Chapter 9

Perturbation expansion of the single-particle propagator

In this chapter several steps are executed which make it possible to express the exact propagator in terms of the noninteracting one and successive powers of the interaction. While these results represent nothing but a reworking of the Schrödinger equation, the end result allows an intuitive and practical analysis of the individual contributions in perturbation theory in terms of so-called Feynman diagrams. A systematic analysis of all these contributions then leads to the Dyson equation discussed in Ch. 10. In the present chapter, Sec. 9.1 summarizes the relevant results from App. A concerning time evolution in the interaction picture. The expansion of the propagator in terms in terms of the interaciton is obtained in Sec. 9.2. The evaluation of individual contributions to this expansion as an expectation value with respect to the noninteracting ground state is greatly facilitated by Wick's theorem which is discussed in Sec. 9.3. All the resulting expressions contributing to the propagator can be represented pictorially in terms of diagrams as discussed in Sec. 9.4. Simple rules providing a dictionary between the diagrams and corresponding mathematical expression in terms of known quantities are given in Sec. 9.5. Diagrams are presented both in time and energy formulation in this section. Additional rules are developed for systems where it is advisable to treat direct and exchange matrix elements together.

9.1 Time evolution in the interaction picture

As discussed in App. A it is convenient to separate the simple time-dependence of the time-evolution operator associated with $\hat{H}_0$ from the full time-evolution operator by introducing the interaction picture. For state kets this is accomplished by defining

$$|\Psi_I(t)\rangle = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}|\Psi_S(t)\rangle\,, \tag{9.1}$$

where the subscripts I and S refer to the interaction and Schrödinger picture, respectively. Note that the latter picture refers to the conventional description of the time dependence in quantum mechanics. The corresponding Schrödinger equation in the Interaction picture then acquires the following form as shown in App. A

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{H}_1(t)\,|\Psi_I(t)\rangle\,, \tag{9.2}$$

with

$$\hat{H}_1(t) = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{H}_1 \exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}. \tag{9.3}$$

Time evolution in the interaction picture is governed by the operator which connects interaction picture kets at different times according to

$$|\Psi_I(t)\rangle = \hat{U}(t,t_0)\,|\Psi_I(t_0)\rangle\,, \tag{9.4}$$

where the I subscript is left out for this special operator and

$$\hat{U}(t_0,t_0) = 1. \tag{9.5}$$

The equation of motion for this operator is obtained by combining Eqs. (9.2) and (9.4) with the following result

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}_1(t)\hat{U}(t,t_0). \tag{9.6}$$

As shown in App. A one may integrate this equation formally and iterate it to all orders to yield

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 ... \int_{t_0}^{t} dt_n\, \mathcal{T}\left[\hat{H}_1(t_1)\hat{H}_1(t_2)...\hat{H}_1(t_n)\right], \tag{9.7}$$

where the $\mathcal{T}$-operation is extended to order the $\hat{H}_1$ operator with the latest time farthest to the left, and so on.

9.2 Perturbation expansion in the interaction

The expression for the time-evolution operator given in Eq. (9.7) can be fruitfully employed to express the correlated single-particle propagator as a sum of known quantities each obtained by taking a corresponding expectation value with respect to the noninteracting ground state involving contributions from the two-body interaction. In order to establish this result it is convenient to separately consider the particle and hole part of the correlated single-particle propagator. In particular, it can be shown that for the particle part of the sp propagator

$$G^{+}(\alpha,\beta;t-t') = \lim_{T'\to-\infty(1-i\eta)} \lim_{T\to+\infty(1-i\eta)} Q(\alpha,\beta;T,T',t-t'), \tag{9.8}$$

where

$$Q = -\frac{i}{\hbar}\frac{\left\langle \Phi_0^A \right| \mathcal{T}\left[\hat{U}(T,T')a_{\alpha_I}(t)a^{\dagger}_{\beta_I}(t')\right]\left|\Phi_0^A\right\rangle}{\left\langle \Phi_0^A \right| \hat{U}(T,T')\left|\Phi_0^A\right\rangle}. \tag{9.9}$$

The choice of the particle part of G implies that $t > t'$. In addition, considering the limits in Eq. (9.8), one has

$$T > t > t' > T'. \tag{9.10}$$

Note that the particle removal and addition operators appearing explicitly and implicitly (inside $\hat{U}$) in Eq. (9.8) are given in the interaction picture. The original definition of G involves the corresponding operators in the Heisenberg picture and is given by

$$G^{+}(\alpha,\beta;t-t') = -\frac{i}{\hbar}\theta(t-t')\left\langle \Psi_0^A \right| a_{\alpha_H}(t)a^{\dagger}_{\beta_H}(t')\left|\Psi_0^A\right\rangle. \tag{9.11}$$

In order to show that Eq. (9.8) is correct we will proceed backwards from Eq. (9.9). One first observes that

$$\hat{U}(T,T') = \hat{U}(T,t)\hat{U}(t,t')\hat{U}(t',T') \tag{9.12}$$

representing the group property. Inserting this result in Eq. (9.9), one can move the addition and removal operators under the $\mathcal{T}$ sign to their location suggested by Eq. (9.12). The latter procedure involves no change in sign since it always involves an even number of interchanges. At this point the

$\mathcal{T}$ symbol can be dropped and one obtains

$$Q = -\frac{i}{\hbar}\frac{\left\langle \Phi_0^A \right| \hat{U}(T,t) a_{\alpha_I}(t) \hat{U}(t,t') a_{\beta_I}^\dagger(t') \hat{U}(t',T') \left| \Phi_0^A \right\rangle}{\left\langle \Phi_0^A \right| \hat{U}(T,T') \left| \Phi_0^A \right\rangle}. \tag{9.13}$$

One may now use Eq. (A.11) for the addition and removal operators and Eq. (A.22) to express $\hat{U}$ in terms of the regular time-evolution operator $\hat{U}_S$ given in Eq. (A.4) to rewrite Q in the following way

$$Q = -\frac{i}{\hbar}\frac{e^{iE^A_{\Phi_0}(T-T')/\hbar} \left\langle \Phi_0^A \right| \hat{U}_S(T-t) a_\alpha \hat{U}_S(t-t') a_\beta^\dagger \hat{U}_S(t'-T') \left| \Phi_0^A \right\rangle}{e^{iE^A\Phi_0(T-T')/\hbar} \left\langle \Phi_0^A \right| \hat{U}_S(T-T') \left| \Phi_0^A \right\rangle}. \tag{9.14}$$

One can now use Eq. (A.4) again to write the particle addition and removal operators in the Heisenberg picture while suitably reexpressing the denominator so that

$$Q = -\frac{i}{\hbar}\frac{\left\langle \Phi_0^A \right| e^{-i\hat{H}T/\hbar} a_{\alpha_H}(t) a_{\beta_H}^\dagger(t') e^{i\hat{H}T'/\hbar} \left| \Phi_0^A \right\rangle}{\left\langle \Phi_0^A \right| e^{-i\hat{H}T/\hbar} e^{i\hat{H}T'/\hbar} \left| \Phi_0^A \right\rangle}. \tag{9.15}$$

One can now insert the completeness relation for the exact Hamiltonian in terms of states in the A-particle system at appropriate places to obtain

$$Q = -\frac{i}{\hbar}\frac{\sum \langle \Phi_0^A \left| \Psi_n^A \right\rangle \langle \Psi_m^A \left| \Phi_0^A \right\rangle e^{-i(E_n^A T - E_m^A T')/\hbar} \left\langle \Psi_n^A \right| a_{\alpha_H}(t) a_{\beta_H}^\dagger(t') \left| \Psi_m^A \right\rangle}{\sum \langle \Phi_0 | \Psi_k^A \rangle \langle \Psi_k^A \left| \Phi_0 \right\rangle e^{-i(E_k^A T - E_k^A T')/\hbar}}. \tag{9.16}$$

It is now possible to perform the limits that are given in Eq (9.8). As $T \to \infty$ (or T'), the quantity ηT will be assumed to go to ∞. Accordingly all exponentials will decay to zero. The slowest decay corresponds to the terms with the lowest energy in the exponentials, so that only that term in the various sums will be important. From the resulting cancellation between numerator and denominator one then obtains the desired expression Eq. (9.11) when taking this limit for Eq. (9.8). The expansion for G^+ is then obtained by inserting Eq. (9.7) for $\hat{U}$ which finally yields

$$\begin{aligned} G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\sum_n^\infty \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty(1-i\eta)}^{+\infty(1-i\eta)} dt_1 ... \int_{-\infty(1-i\eta)}^{+\infty(1-i\eta)} dt_n \\ \times \left\langle \Phi_0^A \right| \mathcal{T}\left[\hat{H}_1(t_1)...\hat{H}_1(t_n) a_{\alpha_I}(t) a_{\beta_I}^\dagger(t')\right] \left| \Phi_0^A \right\rangle \quad (9.17) \\ / \sum_m^\infty \left(\frac{-i}{\hbar}\right)^m \frac{1}{m!} \int_{-\infty(1-i\eta)}^{+\infty(1-i\eta)} dt'_1 ... \int_{-\infty(1-i\eta)}^{+\infty(1-i\eta)} dt'_m \left\langle \Phi_0^A \right| \mathcal{T}\left[\hat{H}_1(t'_1)...\hat{H}_1(t'_m)\right] \left| \Phi_0^A \right\rangle . \end{aligned}$$

Since the result also holds for the hole part of the propagator, the $+$ has been dropped in Eq. (9.17). The critical point in the last step of this derivation is the nonvanishing of $\langle \Phi_0^A | \Psi_0^A \rangle$ expressing the assumption that a nonvanishing overlap exists between the simple state $|\Phi_0^A\rangle$ and the correlated ground state $|\Psi_0^A\rangle$.

9.3 Wick's theorem

Having obtained the expression in Eq. (9.17) for the exact propagator, it remains to be shown how to generate each relevant contribution in this perturbation expansion since important cancellations between numerator and denominator occur. To arrive at these results it is essential to employ a technique referred to as Wick's theorem which facilitates the evaluation of a given time-ordered product of operators. To motivate the use of this technique it is useful to consider a few low-order terms contributing to the numerator and denominator of Eq. (9.17). Before doing this, it is helpful to simplify notation for the rest of this chapter by eliminating the I subscript from the particle addition and removal operators occurring in the terms that contribute to Eq. (9.17). This should not ead to any confusion since the corresponding Heisenberg picture operators will still be labeled by the subscript H. Consider first the $n = 0$ term in the numerator

$$n = 0 \to -\frac{i}{\hbar} \langle \Phi_0^A | \mathcal{T} \left[a_\alpha(t) a_\beta^\dagger(t') \right] | \Phi_0^A \rangle = G^{(0)}(\alpha, \beta; t - t'), \tag{9.18}$$

which just gives the noninteracting propagator as given explicitly in Eq. (8.32). This result is physically reasonable since without interaction one should obtain the noninteracting result for the propagator. The first-order contribution to the numerator in Eq. (9.17) requires the evaluation of

$$\begin{aligned} n = 1 \to & \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty(1-i\eta)}^{\infty(1-i\eta)} dt_1 \; \langle \Phi_0^A | \mathcal{T} \left[\hat{H}_1(t_1) a_\alpha(t) a_\beta^\dagger(t') \right] | \Phi_0^A \rangle \qquad (9.19) \\ &= \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty(1-i\eta)}^{\infty(1-i\eta)} dt_1 \; \frac{1}{2} \sum_{\gamma\delta\epsilon\theta} \langle \gamma\delta | V | \epsilon\theta \rangle \\ &\qquad \times \langle \Phi_0^A | \mathcal{T} \left[a_\gamma^\dagger(t_1) a_\delta^\dagger(t_1) a_\theta(t_1) a_\epsilon(t_1) a_\alpha(t) a_\beta^\dagger(t') \right] | \Phi_0^A \rangle \\ &- \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty(1-i\eta)}^{\infty(1-i\eta)} dt_1 \; \sum_{\gamma\delta} \langle \gamma | U | \delta \rangle \langle \Phi_0^A | \mathcal{T} \left[a_\gamma^\dagger(t_1) a_\delta(t_1) a_\alpha(t) a_\beta^\dagger(t') \right] | \Phi_0^A \rangle , \end{aligned}$$

where $\hat{H}_1$ has been inserted with the inclusion of a contribution from an auxiliary one-body potential in addition to the two-body interaction

$$\hat{H}_1(t_1) = \frac{1}{2}\sum_{\gamma\delta\epsilon\theta} \langle\gamma\delta|\, V\, |\epsilon\theta\rangle\, a^\dagger_\gamma(t_1)a^\dagger_\delta(t_1)a_\theta(t_1)a_\epsilon(t_1) - \sum_{\gamma\delta} \langle\gamma|\, U\, |\delta\rangle\, a^\dagger_\gamma(t_1)a_\delta(t_1). \tag{9.20}$$

An explicit calculation for the $\hat{U}$ term in Eq. (9.19), for example, requires the consideration of the time-ordering of t and t' and a subsequent evaluation of the expectation value of the four operators with respect to the noninteracting ground state. The time dependence of the particle addition and removal operators is given by Eqs. (A.16) and (A.15), respectively. So for $t > t'$ and the part of the integration over t_1 for which $t' > t_1$ one requires the evaluation of

$$\begin{aligned}\left\langle\Phi^A_0\right| a_\alpha a^\dagger_\beta a^\dagger_\gamma a_\delta \left|\Phi^A_0\right\rangle = \\ &\theta(\alpha-F)\theta(F-\delta)\left\langle\Phi^A_0\right| (\delta_{\alpha,\beta} - a^\dagger_\beta a_\alpha)(\delta_{\gamma,\delta} - a_\delta a^\dagger_\gamma) \left|\Phi^A_0\right\rangle \\ &= \theta(\alpha-F)\theta(F-\delta)\Big(\underbrace{\delta_{\alpha,\beta}\delta_{\gamma,\delta}}_{I} - \underbrace{\delta_{\beta,\delta}\delta_{\alpha,\gamma}}_{II}\Big),\end{aligned} \tag{9.21}$$

where the same strategy as in Ch. 3 has been used which involves moving operators which give zero when acting on $\left|\Phi^A_0\right\rangle$ to the right and operators that have the same effect on $\left\langle\Phi^A_0\right|$ to the left. Before starting this moving around, one identifies that no contribution is obtained unless both $\alpha > F$ and $F > \delta$ for the same reasons. The first term in Eq. (9.21) then yields the following contribution

$$\begin{aligned}U_I \Rightarrow &-\left(\frac{-i}{\hbar}\right)^2 \int_{-\infty(1-i\eta)}^{t'} dt_1 \sum_{\gamma\delta} \langle\gamma|\, U\, |\delta\rangle \\ &\times \left\{\frac{i}{\hbar}\theta(t_1^+ - t_1)\delta_{\gamma,\delta}\theta(F-\gamma)e^{i\epsilon_\delta(t_1^+ - t_1)/\hbar}\right\}\hbar \\ &\times \left\{-\frac{i}{\hbar}\theta(t-t')\delta_{\alpha,\beta}\theta(\alpha-F)e^{-i\epsilon_\alpha(t-t')/\hbar}\right\}\hbar \\ = &\left\{\int_{-\infty(1-i\eta)}^{t'} dt_1 \sum_{\gamma\delta} \langle\gamma|\, U\, |\delta\rangle\, G^{(0)}_-(\delta,\gamma;t_1 - t_1^+)\right\} G^{(0)}_+(\alpha,\beta;t-t').\end{aligned} \tag{9.22}$$

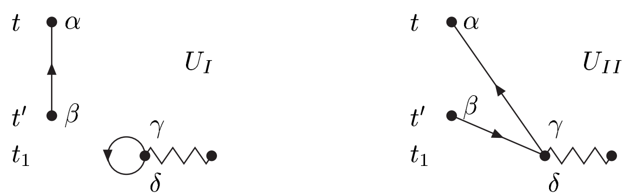

Fig. 9.1 Diagrammatic representation of Eqs. (9.22) and (9.23).

This contribution has been written such that particle and hole parts of noninteracting propagators can be identified even if the time arguments are identical. Note that the order of the operators for this $G_-^{(0)}$ term is dictated by the $a^\dagger a$ form of $\hat{U}$ and these time arguments are therefore uniquely determined. Similar steps for the second term yield

$$U_{II} \Rightarrow -\theta(t-t') \int_{-\infty(1-i\eta)}^{t'} dt_1 \sum_{\gamma\delta} \langle\gamma|\, U \,|\delta\rangle\, G_+^{(0)}(\alpha,\gamma;t-t_1) G_-^{(0)}(\delta,\beta;t_1-t'). \tag{9.23}$$

These contributions have a simple graphical representation shown in Fig. 9.1. In each picture the three times that are involved in the contribution are indicated with time increasing in the vertical direction. Such diagrams are therefore referred to as time-ordered. Each propagator term is represented by a line with an arrow that starts at its second argument accordingly labeled with appropriate sp quantum numbers and ends at its first (also labeled). These beginnings and ends are indicated by a dot to which, where appropriate, a zigzag line ending in another black dot can be attached representing the action of the $\hat{U}$ interaction. These interactions are also labeled with corresponding sp quantum numbers where the final state is shown above and the initial state below the zigzag. The first picture is considered "disconnected" since it consists of two separate pieces unrelated to each other, and, therefore, appear in product form as in Eq. (9.22). This usage of language implies that the second term is "connected" since all parts are linked to each other and no factorization occurs in Eq. (9.23). The propagator in the U_I picture that starts and ends at the $\hat{U}$ vertex also demonstrates how such closed loops occur as it is the result of addition and removal operators from the same interaction operator "contracting" with each other. Since these operators always have addition operators to the left of removal operators such loops always involve the hole parts of the corresponding sp propagator.

The term labeled U_I can now be read as folllows: before time t_1 the system is represented by the ground state of the noninteracting system $|\Phi_0^A\rangle$ which is not explicitly shown; at time t_1 the $\hat{U}$ interaction acts by removing a particle from this state but putting it back at the same time, necessarily in the same sp level. Later, at time t' a particle with quantum numbers β is added to the noninteracting ground state; at a later time t, this particle is removed again, leaving the system in the ground state of the noninteracting system, in turn implying that α should equal β since these quantum numbers correspond to the basis associated with H_0. The second picture represents a different physical process: before t_1 the system is again in the noninteracting ground state; at t_1 the $\hat{U}$ interaction now creates a particle-hole state with the "particle" in an unoccupied state (γ) and the "hole" in the noninteracting ground state indicated by δ. The particle line is drawn with the arrow pointing towards increasing time, whereas the arrow of the hole line points towards decreasing time. At time t', this hole is filled again by adding a particle with quantum numbers β (equating δ and β). This hole line can therefore also be considered as a particle going backward in time from t' to t_1 just as an antiparticle in relativistic field theory. From this time t' to time t one particle propagates above the noninteracting ground state until at t it is also removed, returning the system to the noninteracting ground state. The implied complete equivalence of the pictures and the expressions given in Eqs. (9.22) and (9.23) still requires a set of simple rules that will be discussed in more detail later.

Similar pictures and results can be generated for other time-orderings and corresponding evaluations of the expectation value with respect to the noninteracting ground state for the resulting order of particle addition and removal operators. Indeed, one may continue these calculations generating similar pictures for the term involving the two-body operator $\hat{V}$. This tedious process can then be continued for higher-order terms contributing to the numerator of Eq. (9.17). Similar pictures can also be generated by evaluating the denominator of that equation order by order. Clearly, in every case to be considered in each order a set of noninteracting propagator terms will be generated complemented by a product of matrix elements of $\hat{U}$ and $\hat{V}$ terms. In addition, relevant integrations over time variables and summations over internal sp quantum numbers are to be performed in every case. Order can be brought to this tedious work by employing Wick's theorem which elaborates all the terms that are generated by the "moving" around of operators as discussed in the context of Eq. (9.21).

We will follow the presentation of [Fetter and Walecka (1971)] to establish this result. It is useful to introduce the notion of the normal-ordered product in which the operators are ordered in such a way that those that give zero when acting to the right on $\left|\Phi_0^A\right\rangle$ are placed to the right of those that don't. Normal ordering therefore reorders a product of operators with the property that the usual interchanges of fermion operators are accompanied by appropriate minus signs as in time-ordered products of operators. For the two operators $a_\alpha(t)$ and $a_\beta^\dagger(t')$ this normal ordering yields

$$N\left[a_\alpha(t)a_\beta^\dagger(t')\right] = \begin{cases} -a_\beta^\dagger(t')a_\alpha(t) & \alpha > F,\ \beta > F \\ a_\alpha(t)a_\beta^\dagger(t') & \alpha > F,\ \beta < F \\ a_\alpha(t)a_\beta^\dagger(t') & \alpha < F,\ \beta > F \\ a_\alpha(t)a_\beta^\dagger(t') & \alpha < F,\ \beta < F, \end{cases} \tag{9.24}$$

where the order in the second and third term could be changed (with an attendant extra sign) since both operators have the same effect. In the first and last term in Eq. (9.24) the order is essential. In words, one simply moves removal operators of empty states to the right, addition operators of those same states to the left, removal operators of occupied states to the left, and, finally, addition operators of those states to the right. The extension to normal ordered products of other or more operators is defined in a similar fashion. It is now possible to define the contraction of two operators as the difference between their time-ordered and normal-ordered product. This contraction is identified by two identical symbols (*e.g.* bullets) used as superscripts attached to the operators involved.

$$a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet = \mathcal{T}\left[a_\alpha(t)a_\beta^\dagger(t')\right] - N\left[a_\alpha(t)a_\beta^\dagger(t')\right]. \tag{9.25}$$

For the case $t > t'$ one then obtains

$$a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet = a_\alpha(t)a_\beta^\dagger(t') - N\left[a_\alpha(t)a_\beta^\dagger(t')\right]. \tag{9.26}$$

In the case $\alpha > F$ and $\beta > F$ this time-ordering and the definition of the normal-ordered product generates the following result

$$\begin{aligned} a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet &= \theta(t-t')\left(a_\alpha(t)a_\beta^\dagger(t') + a_\beta^\dagger(t')a_\alpha(t)\right)\theta(\alpha-F)\theta(\beta-F) \\ &= \theta(t-t')\left(a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha\right)\theta(\alpha-F)\theta(\beta-F)e^{-i\epsilon_\alpha t/\hbar}e^{i\epsilon_\beta t'/\hbar} \\ &= i\hbar\left(\frac{-i}{\hbar}\right)\theta(t-t')\delta_{\alpha,\beta}\theta(\alpha-F)e^{i\epsilon_\alpha(t'-t)/\hbar} \\ &= i\hbar\, G_+^{(0)}(\alpha,\beta;t-t'). \end{aligned} \tag{9.27}$$

Applying the definitions of the time-ordered and normal-ordered product it is straightforward to show that for all other combinations of quantum numbers ($\alpha > F$, $\beta < F$, etc.) this contractions vanishes for $t > t'$. In the case $t < t'$, one obtains only a nonvanishing contribution when both α and β correspond to an occupied level in the noninteracting ground state and one obtains

$$a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet = i\hbar\, G_-^{(0)}(\alpha,\beta;t-t'). \tag{9.28}$$

This means that for all quantum numbers α and β and time orderings one can write

$$a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet = i\hbar\, G^{(0)}(\alpha,\beta;t-t'), \tag{9.29}$$

where the particle or hole part is automatically selected by the choice of occupied or empty quantum numbers and the result is simply a c-number. Other pairs of operators like two removal or two addition operators have vanishing contractions. This is to be expected since the corresponding anticommutation relations vanish.

The strategy to rearrange a time-ordered product of operators according to the properties of the individual addition and removal operators with respect to their action on the noninteracting ground state can be accomplished in one stroke by invoking the following form of Wick's theorem:

$$\begin{aligned}\mathcal{T}\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] &= N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] + N\left[\hat{a}^\bullet\hat{b}^\bullet\hat{c}...\hat{x}\hat{y}\hat{z}\right] + N\left[\hat{a}^\bullet\hat{b}\hat{c}^\bullet...\hat{x}\hat{y}\hat{z}\right]\\ &+ ... + N\left[\hat{a}^\bullet\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^\bullet\right] + N\left[\hat{a}\hat{b}^\bullet\hat{c}^\bullet...\hat{x}\hat{y}\hat{z}\right] + ... + N\left[\hat{a}^\bullet\hat{b}^\bullet\hat{b}^{\bullet\bullet}\hat{c}...{}^\bullet...{}^{\bullet\bullet}\hat{x}\hat{y}\hat{z}\right]\\ &+ ... + N\left[\hat{a}^\bullet\hat{b}^{\bullet\bullet}\hat{c}^{\bullet\bullet\bullet}...\hat{x}^\circ\hat{y}^{\circ\circ}\hat{z}^{\circ\circ\circ}\right]\\ &= N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] + N\left[\text{sum over all possible pairs of contractions}\right].\end{aligned} \tag{9.30}$$

The utility of this result is obvious once its expectation value is considered with respect to the noninteracting ground state. Only contributions to Eq. (9.30) involving a fully contracted set of operators (corresponding to an even number) will yield a nonvanishing expectation value. Nonvanishing expectation values of time-ordered products of an even number ($2n$) of operators (with both n addition and removal operators) therefore involve n contractions implying n noninteracting propagators (and n factors of $i\hbar$). The total number of these contractions is simply $n!$ to allow each removal operator to contract will all possible addition operators.

We start with observing that changing the order of operators inside a normal ordered product requires an appropriate sign change according to

$$N\left[\hat{a}\hat{b}\hat{c}\hat{d}...\right] = -N\left[\hat{b}\hat{a}\hat{c}\hat{d}...\right], \tag{9.31}$$

where $\hat{a}, \hat{b}, ...$ represent either particle removal or addition operators. It is also helpful to introduce the following sign convention when contractions inside normal-ordered products are considered

$$N\left[\hat{a}^\bullet\hat{b}\hat{c}^\bullet\hat{d}...\right] = -N\left[\hat{b}\hat{a}^\bullet\hat{c}^\bullet\hat{d}...\right] = -\hat{a}^\bullet\hat{c}^\bullet N\left[\hat{b}\hat{d}...\right]. \tag{9.32}$$

For completeness it is useful to repeat the strategy of moving operators depending on their character. An operator like $a_\alpha^\dagger$ with $\alpha > F$ must be moved to the left and will be considered an operator of type I. If $\alpha < F$ this operator must be moved to the right and will be labeled a type II operator. Similarly, a_α is a type I operator when $\alpha < F$ and type II when $\alpha > F$. Note that this distinction is related to the choice of sp basis as *its* lowest levels are filled in the noninteracting ground state $\left|\Phi_0^A\right\rangle$. This choice of basis is convenient and will be used here. It is not required to make this choice since operators representing particle removal and addition operators with other sp quantum numbers can also be used. Ultimately, the usage of Wick's theorem requires the decomposition of such operators into type I and II operators which is accomplished by a basis transformation according to Eqs. (2.58) and (2.59). This decomposition automatically yields two terms, one referring to occupied states the other to empty states in the summations of Eqs. (2.58) and (2.59). This immediately identifies the type I or II character of this decomposition. The observation that normal ordering is a distributive operation then allows the process of normal ordering etc. to proceed as discussed below with similar results for other choices of sp basis states.

Several steps are involved in demonstrating the validity of Eq. (9.30). First one can prove the following: if $N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\right]$ is a normal-ordered product and the operator $\hat{z}$ has a time earlier than any occurring in this product then

$$\begin{aligned} N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\right]\hat{z} = {} & N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}^\bullet\hat{z}^\bullet\right] + N\left[\hat{a}\hat{b}\hat{c}...\hat{x}^\bullet\hat{y}\hat{z}^\bullet\right] + ... \\ & + N\left[\hat{a}^\bullet\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^\bullet\right] + N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right]. \end{aligned} \tag{9.33}$$

One may note the following points to prove this result. First, if $\hat{z}$ is of type

II, then all contractions vanish with each operator $\hat{i}$ in the set $\hat{a}...\hat{y}$ since

$$\hat{i}^\bullet\hat{z}^\bullet = \mathcal{T}\left[\hat{i}\hat{z}\right] - N\left[\hat{i}\hat{z}\right] = \hat{i}\hat{z} - \hat{i}\hat{z} = 0, \tag{9.34}$$

where in the last equality the earlier time of the operator $\hat{z}$ and its type II property was used. So in this particular case Eq. (9.33) follows since one obviously has

$$N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\right]\hat{z} = N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right]. \tag{9.35}$$

One may now proceed by assuming first that the operators $\hat{a}\hat{b}...\hat{y}$ are already normal ordered. In case they are not, one may reorder Eq. (9.33) accordingly on both sides using the sign conventions introduced in Eqs. (9.31) and (9.32) which are the same on both sides. One now assumes that the operators $\hat{a}, \hat{b}, \hat{c}, ...\hat{x}, \hat{y}$ are all of type II (giving zero when acting on $\left|\Phi_0^A\right\rangle$) and considers the case that $\hat{z}$ is of type I. With these assumptions, one may now use an induction procedure. For two operators Eq. (9.33) is valid since

$$N[\hat{y}]\,\hat{z} = \hat{y}\hat{z} = \mathcal{T}[\hat{y}\hat{z}] = \hat{y}^\bullet\hat{z}^\bullet + N[\hat{y}\hat{z}] = N[\hat{y}^\bullet\hat{z}^\bullet] + N[\hat{y}\hat{z}], \tag{9.36}$$

where the second equality applies on account of the original assumption about the times involved, the third involves the definition of the contraction, and the last one is correct since a contraction is a c-number. Assume now that Eq. (9.33) is valid for n operators and prove its correctness for $n+1$. One can then multiply Eq. (9.33) by a type II operator $\hat{d}$ on the left (also with a time later than that of $\hat{z}$) with the result that

$$\begin{aligned}\hat{d}N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\right]\hat{z} &= N\left[\hat{d}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}^\bullet\hat{z}^\bullet\right] + N\left[\hat{d}\hat{a}\hat{b}\hat{c}...\hat{x}^\bullet\hat{y}\hat{z}^\bullet\right] + ...\\ &+ N\left[\hat{d}\hat{a}^\bullet\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^\bullet\right] + \hat{d}N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right].\end{aligned} \tag{9.37}$$

Since all operators $\hat{a}\hat{b}\hat{c}..\hat{x}\hat{y}$ are also of type II and the contraction of $\hat{d}$ with $\hat{z}$ is a c-number, $\hat{d}$ can be taken inside the normal ordering except for the last term in Eq (9.37) since $\hat{z}$ is still an operator there. For this last term, however, one can write

$$\hat{d}N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] = N\left[\hat{d}^\bullet\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^\bullet\right] + N\left[\hat{d}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] \tag{9.38}$$

since

$$\hat{d}N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] = (-1)^p\hat{d}\hat{z}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y} = (-1)^p\mathcal{T}\left[\hat{d}\hat{z}\right]\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}$$

$$
\begin{aligned}
&= (-1)^p \hat{d}^{\bullet}\hat{z}^{\bullet}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y} + (-1)^p N\left[\hat{d}\hat{z}\right]\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y} \\
&= (-1)^{2p}\hat{d}^{\bullet}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^{\bullet} + (-1)^{2p} N\left[\hat{d}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right] \\
&= N\left[\hat{d}^{\bullet}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^{\bullet}\right] + N\left[\hat{d}\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right]. \qquad (9.39)
\end{aligned}
$$

This completes the proof of Eq. (9.33) for the assumed set of operators. Since Eq. (9.33) is now proven in this form, additional type I operators can be included by multiplying them in on the left; the additional contractions generated in this manner vanish and can therefore be included on the right side of Eq. (9.33) maintaining the same result.

Equation (9.33) can be extended to include normal-ordered products already containing contractions. This point can be understood by multiplying both sides of Eq. (9.33) with the contraction of the operators $\hat{d}$ and $\hat{w}$ (c-number) and making the appropriate sign changes on both sides which then cancel on account of the sign conventions

$$
\begin{aligned}
N\left[\hat{a}\hat{b}\hat{c}\hat{d}^{\circ}...\hat{w}^{\circ}\hat{x}\hat{y}\right]\hat{z} &= N\left[\hat{a}\hat{b}\hat{c}\hat{d}^{\circ}...\hat{w}^{\circ}\hat{x}\hat{y}^{\bullet}\hat{z}^{\bullet}\right] + N\left[\hat{a}\hat{b}\hat{c}\hat{d}^{\circ}...\hat{w}^{\circ}\hat{x}^{\bullet}\hat{y}\hat{z}^{\bullet}\right] + ... \\
&+ N\left[\hat{a}^{\bullet}\hat{b}\hat{c}\hat{d}^{\circ}...\hat{w}^{\circ}\hat{x}\hat{y}\hat{z}^{\bullet}\right] + N\left[\hat{a}\hat{b}\hat{c}\hat{d}^{\circ}...\hat{w}^{\circ}\hat{x}\hat{y}\hat{z}\right]. \quad (9.40)
\end{aligned}
$$

This result also holds when additional contractions are included in Eq. (9.40).

With these preliminary items out of the way, Wick's theorem can now be proven by induction. Eq. (9.30) is clearly correct for two operators

$$
\mathcal{T}\left[\hat{a}\hat{b}\right] = \hat{a}^{\bullet}\hat{b}^{\bullet} + N\left[\hat{a}\hat{b}\right] = N\left[\hat{a}^{\bullet}\hat{b}^{\bullet}\right] + N\left[\hat{a}\hat{b}\right] \qquad (9.41)
$$

Again, assume that Eq. (9.30) is valid for n operators and then multiply it by $\hat{A}$ from the right, where $\hat{A}$ has a time earlier than any of the other operators.

$$
\begin{aligned}
&\mathcal{T}\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right]\hat{A} = \mathcal{T}\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\hat{A}\right] \qquad (9.42) \\
&= N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\right]\hat{A} + N\left[\hat{a}^{\bullet}\hat{b}^{\bullet}\hat{c}...\hat{x}\hat{y}\hat{z}\right]\hat{A} + N\left[\hat{a}^{\bullet}\hat{b}\hat{c}^{\bullet}...\hat{x}\hat{y}\hat{z}\right]\hat{A} + ... \\
&+ N\left[\hat{a}^{\bullet}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}^{\bullet}\right]\hat{A} + N\left[\hat{a}\hat{b}^{\bullet}\hat{c}^{\bullet}...\hat{x}\hat{y}\hat{z}\right]\hat{A} + ... + N\left[\hat{a}^{\bullet}\hat{b}^{\bullet\bullet}\hat{c}...^{\bullet}...^{\bullet\bullet}\hat{x}\hat{y}\hat{z}\right]\hat{A} \\
&+ ... + N\left[\hat{a}^{\bullet}\hat{b}^{\bullet\bullet}\hat{c}^{\bullet\bullet\bullet}...\hat{x}^{\circ}\hat{y}^{\circ\circ}\hat{z}^{\circ\circ\circ}\right]\hat{A} \\
&= N\left[\hat{a}\hat{b}\hat{c}...\hat{x}\hat{y}\hat{z}\hat{A}\right] + N\left[\text{sum over all possible pairs of contractions}\right].
\end{aligned}
$$

The first equality in Eq. (9.42) is obtained directly from the left-hand side of Eq.(9.30) since $\hat{A}$ has a time earlier than any of the other operators. The second equality simply reflects the multiplication of $\hat{A}$ on the right side of Eq. (9.30). To obtain the last equality one simply uses Eq. (9.40) and its generalization (containing more contractions) to arrive at the last line which completes the proof for this particular time-ordering where $\hat{A}$ is earlier than any other operator. This restriction can be lifted by simply reordering each term in Eq. (9.42) without changing the result but lifting the restriction that $\hat{A}$ has the earliest times. The sign conventions introduced earlier ensure that Wick's theorem is valid in these other situations also. This completes the proof of Eq. (9.30).

The usefulness of this result which holds as an operator identity, becomes abundantly clear when the expectation value of a time-ordered product of operators is taken with respect to the noninteracting ground state $\left|\Phi_0^A\right\rangle$. In that case, only those terms in Eq. (9.42) that contain fully contracted contributions give nonvanishing results. If there are $2n$ operators in the time-ordered product, accordingly this results in $n!$ terms with n noninteracting propagators and a factor $(i\hbar)^n$, together with an overal sign to be discussed below.

9.4 Diagrams

The introduction of a graphical representation greatly facilitates the analysis of the perturbation expansion for the sp propagator. The direct application of Wick's theorem for the term with $n = 1$ containing the contribution of the auxiliary potential $\hat{U}$ in the numerator of Eq. (9.17) yields for the expectation values of the corresponding time-ordered product

$$\begin{aligned}
&\left\langle\Phi_0^A\right| \mathcal{T}\left[a_\gamma^\dagger(t_1)a_\delta(t_1)a_\alpha(t)a_\beta^\dagger(t')\right]\left|\Phi_0^A\right\rangle = \\
&\qquad -a_\alpha(t)^\bullet a_\beta^\dagger(t')^\bullet a_\delta(t_1)^\circ a_\gamma^\dagger(t_1^+)^\circ + a_\delta(t_1)^\bullet a_\beta^\dagger(t')^\bullet a_\alpha(t)^\circ a_\gamma^\dagger(t_1^+)^\circ \\
&\quad = -(i\hbar)^2\ G^{(0)}(\alpha,\beta;t-t')G^{(0)}(\delta,\gamma;t_1-t_1^+) \\
&\qquad\qquad +(i\hbar)^2\ G^{(0)}(\delta,\beta;t_1-t')G^{(0)}(\alpha,\gamma;t-t_1),
\end{aligned} \tag{9.43}$$

where an extra $+$ superscript has been added to the propagator with two t_1 arguments referring to the original ordering of the relevant operators as discussed in connection with Eq. (9.22). The resulting two contributions have a graphical representation shown in Fig. 9.2 with corresponding analytical