

IX. SINGLE-PARTICLE PROPAGATOR IN A MANY-PARTICLE SYSTEM

The sp propagator in a many-particle system is defined as an expectation value with respect to the exact ground state of the system of A particles, of an operator which represents both particle propagation as well as hole propagation. The latter term is naturally absent in the one-particle problem.

$$G(\alpha, \beta; t, t') = -i \frac{\langle \Psi_0^A | \mathcal{T}[a_{\alpha H}(t) a_{\beta H}^\dagger(t')] | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle}, \quad (530)$$

where $|\Psi_0^A\rangle$ is the Heisenberg ground state for the A -particle system and E_0^A the corresponding eigenvalue

$$\hat{H} |\Psi_0^A\rangle = E_0^A |\Psi_0^A\rangle. \quad (531)$$

The particle addition and removal operators in the definition of the sp propagator are given in the Heisenberg picture

$$\begin{aligned} a_{\alpha H}(t) &= e^{i\hat{H}t/\hbar} a_\alpha e^{-i\hat{H}t/\hbar} \\ a_{\alpha H}^\dagger(t) &= e^{i\hat{H}t/\hbar} a_\alpha^\dagger e^{-i\hat{H}t/\hbar}. \end{aligned} \quad (532)$$

The time-ordering operation \mathcal{T} is generalized here to include a sign change when two fermion operators are interchanged

$$\mathcal{T}[a_{\alpha H}(t) a_{\beta H}^\dagger(t')] = \theta(t-t') a_{\alpha H}(t) a_{\beta H}^\dagger(t') - \theta(t'-t) a_{\beta H}^\dagger(t') a_{\alpha H}(t). \quad (533)$$

Using the definition of the Heisenberg picture operators and the time-ordering operation for fermion operators one obtains

$$\begin{aligned} G(\alpha, \beta; t-t') &= -i \left\{ \theta(t-t') \frac{\langle \Psi_0^A | e^{i\hat{H}t/\hbar} a_\alpha e^{-i\hat{H}t/\hbar} e^{i\hat{H}t'/\hbar} a_\beta^\dagger e^{-i\hat{H}t'/\hbar} | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right. \\ &\quad \left. - \theta(t'-t) \frac{\langle \Psi_0^A | e^{i\hat{H}t'/\hbar} a_\beta^\dagger e^{-i\hat{H}t'/\hbar} e^{i\hat{H}t/\hbar} a_\alpha e^{-i\hat{H}t/\hbar} | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right\} \\ &= -i \left\{ \theta(t-t') e^{iE_0^A(t-t')/\hbar} \frac{\langle \Psi_0^A | a_\alpha e^{-i\hat{H}(t-t')/\hbar} a_\beta^\dagger | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right. \\ &\quad \left. - \theta(t'-t) e^{iE_0^A(t'-t)/\hbar} \frac{\langle \Psi_0^A | a_\beta^\dagger e^{-i\hat{H}(t'-t)/\hbar} a_\alpha | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right\} \\ &= -i \left\{ \theta(t-t') e^{iE_0^A(t-t')/\hbar} \frac{\langle \Psi_0^A | a_\alpha e^{-i\hat{H}(t-t')/\hbar} \sum_m |\Psi_m^{A+1}\rangle \langle \Psi_m^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right. \\ &\quad \left. - \theta(t'-t) e^{iE_0^A(t'-t)/\hbar} \frac{\langle \Psi_0^A | a_\beta^\dagger e^{-i\hat{H}(t'-t)/\hbar} \sum_n |\Psi_n^{A-1}\rangle \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right\} \\ &= -i \left\{ \theta(t-t') \sum_m e^{i(E_0^A - E_m^{A+1})(t-t')/\hbar} \frac{\langle \Psi_0^A | a_\alpha | \Psi_m^{A+1}\rangle \langle \Psi_m^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right. \\ &\quad \left. - \theta(t'-t) \sum_n e^{i(E_0^A - E_n^{A-1})(t'-t)/\hbar} \frac{\langle \Psi_0^A | a_\beta^\dagger | \Psi_n^{A-1}\rangle \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle}{\langle \Psi_0^A | \Psi_0^A \rangle} \right\}. \end{aligned} \quad (534)$$

As expected, the propagator depends only on the time difference $t-t'$. Note that the completeness of the exact eigenstates of \hat{H} for both the $A+1$ as well as the $A-1$ system has been used. In addition the results

$$\begin{aligned} \hat{H} |\Psi_m^{A+1}\rangle &= E_m^{A+1} |\Psi_m^{A+1}\rangle \\ \hat{H} |\Psi_n^{A-1}\rangle &= E_n^{A-1} |\Psi_n^{A-1}\rangle \end{aligned} \quad (535)$$

were incorporated. As in the sp problem, one can introduce the FT of the sp propagator which is more convenient for practical calculations

$$G(\alpha, \beta; \omega) = \int_{-\infty}^{\infty} d(t-t') e^{i\omega(t-t')} G(\alpha, \beta; t-t'). \quad (536)$$

As before, it is recommended to use the integral representation of the stepfunctions. The result of this *FT* can be expressed in various equivalent ways. The *FT* of the last expression for $G(\alpha, \beta; t-t')$ in Eq. (536) yields

$$\begin{aligned} G(\alpha, \beta; \omega) &= \hbar \sum_m \frac{\langle \Psi_0^A | a_\alpha | \Psi_m^{A+1} \rangle \langle \Psi_m^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle}{\hbar\omega - (E_m^{A+1} - E_0^A) + i\eta} + \hbar \sum_n \frac{\langle \Psi_0^A | a_\beta^\dagger | \Psi_n^{A-1} \rangle \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle}{\hbar\omega - (E_0^A - E_n^{A-1}) - i\eta} \\ &= \hbar \langle \Psi_0^A | a_\alpha \frac{1}{\hbar\omega - (\hat{H} - E_0^A) + i\eta} a_\beta^\dagger | \Psi_0^A \rangle + \hbar \langle \Psi_0^A | a_\beta^\dagger \frac{1}{\hbar\omega - (E_0^A - \hat{H}) - i\eta} a_\alpha | \Psi_0^A \rangle, \end{aligned} \quad (537)$$

where (for the moment) it has been assumed that $|\Psi_0^A\rangle$ is normalized. The first equality is known as the Lehmann representation [60] of the sp propagator. The last line is obtained by removing the complete set of exact $A+1$ -eigenstates in the first term and the complete set of $A-1$ -eigenstates in the second one, after replacing the eigenvalues E_m^{A+1} and E_n^{A-1} by \hat{H} . Note that **any** sp basis can be used in this formulation of the propagator. Many texts choose to specialize either to coordinate space or momentum representation. This does not always represent the appropriate choice especially when dealing with finite systems where comparisons with experimental results are readily possible. It is also instructive to compare this form of the sp propagator with the corresponding one for the sp problem (see Eq. (390)). Apart from the hole term which is naturally absent in the sp case there is a clear similarity between the two results. Indeed, the matrix elements involving the addition and removal operators obey Schrödinger-like equations as will be discussed in more detail later.

A. Spectral Functions and Occupation Numbers

In the case of finite systems, one can relate essentially all the information contained in the sp propagator to relevant experimental results. Consider first the information in the denominator. The positions of the poles signal the location of the excited states in the $A+1$ or $A-1$ particle systems. Note that it should be possible to reach those states by the addition (or removal) of a particle with sp quantum numbers α to (or from) the ground state of the A -particle system. In this context it is useful to visualize the addition or removal of a particle as a physical process that can be realized experimentally. Second, the information in the numerator determines the distribution of the corresponding transition strength from the ground state of the A particle system to these states in the $A \pm 1$ systems. This information is a crucial measure of the strength of the correlations in the system as they induce behavior which deviates from the independent particle model. It will also be possible to interpret the transition matrix elements of the particle addition or removal operator as wave functions when α corresponds to the coordinate representation (see later). A good tool to develop intuition for the effect of correlations on sp properties is provided by the spectral function. The hole part of the spectral function is the combined probability for removing a particle with quantum numbers α from the ground state while leaving the remaining $A-1$ -system at an energy $E_n^{A-1} = E_0^A - \hbar\omega$. It is related to the sp propagator by

$$\begin{aligned} S_h(\alpha, \omega) &= \frac{1}{\pi} \text{Im} G(\alpha, \alpha; \omega) && \hbar\omega < \epsilon_F^- \\ &= \hbar \sum_n \left| \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle \right|^2 \delta(\hbar\omega - (E_0^A - E_n^{A-1})). \end{aligned} \quad (538)$$

A similar probability for the addition of a particle with quantum numbers α leaving the $A+1$ -system at energy $E_m^{A+1} = E_0^A + \hbar\omega$ is obtained from

$$\begin{aligned} S_p(\alpha, \omega) &= -\frac{1}{\pi} \text{Im} G(\alpha, \alpha; \omega) && \hbar\omega > \epsilon_F^+ \\ &= \hbar \sum_m \left| \langle \Psi_m^{A+1} | a_\alpha^\dagger | \Psi_0^A \rangle \right|^2 \delta(\hbar\omega - (E_m^{A+1} - E_0^A)). \end{aligned} \quad (539)$$

This quantity is referred to as the particle spectral function. The corresponding Fermi energies are given by

$$\begin{aligned} \epsilon_F^- &= E_0^A - E_0^{A-1} \\ \epsilon_F^+ &= E_0^{A+1} - E_0^A. \end{aligned} \quad (540)$$

In obtaining the imaginary part of the propagator the very useful identity

$$\frac{1}{\omega \pm i\eta} = \mathcal{P} \frac{1}{\omega} \mp i\pi\delta(\omega) \quad (541)$$

has been used, where the symbol \mathcal{P} denotes the principal value. The above expressions for the spectral functions are particularly useful for analyzing finite systems where discrete bound states exist and for certain problems involving band structure, localization or external magnetic fields in condensed matter systems. In finite systems, like nuclei, there can be a considerable difference between ϵ_F^- and ϵ_F^+ . In infinite systems which are called “normal” this difference vanishes. Normality here refers to the presence of a discontinuity at the Fermi momentum in the momentum distribution. This discontinuity is 1 in the non-interacting system and vanishes for systems with pairing correlations like superfluids or superconductors.

The occupation number of a sp state α can be obtained from the hole part of the spectral function by

$$\begin{aligned} n(\alpha) &= \langle \Psi_0^A | a_\alpha^\dagger a_\alpha | \Psi_0^A \rangle = \sum_n \left| \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle \right|^2 \\ &= \int_{-\infty}^{\epsilon_F^-/\hbar} d\omega \hbar \sum_n \left| \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle \right|^2 \delta(\hbar\omega - (E_0^A - E_n^{A-1})) \\ &= \int_{-\infty}^{\epsilon_F^-/\hbar} d\omega S_h(\alpha, \omega). \end{aligned} \quad (542)$$

In a similar way one can obtain the depletion number from the particle part of the spectral function

$$\begin{aligned} d(\alpha) &= \langle \Psi_0^A | a_\alpha a_\alpha^\dagger | \Psi_0^A \rangle = \sum_m \left| \langle \Psi_m^{A+1} | a_\alpha^\dagger | \Psi_0^A \rangle \right|^2 \\ &= \int_{\epsilon_F^+/\hbar}^{\infty} d\omega \hbar \sum_m \left| \langle \Psi_m^{A+1} | a_\alpha^\dagger | \Psi_0^A \rangle \right|^2 \delta(\hbar\omega - (E_m^{A+1} - E_0^A)) \\ &= \int_{\epsilon_F^+/\hbar}^{\infty} d\omega S_p(\alpha, \omega). \end{aligned} \quad (543)$$

An important sum rule exists for $n(\alpha)$ and $d(\alpha)$ which can be obtained by using the anticommutation relation for a_α and a_α^\dagger

$$n(\alpha) + d(\alpha) = \langle \Psi_0^A | a_\alpha^\dagger a_\alpha | \Psi_0^A \rangle + \langle \Psi_0^A | a_\alpha a_\alpha^\dagger | \Psi_0^A \rangle = \langle \Psi_0^A | \Psi_0^A \rangle = 1. \quad (544)$$

This distribution between occupation and emptiness of a sp orbital in the correlated ground state is a sensitive measure of the strength of correlations provided a suitable sp basis is chosen (to be discussed later). The sp propagator will also provide the expectation value of any one-body operator in the ground state

$$\langle \Psi_0^A | \hat{O} | \Psi_0^A \rangle = \sum_{\alpha, \beta} \langle \alpha | O | \beta \rangle \langle \Psi_0^A | a_\alpha^\dagger a_\beta | \Psi_0^A \rangle = \sum_{\alpha, \beta} \langle \alpha | O | \beta \rangle n_{\alpha\beta}. \quad (545)$$

Here, $n_{\alpha\beta}$ is the one-body density matrix element which can be obtained from the sp propagator using the Lehmann representation

$$\begin{aligned} n_{\beta\alpha} &= \int \frac{d\omega}{2\pi i} e^{i\omega\eta} G(\alpha, \beta; \omega) \\ &= \int \frac{d\omega}{2\pi i} e^{i\omega\eta} \hbar \sum_m \frac{\langle \Psi_0^A | a_\alpha | \Psi_m^{A+1} \rangle \langle \Psi_m^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle}{\hbar\omega - (E_m^{A+1} - E_0^A) + i\eta} + \int \frac{d\omega}{2\pi i} e^{i\omega\eta} \hbar \sum_n \frac{\langle \Psi_0^A | a_\beta^\dagger | \Psi_n^{A-1} \rangle \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle}{\hbar\omega - (E_0^A - E_n^{A-1}) - i\eta} \\ &= \sum_n \langle \Psi_0^A | a_\beta^\dagger | \Psi_n^{A-1} \rangle \langle \Psi_n^{A-1} | a_\alpha | \Psi_0^A \rangle \\ &= \langle \Psi_0^A | a_\beta^\dagger a_\alpha | \Psi_0^A \rangle. \end{aligned} \quad (546)$$

Note the convergence factor in the integral which requires closing the contour in the upper half of the complex plane. Therefore, only the (nondiagonal) hole part of the spectral function contributes.

The energy of the ground state can also be obtained from the sp propagator provided that, as has been assumed up to now, there are only two-body interactions between the particles. This is a quite remarkable result. Again, only the hole part of the propagator is required for this result. Consider the following integral

$$\begin{aligned}
I_\alpha &= \int \frac{d\omega}{2\pi i} e^{i\omega\eta} \hbar\omega G(\alpha, \alpha; \omega) \\
&= \sum_m \int \frac{d(\hbar\omega)}{2\pi i} e^{i\omega\eta} \hbar\omega \frac{\langle \Psi_0^A | a_\alpha^\dagger | \Psi_m^{A-1} \rangle \langle \Psi_m^{A-1} | a_\alpha | \Psi_0^A \rangle}{\hbar\omega - (E_0^A - E_m^{A-1}) - i\eta} \\
&= \sum_m (E_0^A - E_m^{A-1}) \langle \Psi_0^A | a_\alpha^\dagger | \Psi_m^{A-1} \rangle \langle \Psi_m^{A-1} | a_\alpha | \Psi_0^A \rangle \\
&= \langle \Psi_0^A | a_\alpha^\dagger a_\alpha \hat{H} | \Psi_0^A \rangle - \sum_m \langle \Psi_0^A | a_\alpha^\dagger E_m^{A-1} | \Psi_m^{A-1} \rangle \langle \Psi_m^{A-1} | a_\alpha | \Psi_0^A \rangle \\
&= \langle \Psi_0^A | a_\alpha^\dagger a_\alpha \hat{H} | \Psi_0^A \rangle - \langle \Psi_0^A | a_\alpha^\dagger \hat{H} a_\alpha | \Psi_0^A \rangle = \langle \Psi_0^A | a_\alpha^\dagger [a_\alpha, \hat{H}] | \Psi_0^A \rangle \\
&= \sum_\beta \langle \alpha | T | \beta \rangle \langle \Psi_0^A | a_\alpha^\dagger a_\beta | \Psi_0^A \rangle + \sum_{\beta\gamma\delta} (\alpha\beta | V | \gamma\delta) \langle \Psi_0^A | a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma | \Psi_0^A \rangle.
\end{aligned} \tag{547}$$

Summing this expression over α one then obtains

$$\sum_\alpha I_\alpha = \langle \Psi_0^A | \hat{T} | \Psi_0^A \rangle + 2 \langle \Psi_0^A | \hat{V} | \Psi_0^A \rangle. \tag{548}$$

In arriving at Eq. (547) the result

$$[a_\alpha, \hat{H}] = \sum_\beta \langle \alpha | T | \beta \rangle a_\beta + \sum_{\beta\gamma\delta} (\alpha\beta | V | \gamma\delta) a_\beta^\dagger a_\delta a_\gamma \tag{549}$$

has been used (see Eqs. (131) and (136)). Combining the result of Eq. (548) with the expectation value for the kinetic energy one obtains the desired result

$$\begin{aligned}
E_0^A &= \langle \Psi_0^A | \hat{H} | \Psi_0^A \rangle \\
&= \int \frac{d\omega}{4\pi i} e^{i\omega\eta} \sum_{\alpha,\beta} \{ \langle \alpha | T | \beta \rangle + \hbar\omega \delta_{\alpha,\beta} \} G(\beta, \alpha; \omega) \\
&= \frac{1}{2} \sum_{\alpha,\beta} \langle \alpha | T | \beta \rangle n_{\alpha\beta} + \frac{1}{2} \sum_\alpha \int_{-\infty}^{\epsilon_F^-/\hbar} d\omega \hbar\omega S_h(\alpha, \omega),
\end{aligned} \tag{550}$$

where the validity of the last equality can be checked by inserting the definition of $S_h(\alpha, \omega)$ given in Eq. (538).

B. Single-Particle Propagator for \hat{H}_0 Problem

In the case the many-particle problem does not contain a two-body interaction operator, for example with hamiltonian \hat{H}_0 and ground state $|\Phi_0\rangle$, the sp propagator becomes

$$G^{(0)}(\alpha, \beta; t - t') = -i \langle \Phi_0 | \mathbb{T}[a_{\alpha_I}(t) a_{\beta_I}^\dagger(t')] | \Phi_0 \rangle, \tag{551}$$

where $|\Phi_0\rangle$ is the nondegenerate ground state of \hat{H}_0 for A particles with eigenvalue

$$E_0 = \sum_{\lambda < F} \epsilon_\lambda \tag{552}$$

and therefore

$$\hat{H}_0 |\Phi_0\rangle = E_0 |\Phi_0\rangle. \tag{553}$$

The extension to treating propagators for open shell systems is non-trivial and not well developed. It will not be further discussed here. For example, the state $|\Phi_0\rangle$ can correspond to the Slater determinant of an infinite Fermi

system, a closed-shell atom, or a closed-shell nucleus. The particle addition and removal operators in the definition of the so-called unperturbed sp propagator, are given in the interaction picture

$$\begin{aligned} a_{\alpha_I}(t) &= e^{i\hat{H}_0 t/\hbar} a_{\alpha} e^{-i\hat{H}_0 t/\hbar} \\ a_{\alpha_I}^{\dagger}(t) &= e^{i\hat{H}_0 t/\hbar} a_{\alpha}^{\dagger} e^{-i\hat{H}_0 t/\hbar}. \end{aligned} \quad (554)$$

Choosing the sp basis $\{|\lambda\rangle\}$ in which H_0 is diagonal, and using the definition of the interaction picture operators and the time-ordering operation for fermion operators, one obtains

$$\begin{aligned} G^{(0)}(\lambda, \lambda'; t - t') &= -i\{\theta(t - t') \langle \Phi_0 | e^{i\hat{H}_0 t/\hbar} a_{\lambda} e^{-i\hat{H}_0 t/\hbar} e^{i\hat{H}_0 t'/\hbar} a_{\lambda'}^{\dagger} e^{-i\hat{H}_0 t'/\hbar} | \Phi_0 \rangle \\ &\quad - \theta(t' - t) \langle \Phi_0 | e^{i\hat{H}_0 t'/\hbar} a_{\lambda'}^{\dagger} e^{-i\hat{H}_0 t'/\hbar} e^{i\hat{H}_0 t/\hbar} a_{\lambda} e^{-i\hat{H}_0 t/\hbar} | \Phi_0 \rangle\} \\ &= -i\{\theta(t - t') \delta_{\lambda, \lambda'} \theta(\lambda - F) e^{iE_0(t-t')/\hbar} e^{-i(E_0 + \epsilon_{\lambda})(t-t')/\hbar} \\ &\quad - \theta(t' - t) \delta_{\lambda, \lambda'} \theta(F - \lambda) e^{iE_0(t'-t)/\hbar} e^{-i(E_0 - \epsilon_{\lambda})(t'-t)/\hbar}\} \\ &= -i\{\theta(t - t') \delta_{\lambda, \lambda'} \theta(\lambda - F) e^{-i\epsilon_{\lambda}(t-t')/\hbar} \\ &\quad - \theta(t' - t) \delta_{\lambda, \lambda'} \theta(F - \lambda) e^{i\epsilon_{\lambda}(t'-t)/\hbar}\} \end{aligned} \quad (555)$$

which represents the propagation of a particle or a hole on top of the non-interacting ground state. Note that one has to use

$$\begin{aligned} \hat{H}_0 a_{\lambda}^{\dagger} | \Phi_0 \rangle &= (E_0 + \epsilon_{\lambda}) a_{\lambda}^{\dagger} | \Phi_0 \rangle & \lambda > F \\ \hat{H}_0 a_{\lambda} | \Phi_0 \rangle &= (E_0 - \epsilon_{\lambda}) a_{\lambda} | \Phi_0 \rangle & \lambda < F \end{aligned} \quad (556)$$

in obtaining the above result. Choosing another sp basis leads to a slightly more involved result which can be related to the present one by a double basis transformation both for the particle addition as well as the particle removal operator.

Again it is fruitful to consider the FT of the unperturbed sp propagator

$$G^{(0)}(\lambda, \lambda'; \omega) = \delta_{\lambda, \lambda'} \hbar \left\{ \frac{\theta(\lambda - F)}{\hbar\omega - \epsilon_{\lambda} + i\eta} + \frac{\theta(F - \lambda)}{\hbar\omega - \epsilon_{\lambda} - i\eta} \right\}. \quad (557)$$

This result can also be obtained directly from the definition of the unperturbed sp propagator in a general sp basis

$$G^{(0)}(\alpha, \beta; \omega) = \hbar \langle \Phi_0 | a_{\alpha} \frac{1}{\hbar\omega - (\hat{H}_0 - E_0) + i\eta} a_{\beta}^{\dagger} | \Phi_0 \rangle + \hbar \langle \Phi_0 | a_{\beta}^{\dagger} \frac{1}{\hbar\omega - (E_0 - \hat{H}_0) - i\eta} a_{\alpha} | \Phi_0 \rangle \quad (558)$$

which can be compared to the exact sp propagator and the one for the sp problem.

The spectral functions for the non-interacting system are particularly simple. Using again the sp basis $\{|\lambda\rangle\}$ which diagonalizes H_0 , one has the following hole spectral function

$$\begin{aligned} S_h(\lambda, \omega) &= \frac{1}{\pi} \text{Im} g^{(0)}(\lambda, \lambda; \omega) \\ &= \delta\left(\omega - \frac{\epsilon_{\lambda}}{\hbar}\right) \theta(F - \lambda) & \hbar\omega < \epsilon_F^{(0)-} \end{aligned} \quad (559)$$

and particle spectral function

$$\begin{aligned} S_p(\lambda, \omega) &= -\frac{1}{\pi} \text{Im} g^{(0)}(\lambda, \lambda; \omega) \\ &= \delta\left(\omega - \frac{\epsilon_{\lambda}}{\hbar}\right) \theta(\lambda - F) & \hbar\omega > \epsilon_F^{(0)+}. \end{aligned} \quad (560)$$

This shows that the poles in the unperturbed spectral function occur at the sp energies which correspond to the eigenvalues of the sp hamiltonian H_0 . The sp states that are occupied yield contributions to the hole spectral function, those that are empty contribute to the particle spectral function. In this independent particle model description for an atom, a nucleus, or a Fermi gas, the hole spectral function displays δ -function peaks with strength 1 which corresponds to the certainty that it is possible to remove a particle from such an occupied orbital. The same holds for the particle spectral function where this certainty relates to the possibility of adding a particle to an empty orbit. The simplicity

of these results is related to the choice of the sp basis. The position of the poles in the sp propagator does not change of course but the numerator changes. As an example, consider the sp propagator in the $\{|\mathbf{r}m_s\rangle\}$ representation

$$\begin{aligned}
G^{(0)}(\mathbf{r}m_s, \mathbf{r}'m'_s; \omega) &= \hbar \langle \Phi_0 | a_{\mathbf{r}m_s} \frac{1}{\hbar\omega - (\hat{H}_0 - E_0) + i\eta} a_{\mathbf{r}'m'_s}^\dagger | \Phi_0 \rangle + \hbar \langle \Phi_0 | a_{\mathbf{r}'m'_s}^\dagger \frac{1}{\hbar\omega - (E_0 - \hat{H}_0) - i\eta} a_{\mathbf{r}m_s} | \Phi_0 \rangle \\
&= \hbar \sum_{\lambda\lambda'} \langle \mathbf{r}m_s | \lambda \rangle \langle \lambda' | \mathbf{r}'m'_s \rangle \langle \Phi_0 | a_\lambda \frac{1}{\hbar\omega - (\hat{H}_0 - E_0) + i\eta} a_{\lambda'}^\dagger | \Phi_0 \rangle \\
&\quad + \hbar \sum_{\lambda\lambda'} \langle \mathbf{r}m_s | \lambda \rangle \langle \lambda' | \mathbf{r}'m'_s \rangle \langle \Phi_0 | a_{\lambda'}^\dagger \frac{1}{\hbar\omega - (E_0 - \hat{H}_0) - i\eta} a_\lambda | \Phi_0 \rangle \\
&= \hbar \sum_\lambda \left\{ \frac{\langle \mathbf{r}m_s | \lambda \rangle \langle \lambda | \mathbf{r}'m'_s \rangle \theta(\lambda - F)}{\hbar\omega - \epsilon_\lambda + i\eta} + \frac{\langle \mathbf{r}m_s | \lambda \rangle \langle \lambda | \mathbf{r}'m'_s \rangle \theta(F - \lambda)}{\hbar\omega - \epsilon_\lambda - i\eta} \right\} \\
&= \hbar \sum_\lambda \left\{ \frac{u_\lambda(\mathbf{r}m_s) u_\lambda^*(\mathbf{r}'m'_s) \theta(\lambda - F)}{\hbar\omega - \epsilon_\lambda + i\eta} + \frac{u_\lambda(\mathbf{r}m_s) u_\lambda^*(\mathbf{r}'m'_s) \theta(F - \lambda)}{\hbar\omega - \epsilon_\lambda - i\eta} \right\}. \tag{561}
\end{aligned}$$

Note that the numerators in Eq. (561) contain again the relevant sp wave functions which in this simple example represent the transition matrix elements of the particle addition and removal operators in the coordinate representation. Occupation numbers are most easily evaluated in the $\{|\lambda\rangle\}$ basis. The resulting occupation numbers then read (not surprisingly)

$$n(\lambda) = \int_{-\infty}^{\epsilon_F^{(0)-}/\hbar} d\omega \delta\left(\omega - \frac{\epsilon_\lambda}{\hbar}\right) \theta(F - \lambda) = \theta(F - \lambda). \tag{562}$$