Lecture Notes: Ch. 7 Particles and Quasiparticles

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1 Greens Functions for Coupled Systems

In many areas of modern theoretical physics—especially in the study of interacting many-body systems—it is common to treat only a few degrees of freedom explicitly while incorporating the effects of the remainder of the system through effective interactions. Such an approach allows one to work in a reduced Hilbert space and replace the original static potentials by *frequency-dependent* effective fields. This section develops the basic framework that underpins many methods in electronic structure and many-body theory.

1.1 Reduction of the Full Problem

Suppose we begin with a full $m \times m$ eigenvalue problem that is partitioned into two parts. The first part is a "small" subsystem of dimension n, and the second part (of dimension $m-n$) represents the rest of the system. In block-matrix form the eigenvalue problem is written as

$$\begin{pmatrix} S & C_1 \\ C_2 & R \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \omega \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \tag{7.1}$$

where S is an operator in the small space, R acts in the rest of the system, and C_1, C_2 describe the coupling between the two subspaces.

If we assume that $(R-\omega)$ is invertible, the degrees of freedom in the larger space can be formally eliminated. In fact, one immediately obtains

$$\phi_2 = -(R-\omega)^{-1} C_2 \, \phi_1. \tag{7.2}$$

Substituting Eq. (7.2) into the equation for ϕ_1, the effective equation in the small space becomes

$$\Big[S - C_1 (R-\omega)^{-1} C_2 \Big] \phi_1 \equiv \tilde{S}(\omega) \phi_1 = \omega \, \phi_1. \tag{7.3}$$

Here the operator $\tilde{S}(\omega)$ is frequency dependent due to the elimination of the larger space. Even though this transformation is exact when solved together with Eq. (7.2), if one retains only the solution in the small space, some information about the full eigenvectors is lost. The price to pay is that one must solve the non-linear eigenvalue problem in Eq. (7.3).

1.2 Green's Function Formulation

An alternative approach to treating the coupled system is provided by Green's function techniques. The Green's function for the entire system, G^{tot}, is defined by

$$\big[\omega - H\big] G^{\text{tot}} = I, \tag{7.4}$$

where I is the identity operator and H is the full Hamiltonian. We can partition H as well as G^{tot} into blocks corresponding to the small space and the rest:

$$H = \begin{pmatrix} H_S & H_{SR} \\ H_{RS} & H_R \end{pmatrix}, \quad G^{\text{tot}} = \begin{pmatrix} G_S & G_{SR} \\ G_{RS} & G_R \end{pmatrix}, \quad I = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}. \tag{7.5}$$

Here, H_S is the Hamiltonian in the small subspace, H_R is the Hamiltonian for the remaining part, and H_{SR} (with its adjoint H_{RS}) mediates the coupling.

Algebraic manipulations analogous to those in the eigenvalue problem lead to an expression for the Green's function restricted to the small subspace:

$$G_S(\omega) = \Big[\omega - H_S - H_{SR}(\omega - H_R)^{-1} H_{RS}\Big]^{-1} = \Big[[G_S^0(\omega)]^{-1} - H_{SR} G_R^0(\omega) H_{RS}\Big]^{-1}, \tag{7.6}$$

where

$$G_S^0(\omega) = (\omega - H_S)^{-1}, \quad G_R^0(\omega) = (\omega - H_R)^{-1}$$

are the Green's functions for the decoupled small system and the rest, respectively.

1.3 The Dyson Equation and Self-Energy

Equation (7.6) can be re-expressed in the compact form of a Dyson equation:

$$G_S(\omega) = \Big[[G_S^0(\omega)]^{-1} - \Sigma_S(\omega)\Big]^{-1}, \tag{7.7}$$

where the frequency-dependent self-energy is defined as

$$\Sigma_S(\omega) = [G_S^0(\omega)]^{-1} - [G_S(\omega)]^{-1} = H_{SR} G_R^0(\omega) H_{RS}. \tag{7.8}$$

This self-energy $\Sigma_S(\omega)$ summarizes all the effects of the coupling to the rest of the system on the dynamics of the small subsystem. It effectively renormalizes the bare propagator $G_S^0(\omega)$ into the full Green's function $G_S(\omega)$.

1.4 Implications

The key outcomes of this analysis can be summarized as follows:

- **Frequency Dependence:** Even if the original Hamiltonian contains only static interactions, eliminating the larger space introduces a dynamical (frequency-dependent) self-energy. This feature is crucial in many-body theory where interactions renormalize the energies and lifetimes of excitations.

- **Effective Reduction:** The reduction of the full eigenvalue problem to the small space leads to an effective operator $\tilde{S}(\omega)$ (or, equivalently, an effective Green's function via the Dyson equation) that encapsulates the influence of the remainder of the system.

- **Approximation Strategies:** In practical calculations (such as in the GW approximation or dynamical mean-field theory), the larger space is treated approximately. The only required information is its projection onto the small subspace, as embodied in the self-energy $\Sigma_S(\omega)$.
- **Nonlinearity:** The effective eigenvalue problem in Eq. (7.3) is nonlinear in ω, which reflects the complexity introduced by the coupling.

These points illustrate the power and generality of the Green's function formalism. By reformulating the problem in terms of an effective dynamical self-energy, one can systematically incorporate the influence of a vast number of degrees of freedom into a manageable description.

2 Focus: Self Energy and Dyson Equations

In the treatment of interacting many-body systems it is often advantageous to focus on a reduced (or "small") subspace in which the key degrees of freedom are treated explicitly. In this approach the effects of the remainder of the system are incorporated via a frequency-dependent self-energy, $\Sigma(\omega)$. In practice the quantity of interest is the Green's function $G(\omega)$ in the small space, and all quantities (such as $G_0(\omega)$ and $\Sigma(\omega)$) are defined there. In this section we elaborate on the fundamental relation between $G(\omega)$ and $\Sigma(\omega)$, derive the Dyson series, and then extend the discussion to screening effects.

2.1 The Dyson Equation and the Self-Energy

Starting from the result derived earlier (Eq. (7.7)) for the Green's function in the small subspace, one may recast it in an expansion that highlights the role of the self-energy:

$$G(\omega) = \left[1 - G_0(\omega)\Sigma(\omega)\right]^{-1} G_0(\omega) = G_0(\omega)+G_0(\omega)\Sigma(\omega)G_0(\omega)+G_0(\omega)\Sigma(\omega)G_0(\omega)\Sigma(\omega)G_0(\omega)+\cdots , \tag{7.9}$$

where $G_0(\omega)$ is the bare (or unperturbed) Green's function. This expansion illustrates the picture of a particle propagating first as a bare particle, then interacting via $\Sigma(\omega)$, then propagating again via $G_0(\omega)$, and so on. In other words, the self-energy includes *all* processes that cannot be decomposed into simpler propagation events connected solely by $G_0(\omega)$. In many contexts, $\Sigma(\omega)$ is said to be *proper* or *irreducible*, in contrast to the *reducible* self-energy defined by

$$\Sigma_{\text{red}} = \Sigma + \Sigma G_0 \Sigma + \Sigma G_0 \Sigma G_0 \Sigma + \cdots ,$$

which would lead to an expression for the full Green's function as $G = G_0\, \Sigma_{\text{red}}\, G_0$.

The infinite series of terms in Eq. (7.9) can be summed compactly, yielding the standard Dyson equation:

$$G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega). \tag{7.10}$$

This form is very general. It represents an integral equation that links the bare propagation $G_0(\omega)$ to the dressed propagation $G(\omega)$ through the kernel $\Sigma(\omega)$ which encodes the effects of all interactions (or couplings) beyond the unperturbed system.

Interpretation and Applications

The Dyson equation, whether written as Eq. (7.9) or (7.10), provides a unified framework to account for the effects of interactions. In the case of electrons, the self-energy $\Sigma(\omega)$ may include contributions from exchange, correlation, and screening effects. For example:

- In the GW approximation, one approximates the exchange-correlation part of the self-energy by $\Sigma_{xc} = iGW$, where W is the dynamically screened Coulomb interaction.
- In dynamical mean-field theory (DMFT), the self-energy is typically assumed to be short range in real space.

Explicit rules and approximations for constructing $\Sigma(\omega)$ can be found in various texts (see, e.g., Refs. [38, 47, 149, 227]).

2.2 Dyson Equation for Screening

The concept behind the Dyson equation is not limited to the one-particle Green's function. A completely analogous formalism applies to the problem of screening. Consider two particles interacting via the bare Coulomb interaction, v_c. When a particle is inserted into the system it induces a polarization in the surrounding medium, which in turn modifies the interaction between the particles. If we denote by $P(\omega)$ the *proper* (irreducible) polarizability (as opposed to the reducible polarizability $\chi(\omega)$ which includes chains of Coulomb interactions), then the screened interaction $W(\omega)$ can be written as an infinite series analogous to Eq. (7.9):

$$W(\omega) = v_c + v_c\chi(\omega)v_c = v_c + v_cP(\omega)v_c + \cdots .$$

This series can be summed to give

$$W(\omega) = v_c + v_cP(\omega)W(\omega) \quad \Longrightarrow \quad W(\omega) = \Big[v_c^{-1} - P(\omega)\Big]^{-1}. \tag{7.11}$$

Here, v_c is the bare Coulomb interaction, and $W(\omega)$ is the dressed (or screened) interaction. The kernel $P(\omega)$ captures the dynamic polarization effects induced in the system.

Physical Interpretation

The Dyson equation for screening, Eq. (7.11), has the following features:

- Just as $\Sigma(\omega)$ encapsulates all processes that renormalize the one-particle propagator, $P(\omega)$ accounts for the collective response of the electrons to an external perturbation.
- The dressed interaction $W(\omega)$ is central to many-body perturbation theory. For example, in the GW approximation, it is this dynamically screened interaction that enters the expression for Σ_{xc}.
- The dependence of both $G(\omega)$ and $W(\omega)$ on the complex frequency ω (or z) determines the causal (retarded, advanced, or time-ordered) properties of these quantities.

3 Example: A Single State Coupled to a Continuum

In this section we consider a simple, exactly solvable example: a single discrete state (labeled 0) that is coupled to a continuum of non-interacting states. Despite its simplicity, this model captures many of the qualitative features of more complex systems such as an impurity embedded in a crystal or an interacting electron coupled to a continuum of excitations.

3.1 The Model Hamiltonian

We consider a state with energy ε_0 that is coupled to a set of states labeled by $l = 1, 2, \dots$ with eigenvalues ε_l. The coupling between the state 0 and state l is given by the matrix element t_{0l}. The Hamiltonian can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_{0,\text{rest}} + \hat{H}_{\text{rest}} = \varepsilon_0\, c_0^\dagger c_0 + \sum_{l=1} t_{0l}\left(c_l^\dagger c_0 + c_0^\dagger c_l\right) + \sum_{l=1} \varepsilon_l\, c_l^\dagger c_l, \tag{7.12}$$

where $c_0^\dagger$ (c_0) creates (annihilates) a particle in the discrete state (space S) and $c_l^\dagger$ (c_l) acts on the continuum states (space R).

3.2 Green's Function and Coupled Equations

The Green's function for the entire system is defined via

$$\left[\omega - \hat{H}\right] G(\omega) = I,$$

where ω can be real or complex. Following the general procedure outlined in Section 7.1, the equations for the relevant components of the Green's function become:

$$\begin{aligned}(\omega - \varepsilon_0)\, G_{00}(\omega) - \sum_{l=1} t_{0l}\, G_{l0}(\omega) &= 1,\\ (\omega - \varepsilon_l)\, G_{l0}(\omega) - t_{l0}\, G_{00}(\omega) &= 0,\end{aligned} \tag{7.13}$$

where an equation for $G_{ll'}(\omega)$ exists but is not needed for our purposes.

Solving these equations for $G_{00}(\omega)$, one finds

$$G_{00}(\omega) = \frac{1}{\omega - \varepsilon_0 - \Delta(\omega)}, \tag{7.14}$$

where the *hybridization function* $\Delta(\omega)$ (a specific example of a generalized self-energy as defined in Eq. (7.8)) is given by

$$\Delta(\omega) = \sum_{l=1} \frac{t_{0l}^2}{\omega - \varepsilon_l} \quad \longrightarrow \quad \Delta(\omega) = \int d\varepsilon\, \frac{t(\varepsilon)^2\, \rho(\varepsilon)}{\omega - \varepsilon}. \tag{7.15}$$

Here, $\rho(\varepsilon)$ is the unperturbed density of states of the continuum, and $t(\varepsilon)$ represents the coupling strength (with, for example, $t(\varepsilon) = t_{0l}/\sqrt{N}$ when the sum is over N states so that the coupling to each state decreases appropriately in the continuum limit). In this limit, the discrete poles merge to form a branch cut along the real axis.

3.3 The Spectral Function

Using Eqs. (5.91) and (5.92) (from earlier chapters), the spectral function for the discrete state is given by

$$A(\omega) = \frac{1}{\pi} \frac{|\operatorname{Im}\Delta(\omega)|}{\left[\omega - \varepsilon_0 - \operatorname{Re}\Delta(\omega)\right]^2 + \left[\operatorname{Im}\Delta(\omega)\right]^2}. \tag{7.16}$$

In the absence of coupling, $A(\omega)$ reduces to $\delta(\omega - \varepsilon_0)$; when coupling is present, the peak is shifted by $\operatorname{Re}\Delta(\omega)$ and broadened by $\operatorname{Im}\Delta(\omega)$.

To extract $\operatorname{Im}\Delta(\omega)$, one considers the analytic continuation slightly off the real axis:

$$\lim_{\eta\to 0^+} \Delta(\omega \pm i\eta) = \mathcal{P} \int d\varepsilon \, \frac{t(\varepsilon)^2 \, \rho(\varepsilon)}{\omega - \varepsilon} \mp i\pi \, \rho(\omega) \, t(\omega)^2, \tag{7.17}$$

where $\mathcal{P}$ denotes the principal value.

If the coupling $t(\varepsilon)$ and density of states $\rho(\varepsilon)$ are approximately constant (denoted $\bar{t}$ and $\bar{\rho}$), then $\Delta(\omega \pm i\eta)$ simplifies to a purely imaginary constant:

$$\Delta = \mp i\pi \, \bar{\rho} \, \bar{t}^2.$$

Under these approximations, the spectral function becomes a Lorentzian,

$$A(\omega) = \frac{1}{\pi|\Delta|} \frac{1}{(\omega - \varepsilon_0)^2 + |\Delta|^2}. \tag{7.18}$$

This Lorentzian profile can be interpreted as a resonance, where the width $|\Delta|$ is related to the lifetime for the decay of the discrete state into the continuum.

3.4 Physical Interpretation and Applications

This model is directly analogous to the problem of an impurity embedded in a crystal: the discrete level with energy ε_0 represents an impurity state, while the continuum represents the host crystal's states. In this context, the magnitude $|\Delta|$ corresponds to the escape rate (or decay rate) of a particle from the impurity state into the continuum. Moreover, the structure of $\Delta(\omega)$ can lead to additional features in the spectral function beyond a simple Lorentzian, illustrating how coupling to a continuum can produce complex many-body effects. Such ideas are central to understanding the Anderson impurity model (see Sec. 3.5) and form the basis for dynamical mean-field theory (DMFT) as discussed in later chapters.

4 Interacting Systems – The Self-Energy and Spectral Function

Thus far we have seen how coupling a small subspace to a larger one produces a frequency-dependent self-energy even in non-interacting systems. In this section we extend these ideas to *interacting* electrons. Our aim is to understand how the many-body interaction

$$\hat{V} = \frac{1}{2} \sum_{ijkl} v_{ijkl} \, c_i^\dagger c_j^\dagger c_k c_l$$

modifies the one-particle Green's function and gives rise to a self-energy $\Sigma(\omega)$ that encapsulates the effects of coupling between a state in which a particle is added (or removed) and the excited states of the $(N \pm 1)$-electron system.

4.1 The Interacting Green's Function

Consider a system described by

$$\hat{H} = \hat{H}_0 + \hat{V}, \quad \text{with} \quad \hat{H}_0 = \sum_{ij} h_{ij}\, c_i^\dagger c_j.$$

At zero temperature, the one-electron Green's function for electron addition (in a basis labeled by $i, j, \ldots$) is defined as

$$G^{\text{el}}_{ij}(\omega) = \langle N, 0|\, c_i \left[\omega - \hat{H} + E_N\right]^{-1} c_j^\dagger\, |N, 0\rangle, \tag{7.19}$$

where $|N, 0\rangle$ is the ground state of the N-electron system with energy E_N. In the absence of interactions, one can choose the states $c_j^\dagger|N, 0\rangle$ to be eigenstates of $\hat{H}_0$ so that

$$G^{\text{el}}_{ij}(\omega) \sim \frac{\delta_{ij}}{\omega - \varepsilon_i^0},$$

with ε_i^0 the independent-particle eigenenergies. In the interacting case, however, the added (or removed) particle becomes coupled to a continuum of excited states. In our earlier discussion the decoupled (or mean-field) Green's function is denoted G_0, while the full, interacting Green's function is G.

4.2 Defining the Self-Energy

Following the general approach of Secs. 7.1 and 7.2, one can relate the interacting and non-interacting Green's functions via the self-energy:

$$\Sigma(\omega) = [G_0(\omega)]^{-1} - G^{-1}(\omega). \tag{7.20}$$

In this expression each quantity is understood to be a matrix in the chosen one-particle basis. Physically, $\Sigma(\omega)$ contains all the processes in which an added particle (or hole) couples to the excitations of the system. In a perturbative expansion, the zero-order term yields $G_0(\omega)$ (corresponding to no coupling), the first-order terms produce the Hartree and Fock contributions, and higher-order terms describe the correlation effects.

4.3 Application to Crystalline Solids

For electrons in a crystal the independent-particle Green's function can be written as

$$G_k^0(\omega) = \frac{1}{\omega - \varepsilon_k^0}, \tag{5.106 (recalled)}$$

where ε_k^0 is the energy for momentum k. In the presence of interactions the Green's function becomes

$$G_k(\omega) = \frac{1}{\omega - \varepsilon_k^0 - \Sigma_k(\omega)}. \tag{7.21}$$

Thus, the self-energy $\Sigma_k(\omega)$ induces a shift in the energy levels (through its real part) and introduces a finite lifetime (through its imaginary part).

4.4 Spectral Function and Quasi-Particles

The spectral function is defined as

$$A_k(\omega) = \frac{1}{\pi} \, |\operatorname{Im} G_k(\omega)| = \frac{1}{\pi} \frac{|\operatorname{Im} \Sigma_k(\omega)|}{\Big[\omega - \varepsilon_k^0 - \operatorname{Re} \Sigma_k(\omega)\Big]^2 + [\operatorname{Im} \Sigma_k(\omega)]^2}. \tag{7.22}$$

In the non-interacting limit, $\Sigma_k(\omega)$ vanishes and $A_k(\omega)$ reduces to a delta function centered at ε_k^0. In the interacting system, the real part of $\Sigma_k(\omega)$ shifts the peak position, while the imaginary part leads to a broadening. The new peak position, corresponding to the quasi-particle energy, is determined by the solution of

$$\varepsilon_k = \varepsilon_k^0 + \operatorname{Re} \Sigma_k(\omega = \varepsilon_k). \tag{7.23}$$

When the imaginary part is small, the spectral function exhibits a sharp quasi-particle peak. However, additional structure (often termed “satellites” or “sidebands”) may appear in $A_k(\omega)$, reflecting the coupling of the single-particle state to multiple excitation channels. The conservation of total spectral weight (as imposed by sum rules such as Eq. (5.95)) implies that weight lost from the quasi-particle peak appears in these satellite features—a signature of strong correlation effects.

4.5 Discussion

Even though the derivation of the exact self-energy is generally intractable, the formalism outlined here shows that the complex interaction effects can be systematically incorporated into a Dyson equation framework:

$$G = G_0 + G_0 \, \Sigma \, G,$$

where all the many-body effects are subsumed into the self-energy $\Sigma(\omega)$. Approximations such as the GW method explicitly include the frequency dependence of $\Sigma(\omega)$ by coupling the electrons to dynamically screened interactions, while other approaches (e.g., dynamical mean-field theory) treat $\Sigma(\omega)$ in a local or short-ranged approximation.

Moreover, the formulation is not limited to electron–electron interactions. Similar Dyson equations can be written for phonons, polarons, or even two-particle Green’s functions. The key feature is that the self-energy, whether arising from Coulomb, electron–boson, or other interactions, acts as an effective dynamical field that renormalizes the independent-particle excitations.

5 Quasi-particles

In many-body calculations the focus is often on the quasi-particle part of the spectrum since the quasi-particle energies form the basis of the band structure of a solid. Quasi-particles are essentially dressed versions of the non-interacting particles, modified by many-body interactions. Unlike Landau’s ideal quasi-particles (which carry the full spectral weight), the quasi-particle peaks observed in interacting systems are broadened due to finite lifetimes, and part of the spectral weight is transferred to satellite structures.

5.1 Quasi-particles in Fermi Liquids

Within Fermi liquid theory (see Sec. 3.4), the notion of a quasi-particle arises as an electron dressed by interactions. Near the Fermi energy E_F, the lifetime of these quasi-particles increases. In fact, the imaginary part of the self-energy, which governs the scattering rate, behaves as

$$\operatorname{Im}\Sigma_k(\omega) \sim (\omega - E_F)^2. \tag{7.24}$$

This quadratic dependence is a hallmark of a "normal" Fermi liquid and implies that quasi-particle states are well-defined near E_F, allowing the Fermi surface to be identified as the locus in k-space where the quasi-particle energy ε_k equals E_F.

5.2 Renormalization and the Quasi-particle Energy

For interacting systems, the independent-particle energy ε_k^0 is renormalized by the real part of the self-energy. Since the self-energy is approximately linear near the Fermi energy, one may expand

$$\operatorname{Re}\Sigma_k(\omega) \approx \operatorname{Re}\Sigma_k(\varepsilon_k^0) + (\omega - \varepsilon_k^0)\, \frac{\partial\, \operatorname{Re}\Sigma_k(\omega)}{\partial\omega}\bigg|_{\omega=\varepsilon_k^0}. \tag{7.25}$$

The renormalization factor (or quasi-particle weight) is then defined by

$$Z_k = \frac{1}{1 - \frac{\partial\, \operatorname{Re}\Sigma_k(\omega)}{\partial\omega}\Big|_{\omega=\varepsilon_k^0}}. \tag{7.26}$$

With this definition, the quasi-particle energy satisfies the implicit equation

$$\varepsilon_k = \varepsilon_k^0 + Z_k\, \operatorname{Re}\Sigma_k(\omega = \varepsilon_k^0). \tag{7.27}$$

In practice, this "on-shell" approximation is often used to compute band structures close to the Fermi energy.

5.3 Spectral Function and Lorentzian Peak

The spectral function for the interacting system is given by

$$A_k(\omega) = \frac{1}{\pi}\frac{|\operatorname{Im}\Sigma_k(\omega)|}{\left[\omega - \varepsilon_k^0 - \operatorname{Re}\Sigma_k(\omega)\right]^2 + \left[\operatorname{Im}\Sigma_k(\omega)\right]^2}. \tag{7.22}$$

Using the linear expansion around ε_k and evaluating the imaginary part at $\omega = \varepsilon_k$, one finds that near the quasi-particle energy the spectral function can be approximated as a Lorentzian:

$$A_k(\omega) \approx \frac{Z_k}{\pi}\frac{Z_k\, \operatorname{Im}\Sigma_k(\varepsilon_k)}{(\omega - \varepsilon_k)^2 + \left[Z_k\, \operatorname{Im}\Sigma_k(\varepsilon_k)\right]^2}. \tag{7.28}$$

Here, Z_k not only reduces the spectral weight of the quasi-particle peak (with the missing weight transferred to satellite features) but also scales the discontinuity in the occupation number at the Fermi surface.

5.4 Renormalization and Effective Mass

The renormalization factor Z_k also influences the dispersion of the quasi-particles. Differentiating the quasi-particle condition (7.27) with respect to k, one obtains

$$\frac{d\varepsilon_k}{dk} = Z_k \left[\frac{d\varepsilon_k^0}{dk} + \left. \frac{\partial \, \mathrm{Re}\, \Sigma_k(\omega)}{\partial k} \right|_{\omega=\varepsilon_k} \right]. \tag{7.29}$$

This shows that both the frequency and momentum dependence of $\Sigma_k(\omega)$ contribute to the effective mass, which in an isotropic system is given by

$$m^* \propto \frac{1}{\left. \frac{d\varepsilon_k}{dk} \right|_{k=k_F}}.$$

Thus, the effective mass of the quasi-particles is enhanced relative to the bare mass, a signature commonly used as a measure of correlation strength.

5.5 Quasi-particles in the Time Domain

Beyond their energy and momentum properties, quasi-particles can be characterized in the time domain. The analytic continuation of the spectral function $A_k(z)$ into the complex plane reveals a pole at

$$z \approx \varepsilon_k - i \big| Z_k \, \mathrm{Im}\, \Sigma_k(\varepsilon_k) \big|.$$

By taking a Fourier transform, the time-dependent Green's function is approximately given by

$$G_k(t) \approx -i \, Z_k \, e^{-i\varepsilon_k t - |Z_k \, \mathrm{Im}\, \Sigma_k(\varepsilon_k)| t}. \tag{7.32}$$

This expression shows that the finite quasi-particle width $|Z_k \, \mathrm{Im}\, \Sigma_k(\varepsilon_k)|$ leads to an exponential damping of the quasi-particle amplitude. The validity of this result is limited to times satisfying

$$\frac{1}{|\varepsilon_k - \mu|} \ll t \ll \frac{1}{|Z_k \, \mathrm{Im}\, \Sigma_k(\varepsilon_k)|}, \tag{7.33}$$

where the lower limit is the time needed to form the quasi-particle and the upper limit reflects the finite lifetime of the excitation.

6 Quasiparticle Equations

The idea of representing a strongly interacting system in terms of weakly interacting quasi-particles is very appealing because it brings us close to an independent-particle picture. In this section we derive the so-called quasi-particle equations from the Dyson equation. While the full derivation is somewhat tedious, the basic principles clarify differences between the poles of the full Green's function (which correspond to total energy differences) and the complex quasi-particle energies that appear when only the quasi-particle part of the spectrum is retained. Throughout this discussion frequencies in the complex plane are denoted by z.

6.1 Derivation of the Quasi-particle Equation

In an ideal scenario one would like to write an effective one-particle Schrödinger-like equation

$$\hat{H}^{\text{eff}}(z)\,\tilde{\psi}_k(r,z) = \tilde{\varepsilon}_k(z)\,\tilde{\psi}_k(r,z)$$

whose eigenvalues $\tilde{\varepsilon}_k(z)$ approximate the quasi-particle energies near the Fermi level and whose eigenfunctions $\tilde{\psi}_k(r,z)$ carry information about the dressing (e.g., the renormalization factor Z_k). In practice, one begins by noting that in the Dyson equation the self-energy acts as a frequency-dependent potential.

One expands the eigenfunctions in a chosen single-particle basis $\{\psi_{mk}(r)\}$:

$$\tilde{\psi}_{nk}(r,z) = \sum_m b_{mk}(z)\,\psi_{mk}(r). \tag{7.34}$$

In this basis the effective Schrödinger-like equation takes the form

$$\sum_m \Big[\varepsilon_k^0\,\delta_{nm} + \Sigma_{nm}^{\text{cont}}(z)\Big] b_{mk}(z) = \tilde{\varepsilon}_k(z)\,b_{nk}(z), \tag{7.35}$$

where ε_k^0 is the independent-particle energy and $\Sigma^{\text{cont}}(z)$ is the analytic continuation of the self-energy (which, in general, is non-Hermitian). Since $\Sigma^{\text{cont}}(z)$ is non-Hermitian, one must also define left eigenfunctions $\bar{b}_k(z)$ such that a bilinear representation of the Green's function holds:

$$G_k^{\text{cont}}(z) = \frac{b_k(z)\,\bar{b}_k(z)}{z - \tilde{\varepsilon}_k(z)}. \tag{7.36}$$

6.2 Quasi-particle Pole and Renormalization

We are interested in the solution where z is close to the quasi-particle pole, i.e., for

$$z \approx \tilde{\varepsilon}_k \quad \text{with} \quad \tilde{\varepsilon}_k \equiv \tilde{\varepsilon}_k(z = \tilde{\varepsilon}_k).$$

Expanding to first order in $(z - \tilde{\varepsilon}_k)$, one finds the quasi-particle part of the Green's function:

$$G_k^{QP}(z) = \frac{Z_k\,b_k(\tilde{\varepsilon}_k)\,\bar{b}_k(\tilde{\varepsilon}_k)}{z - \tilde{\varepsilon}_k}, \tag{7.37}$$

where the renormalization factor Z_k (which is less than one in an interacting system) arises from the first-order expansion. The quasi-particle energy $\tilde{\varepsilon}_k$ itself is determined from

$$\Big[\varepsilon_k^0 + \Sigma_k^{\text{cont}}(\tilde{\varepsilon}_k)\Big]\,b_k(\tilde{\varepsilon}_k) = \tilde{\varepsilon}_k\,b_k(\tilde{\varepsilon}_k). \tag{7.38}$$

In many practical applications one neglects the imaginary part of $\tilde{\varepsilon}_k$, thereby obtaining a spectrum of ideal quasi-particles with sharp peaks. In this approximation the equation becomes Hermitian:

$$\Big[\varepsilon_k^0 + \operatorname{Re}\Sigma_k(\varepsilon_k)\Big]\,b_k(\varepsilon_k) = \varepsilon_k\,b_k(\varepsilon_k), \tag{7.39}$$

which is equivalent to the quasi-particle condition derived earlier (see Eq. (7.23)). Equation (7.39) is most commonly used to compute quasi-particle energies (i.e., the band structure) near the Fermi level.

6.3 Discussion

The derivation above shows that by treating the self-energy as a frequency-dependent potential one can formulate an effective one-particle equation. The resulting quasi-particle energies $\tilde{\varepsilon}_k$ (or ε_k when the imaginary part is neglected) and the renormalization factor Z_k capture the effects of many-body interactions. Although the full Green's function has poles corresponding to exact total energy differences, the quasi-particle equation focuses solely on the pole associated with the dressed single-particle excitation. In practice, methods that compute the spectral function directly and then extract the quasi-particle peak (by locating its maximum) tend to yield similar results near the Fermi level, although differences can arise further away from it due to larger imaginary parts of the self-energy.

7 Separating Different Contributions to a Dyson Equation

In many-body theory, Dyson equations provide a compact way to incorporate interaction effects via a self-energy (or, for screening, a polarizability). In this section the focus is on a general strategy for *decomposing* a Dyson equation into coupled equations that may simplify calculations. It is important to distinguish this separation from the decoupling due to symmetry (for example, momentum conservation in a crystal).

7.1 Coupled Dyson Equations

For a given momentum (or momentum transfer), the standard Dyson equation for the one-particle Green's function is

$$G_k(\omega) = \Big[\omega - \varepsilon_k^0 - \Sigma_k(\omega)\Big]^{-1},$$

where all quantities are labeled by the crystal momentum k. Now suppose the self-energy can be split into two parts,

$$\Sigma(\omega) = \Sigma_1(\omega) + \Sigma_2(\omega).$$

A simple mathematical property of the Dyson equation allows us to introduce an intermediate Green's function, $G_1(\omega)$, defined by

$$G_1(\omega) = G_0(\omega) + G_0(\omega)\,\Sigma_1(\omega)\,G_1(\omega), \tag{7.40}$$

so that the full Green's function is then given by

$$G(\omega) = G_1(\omega) + G_1(\omega)\,\Sigma_2(\omega)\,G(\omega). \tag{7.41}$$

In this way, the fully dressed $G(\omega)$ is determined in two steps. In the first step, $G_1(\omega)$ incorporates contributions from $\Sigma_1(\omega)$; in the second step the remaining part $\Sigma_2(\omega)$ is added to yield the final result.

7.2 Extension to Screening

An analogous decomposition applies to the screening problem. For the screened Coulomb interaction, one typically starts from

$$W(q,\omega) = \Big[v_c(q)^{-1} - P(q,\omega)\Big]^{-1},$$

with $P(q,\omega)$ being the proper polarizability. By expressing the polarizability as

$$P(q,\omega) = P_1(q,\omega) + P_2(q,\omega),$$

one can define an intermediate screened interaction via

$$W_1(\omega) = v_c + v_c\, P_1(\omega)\, W_1(\omega), \tag{7.42}$$

and then write

$$W(\omega) = W_1(\omega) + W_1(\omega)\, P_2(\omega)\, W(\omega). \tag{7.43}$$

Here the bare Coulomb interaction v_c (which is frequency independent) is dressed in two stages: first by transitions described by P_1, then by additional processes captured in P_2.

7.3 Practical Examples and Applications

Several important applications of this decomposition include:

- **Static and Dynamical Separation:** One may separate the self-energy into a static part Σ_1 (often chosen to be a Kohn–Sham potential or a COHSEX-like approximation) and a dynamical contribution Σ_2 that is treated perturbatively (as in the common "G_0W_0" approach).
- **Bethe–Salpeter Equation:** The kernel in the Bethe–Salpeter equation for the two-particle correlation function is composed of two parts—the variation of the Hartree potential with respect to the density and the variation of the exchange–correlation self-energy. Because these terms have different space–spin structures, they are often treated separately.
- **DMFT for Real Materials:** In dynamical mean-field theory, especially when applied to complex materials, localized orbitals (e.g., d or f states) are treated at a different level than delocalized ones (e.g., s and p states). This requires a division of the self-energy into contributions from different orbital subspaces.
- **Screening in RPA:** In the random phase approximation, the proper polarizability P is expressed as a sum over electron–hole pairs. One may separate transitions of interest (e.g., those within a subset of orbitals) into P_2, while including all others in P_1. This leads to an effective screened interaction W_1 that acts in the reduced subspace.

7.4 Self-Consistency Relations

In many cases the separation is not independent. For example, if Σ_1 is expressed in terms of the full Green's function G, then the two coupled equations (7.40) and (7.41) must be solved self-consistently. This situation arises in methods such as DMFT, where the effective impurity problem (described by G_1) is embedded in a self-consistent bath. Self-consistency ensures that the quantities used as input for one part of the calculation are consistent with the final, fully dressed solution.