Appendix H

Multi-electron propagator

In this appendix, we derive the expressions for the multi-electron propagator heavily used in Chapters 7 and 11 and in Appendix I. We choose to give the details for the derivations to introduce various techniques that are useful for other analyses and to engender a keener appreciation of the physical content of the multipropagator relation.

Our main objective is proving the identity

$$\left\langle 0 \left| c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma}} \left[\mathcal{T} \exp\left(-\int_{\tau_1}^{\tau_2} H(\tau)\, d\tau \right) \right] c_{j_{N_\sigma}}^\dagger \cdots c_{j_2}^\dagger c_{j_1}^\dagger \right| 0 \right\rangle =$$
$$\det \begin{pmatrix} B_{i_1 j_1}(\tau_2,\tau_1) & B_{i_1 j_2}(\tau_2,\tau_1) & \cdots & B_{i_1 j_{N_\sigma}}(\tau_2,\tau_1) \\ B_{i_2 j_1}(\tau_2,\tau_1) & B_{i_2 j_2}(\tau_2,\tau_1) & \cdots & B_{i_2 j_{N_\sigma}}(\tau_2,\tau_1) \\ \vdots & \vdots & \ddots & \vdots \\ B_{i_{N_\sigma} j_1}(\tau_2,\tau_1) & B_{i_{N_\sigma} j_2}(\tau_2,\tau_1) & \cdots & B_{i_{N_\sigma} j_{N_\sigma}}(\tau_2,\tau_1) \end{pmatrix}, \tag{H.1}$$

which expresses the multielectron propagator as a determinant of a matrix of single-electron propagators

$$B_{ij}(\tau_2,\tau_1) = \left\langle 0 \left| c_i \left[\mathcal{T} \exp\left(-\int_{\tau_1}^{\tau_2} H(\tau)\, d\tau \right) \right] c_j^\dagger \right| 0 \right\rangle. \tag{H.2}$$

As a preliminary step, we prove a related result for electrons in nonoverlapping states, whose creation and destruction operators satisfy

$$\{c_i^\dagger, c_j\} = \mathcal{B}_{ij}, \tag{H.3}$$

where $\mathcal{B}_{ij} \equiv \langle 0|c_i c_j^\dagger|0\rangle$ is the overlap. The result we first prove is

$$\langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma}} c_{j_{N_\sigma}}^\dagger \cdots c_{j_2}^\dagger c_{j_1}^\dagger \,|0\rangle = \det \begin{pmatrix} \mathcal{B}_{i_1 j_1} & \mathcal{B}_{i_1 j_2} & \cdots & \mathcal{B}_{i_1 j_{N_\sigma}} \\ \mathcal{B}_{i_2 j_1} & \mathcal{B}_{i_2 j_2} & \cdots & \mathcal{B}_{i_2 j_{N_\sigma}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{B}_{i_{N_\sigma} j_1} & \mathcal{B}_{i_{N_\sigma} j_2} & \cdots & \mathcal{B}_{i_{N_\sigma} j_{N_\sigma}} \end{pmatrix}. \tag{H.4}$$

To demystify this result let us remark that if the electrons were in orthonormal states, $\mathcal{B}_{ij} = \delta_{ij}$, the determinant would equal a product of δ-functions and would simply express the normalization of the many-electron basis.

We first note that (H.4) is trivially true for $N_\sigma = 1$. We next assume that it is true for $N_\sigma - 1$. Then, in the inner product on the left-hand side of (H.3), we commute electron operators until we move $c_{j_{N_\sigma}}$ all the way to the right, so it operates directly on the vacuum state $|0\rangle$ and produces 0. The anticommutation relation (H.3) says this sequence of commutations generates

$$
\begin{aligned}
\langle 0|\, & c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma}} c^\dagger_{j_{N_\sigma}} \cdots c^\dagger_{j_2} c^\dagger_{j_1}\, |0\rangle \\
&= \mathcal{B}_{i_{N_\sigma} j_{N_\sigma}}\, \langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma-1}} \cdots c^\dagger_{j_2} c^\dagger_{j_1}\, |0\rangle \\
&\quad - \mathcal{B}_{i_{N_\sigma} j_{N_\sigma-1}}\, \langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma}} c^\dagger_{j_{N_\sigma-2}} \cdots c^\dagger_{j_2} c^\dagger_{j_1}\, |0\rangle \\
&\quad + \mathcal{B}_{i_{N_\sigma} j_{N_\sigma-2}}\, \langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma}} c^\dagger_{j_{N_\sigma-1}} c^\dagger_{j_{N_\sigma-3}} \cdots c^\dagger_{j_2} c^\dagger_{j_1}\, |0\rangle \\
&\quad - \cdots .
\end{aligned}
$$

By assumption, the inner products on the right-hand side of the above equation are determinants for $N_\sigma - 1$ electrons, and accordingly the right side is the cofactor expansion of the determinant we would obtain by expanding down the far right-hand column of the matrix for the N_σ electron system. Thus, we have proven the identity (H.4).

To start the proof of (H.1), we consider the imaginary-time propagation of an N_σ-state piecewise in $\Delta\tau$ steps:

$$
\mathcal{T} \exp\left(- \int_0^\beta H(\tau) d\tau \right) \equiv e^{-\Delta\tau H(\beta)} \cdots e^{-\Delta\tau H(2\Delta\tau)} e^{-\Delta\tau H(\Delta\tau)}.
$$

Because of the Hubbard-Stratonovich transformation, the electron operator $H(\ell\Delta\tau)$ is a quadratic form in the electron creation and destruction operators. Designating the $N \times N$ matrix that defines this form as M_ℓ and defining vectors of creation and destruction operators as

$$
c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}, \qquad c^\dagger = \begin{pmatrix} c_1^\dagger & c_2^\dagger & \cdots & c_N^\dagger \end{pmatrix}
$$

yields

$$
\mathcal{T} \exp\left(- \int_0^\beta H(\tau)\, d\tau \right) \propto e^{-\Delta\tau c^\dagger M_{N_\tau} c} \cdots e^{-\Delta\tau c^\dagger M_2 c} e^{-\Delta\tau c^\dagger M_1 c}. \tag{H.5}
$$

Our task now is propagating the right-hand N_σ-body state $|i_{N_\sigma},\ldots,i_2,i_1\rangle = c^\dagger_{i_{N_\sigma}}\cdots c^\dagger_{i_2}c^\dagger_{i_1}|0\rangle$ in (H.1) by the product of these exponentials. We first prove that

$$e^{-\Delta\tau c^\dagger Mc}c^\dagger = c^\dagger e^{-\Delta\tau M}e^{-\Delta\tau c^\dagger Mc}, \tag{H.6}$$

where $c^\dagger Mc = \sum_{ij} c^\dagger_i M_{ij} c_j$. For this, we note that

$$\left(\sum_{ij} c^\dagger_i M_{ij} c_j\right)c^\dagger_k = \sum_i c^\dagger_i \left[M_{ik} + \delta_{ik}\sum_j c^\dagger_i M_{ij} c_j\right],$$

or more compactly that $\left(c^\dagger Mc\right)c^\dagger = c^\dagger\left[M + I\left(c^\dagger Mc\right)\right]$. Using this commutation relation n times, we obtain

$$\left(c^\dagger Mc\right)^n c^\dagger = c^\dagger\left[M + I\left(c^\dagger Mc\right)\right]^n.$$

Then, using the power series representation of the exponential of an operator, $\exp(A) = I + A + \frac{1}{2!}A^2 + \cdots$, we find $e^{-\Delta\tau c^\dagger Mc}c^\dagger = c^\dagger e^{-\Delta\tau M - \Delta\tau\left(c^\dagger Mc\right)I}$ and, noting that M and $c^\dagger Mc$ commute, the relation (H.6).

To get (H.1), we make a proof by induction similar to the one used to go from (H.3) to (H.4). We first note that after a Trotter breakup (H.5) and an application of Thouless's theorem (Appendix F)

$$\mathcal{T}\exp\left(-\int_{\tau_1}^{\tau_2} H(\tau)\,d\tau\right)c^\dagger_{j_{N_\sigma}}\cdots c^\dagger_{j_2}c^\dagger_{j_1}|0\rangle$$

equals (F.1) and

$$b^\dagger_i = \sum_j c^\dagger_j\left[e^{-\Delta\tau M_{N_\tau}}\cdots e^{-\Delta\tau M_2}e^{-\Delta\tau M_1}\right]_{ji}. \tag{H.7}$$

We now define

$$B_{ij}(\tau_2,\tau_1) = \left[e^{-\Delta\tau M_{N_\tau}}\cdots e^{-\Delta\tau M_2}e^{-\Delta\tau M_1}\right]_{ij}.$$

With this definition, we see that the inner product in (H.1) is trivially true for $N_\sigma = 1$:

$$\begin{aligned} B_{i_1 j_1}(\tau_2,\tau_2) &= \left\langle 0\middle| c_{i_1}\mathcal{T}\exp\left(-\int_{\tau_1}^{\tau_2} H(\tau)\,d\tau\right)c^\dagger_{j_1}\middle|0\right\rangle \\ &= \langle 0|c_{i_1}b^\dagger_{j_1}|0\rangle = B_{i_1 j_1}(\tau_2,\tau_1)\langle 0|c_{i_1}c^\dagger_{j_1}|0\rangle. \end{aligned}$$

We next assume that it is true for $N_\sigma - 1$. Then, in the inner product on the left-hand side, we commute electron operators until we move $c_{j_{N_\sigma}}$ all the way to the right so

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it operates directly on the vacuum state $|0\rangle$ and produces 0. The relation (H.7) says that this sequence of commutations generates

$$
\begin{aligned}
&\langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma}} c^\dagger_{j_{N_\sigma}} \cdots c^\dagger_{j_2} c^\dagger_{j_1} \,|0\rangle \\
&\qquad = B_{i_{N_\sigma} j_{N_\sigma}} \,\langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma-1}} \cdots c^\dagger_{j_2} c^\dagger_{j_1} \,|0\rangle \\
&\qquad\quad - B_{i_{N_\sigma} j_{N_\sigma-1}} \,\langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma}} c^\dagger_{j_{N_\sigma-2}} \cdots c^\dagger_{j_2} c^\dagger_{j_1} \,|0\rangle \\
&\qquad\quad + B_{i_{N_\sigma} j_{N_\sigma-2}} \,\langle 0|\, c_{i_1} c_{i_2} \cdots c_{i_{N_\sigma-1}} c^\dagger_{j_{N_\sigma}} c^\dagger_{j_{N_\sigma-1}} c^\dagger_{j_{N_\sigma-3}} \cdots c^\dagger_{j_2} c^\dagger_{j_1} \,|0\rangle \\
&\qquad\quad - \cdots,
\end{aligned}
$$

where we left out the τ dependence of the B matrix elements for notational simplicity. By assumption, the inner products on the right-hand side are determinants for $N_\sigma - 1$ electrons, and accordingly, the right side is the cofactor expansion of the determinant we would obtain by expanding down the far right-hand column of the matrix for the N_σ-electron system. Thus, we have proven the identity (H.1).