0\rangle = |0\rangle$ and hence

$$\begin{aligned} e^{-\Delta\tau c^\dagger Mc} a_{N_\sigma}^\dagger \cdots a_2^\dagger a_1^\dagger |0\rangle = &\left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{jN_\sigma}\right] \left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{j,N_\sigma-1}\right] \\ &\cdots \left[\sum_{ij} c_i^\dagger \left[e^{-\Delta\tau M}\right]_{ij} \Phi_{j1}\right] |0\rangle . \end{aligned}$$

We could stop here, but we will add multiple propagator steps because they are required for the Trotterized path integrals in several algorithms. Each propagator step inherits the Slater determinant from the previous step. Multiple steps simply use multiple applications of the theorem.

Repeating this multiplication for each exponential produces

$$e^{-\Delta\tau c^\dagger M_{N_\tau} c} \cdots e^{-\Delta\tau c^\dagger M_2 c} e^{-\Delta\tau c^\dagger M_1 c} a^\dagger_{N_\sigma} \cdots a^\dagger_2 a^\dagger_1 |0\rangle =$$
$$\left[\sum_{ij} c^\dagger_i \left[e^{-\Delta\tau M_{N_\tau}} \cdots e^{-\Delta\tau M_2} e^{-\Delta\tau M_1}\right]_{ij} \Phi_{jN_\sigma}\right] \cdots$$
$$\cdots \left[\sum_{ij} c^\dagger_i \left[e^{-\Delta\tau M_{N_\tau}} \cdots e^{-\Delta\tau M_2} e^{-\Delta\tau M_1}\right]_{ij} \Phi_{j2}\right]$$
$$\times \left[\sum_{ij} c^\dagger_i \left[e^{-\Delta\tau M_{N_\tau}} \cdots e^{-\Delta\tau M_2} e^{-\Delta\tau M_1}\right]_{ij} \Phi_{j1}\right] |0\rangle .$$

After defining $b^\dagger_i = \sum_{jk} c^\dagger_j \left[e^{-\Delta\tau M_{N_\tau}} \cdots e^{-\Delta\tau M_2} e^{-\Delta\tau M_1}\right]_{jk} \Phi_{ki}$, we get

$$e^{-\Delta\tau c^\dagger M_{N_\tau} c} \cdots e^{-\Delta\tau c^\dagger M_2 c} e^{-\Delta\tau c^\dagger M_1 c} |\phi\rangle = b^\dagger_{N_\sigma} \cdots b^\dagger_2 b^\dagger_1 |0\rangle \equiv \left|\phi'\right\rangle . \qquad \text{(F.1)}$$

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