6 Green Functions and Self-Energy Functionals

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1 Introduction

Green functions are quantities of central importance in the theory of interacting many-particle systems. In simplest terms they may be viewed as describing the propagation of some kind of 'perturbation' through a system of interacting particles. On one hand, by their very definition Green functions contain information about the system which can be directly compared to experiments, on the other hand they are a useful mathematical tool because there is a wide variety of techniques to calculate them approximately, and thus overcome the, in general, insoluble nature of the many-particle problem. Of particular importance is the single-particle Green function $G(\mathbf{k}, \omega)$, which describes the propagation of an added particle with wave number $\mathbf{k}$ and energy $\hbar\omega$ through the system and which is directly related to the experimentally measurable photoemission and inverse photoemission spectrum. The famous Dyson equation then expresses the single-particle Green function in terms of another central quantity in many-body physics, the self-energy $\Sigma(\mathbf{k}, \omega)$. This may be viewed as a $\mathbf{k}$- and ω-dependent potential which mimics the effect of the other particles on the propagation of the added particle (it is therefore hardly a surprise that to simplest approximation the self-energy equals the Hartree-Fock potential). However, the physical significance of the self-energy is considerably wider. Namely, in 1961 Luttinger and Ward (LW) published a seminal paper [1] which became the foundation of many important developments in the quantum theory of many-particle systems. They showed that the grand canonical potential Ω of an interacting Fermion system can be expressed as a functional of the single-particle Green function $G(\mathbf{k}, \omega)$ and the self-energy $\Sigma(\mathbf{k}, \omega)$. A key step thereby was the construction of the Luttinger-Ward functional $\Phi[G]$, a functional of the Green function which essentially describes the deviation of Ω from a non-interacting system with the same band structure as the interacting one. Luttinger and Ward gave an explicit expression for $\Phi[G]$ as a sum over infinitely many Feynman diagrams and also showed that Σ is the functional derivative of $\Phi[G]$ with respect to G and that Ω is stationary under variations of Σ. The expression for Ω and the properties of $\Phi[G]$ became the basis for many important results, such as the Luttinger theorem [2] which states that interactions between electrons do not change the volume of the Fermi surface, or the construction of conserving approximations by Baym and Kadanoff [3, 4], where $\Phi[G]$ is approximated by keeping only a subclass of Feynman diagrams. While the representation of Green functions in terms of Feynman diagrams was highly successful for systems such as the electron gas, a new challenge arose with increasing interest in strongly correlated electron systems such as the Hubbard model. Namely any Feynman diagram expansion implicitly treats the interaction between the particles as a perturbation and assumes a continuous evolution from the noninteracting case, which is highly questionable for systems such as Mott-insulators. It is the purpose of the present lecture to sketch a further development of the ideas of Luttinger and Ward which is mainly due to Potthoff, the so-called self-energy functional theory. We present Potthoff's non-perturbative re-derivation of the results of Luttinger and Ward [5, 6] and the application of their theorems to strongly correlated electron systems by combining them with numerical methods. As an application, we discuss the metal-insulator transition in the single-band Hubbard model.

2 Green functions and the self-energy

2.1 The Green function and its analytical properties

We start with a discussion of Green functions and their properties and use. We will not cover the representation of Green functions in terms of Feynman diagrams, since excellent introductions to this subject can be found in various textbooks [7–9]. In the present notes we try to be consistent with Fetter/Walecka (FW) [8].

We consider a system of interacting fermions and assume that there is some complete basis of single electron states $\varphi_\alpha(x)$. Here $x = (\mathbf{r}, \sigma)$ is the combined real-space and spin coordinate, whereas α is shorthand for a set of quantum numbers. For example, in an LCAO-type description of a solid – which is what we mostly have in mind – we would have $\alpha = (i, n, \nu, \sigma)$ where $i \in \{1, \ldots, N\}$ denotes the unit cell, $n \in \{1, \ldots, n_{Atom}\}$ the number of the atoms in the basis, $\nu \in \{s, p_x, p_y, p_z, d_{xy} \ldots\}$ the type of orbital on the respective atom, and σ the z-component of spin. We denote the number of orbitals in a unit cell by n_{orb}, the total number of α's thus is $N_\alpha = 2Nn_{orb}$. Upon Fourier transformation one would replace $i \to \mathbf{k}$, the wave vector.

In all that follows we consider a grand canonical ensemble with inverse temperature $\beta = 1/k_BT$ and chemical potential μ. Introducing fermionic creation/annihilation operators $c^\dagger_\alpha/c_\alpha$ for electrons in the states $\varphi_\alpha(x)$, the grand canonical Hamiltonian $K = H - \mu\hat{N}$ (with $\hat{N}$ the operator for the number of electrons) can be written as $K = K_0 + K_1$ with [7–9]

$$K_0 = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta}\right) c^\dagger_\alpha c_\beta \quad \text{and} \qquad K_1 = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\, c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta. \tag{1}$$

The matrix elements in this Hamiltonian are given by

$$t_{\alpha,\beta} = \int dx\, \varphi^*_\alpha(x) \Big(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \Big) \varphi_\beta(x),$$
$$V_{\alpha,\beta,\delta,\gamma} = \int dx \int dx'\, \varphi^*_\alpha(x)\, \varphi^*_\beta(x')\, V(x - x')\, \varphi_\gamma(x')\, \varphi_\delta(x).$$

For later reference we calculate

$$[c_\alpha, K] = \sum_\beta \Big(t_{\alpha,\beta} - \mu\delta_{\alpha,\beta} \Big) c_\beta + \sum_{\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\, c^\dagger_\beta c_\gamma c_\delta, \tag{2}$$

where we have used the identity $V_{\alpha,\beta,\gamma,\delta} = V_{\beta,\alpha,\delta,\gamma}$ obtained by exchanging the integration variables $x \leftrightarrow x'$ in the definition of V. It obviously holds that $[H, \hat{N}] = 0$ so that eigenstates of H have a fixed particle number. The thermal average of any operator $\hat{O}$ is

$$\left\langle \hat{O} \right\rangle_{th} = \frac{1}{Z} \operatorname{Tr} \left(e^{-\beta K} \hat{O} \right) = \frac{1}{Z} \sum_i e^{-\beta K_i} \langle i | \hat{O} | i \rangle. \tag{3}$$

Here $|i\rangle$ are the eigenstates of H, $H|i\rangle = E_i|i\rangle$, and $K_i = E_i - \mu N_i$ the corresponding eigenvalues of K. Also,

$$Z = \operatorname{Tr} \left(e^{-\beta K} \right) = \sum_i e^{-\beta K_i} \tag{4}$$

is the grand partition function, which is a quantity of interest by itself, because the grand canonical potential of the system is given by $\Omega = -k_B T \ \log(Z)$.
We proceed to the definition of *Green functions* which basically describe the following *gedanken experiment*: the system is initially in thermal equilibrium, but at a certain time t we do something to the system by acting with an operator $\hat{A}$. $\hat{A}$ could add or remove an electron, flip a spin or similar. We then let the system evolve for some time and undo the change at a time t' by acting with an operator $\hat{B}$, which often is $\hat{A}^\dagger$. We then form the overlap with the state we would have obtained had the system evolved without perturbation. In other words, the Green function describes how the 'perturbation' created by $\hat{A}$ propagates in the interval $t \to t'$ before it is removed by $\hat{B}$.
We now formalize this idea, but for reasons which will become clear only later we make a digression and first introduce *imaginary time Green functions*. Moreover, we specialize to the *single particle Green function*, where the perturbation is removing or adding a particle, i.e. $\hat{A} = c_\alpha$ and $\hat{B} = c_\beta^\dagger$, or vice versa. For any operator $\hat{O}$ the imaginary time Heisenberg operator is $\hat{O}(\tau) = e^{\tau K/\hbar}\, \hat{O}\, e^{-\tau K/\hbar}$ and the imaginary time Green function is

$$\begin{aligned} G_{\alpha,\beta}(\tau,\tau') &= -\big\langle T\ c_\alpha(\tau) c_\beta^\dagger(\tau') \big\rangle_{th} \\ &= -\Theta(\tau{-}\tau') \left\langle c_\alpha(\tau) c_\beta^\dagger(\tau') \right\rangle_{th} + \Theta(\tau'{-}\tau) \left\langle c_\beta^\dagger(\tau') c_\alpha(\tau) \right\rangle_{th} \qquad (5) \\ &= \frac{1}{Z}\Bigg(-\Theta(\tau{-}\tau') \sum_{i,j} e^{-\beta K_i}\, e^{\frac{\tau-\tau'}{\hbar}(K_i - K_j)}\, \langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle \\ &\qquad + \Theta(\tau'{-}\tau) \sum_{i,j} e^{-\beta K_i}\, e^{\frac{\tau-\tau'}{\hbar}(K_j - K_i)}\, \langle i|c_\beta^\dagger|j\rangle \langle j|c_\alpha|i\rangle \Bigg). \qquad (6) \end{aligned}$$

T in the first line is the *time ordering operator*, which reorders the following Heisenberg operators such that their times decrease from left to right and multiplies by (-1) for each exchange of two Fermion operators, as can be seen in the second line. In going from the second to last line we have used (3), inserted a resolution of unity $\sum_j |j\rangle\langle j| = 1$, and used $\langle i|\hat{O}(\tau)|j\rangle = e^{\frac{\tau}{\hbar}(K_i - K_j)}\ \langle i|\hat{O}|j\rangle$. Eq. (6) shows that $G_{\alpha,\beta}$ really is a function of $\tau{-}\tau'$ only: $G_{\alpha,\beta}(\tau,\tau') = G_{\alpha,\beta}(\tau{-}\tau')$. To simplify the notation we henceforth replace $\tau{-}\tau' \to \tau$, which is equivalent to choosing $\tau' = 0$. The τ-dependence of both terms in (6) is $e^{(-\beta + \frac{|\tau|}{\hbar})K_i}\ e^{-\frac{|\tau|}{\hbar}K_j}$. Since the K_i are bounded from below, namely by K_0 for the ground state with the given μ, but unbounded from above in the thermodynamical limit, $\mathbf{G}$ is therefore well-defined only for $\tau \in [-\beta\hbar, \beta\hbar]$ [10]. It therefore can be written as a Fourier series with frequencies $n\pi/\hbar\beta$. However, it is easy to see from (6) that for $\tau \in [-\beta\hbar, 0]$ one has $G(\tau{+}\beta\hbar) = -G(\tau)$, so that only odd n can contribute. All in all we find the Fourier expansion

$$G(\tau) = \frac{1}{\beta\hbar} \sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu \tau}\, G(i\omega_\nu), \qquad (7)$$

$$G(i\omega_\nu) = \int_0^{\beta\hbar} d\tau\ e^{i\omega_\nu \tau}\, G(\tau), \qquad (8)$$

with $\omega_\nu = (2\nu + 1)\pi/\beta\hbar$ and integer ν. The ω_ν are the Fermionic *Matsubara frequencies*.

Performing the integral (8) with (6) for $G_{\alpha,\beta}(\tau)$, thereby using $e^{i\omega_\nu \beta\hbar} = -1$ for any ν, we obtain

$$G_{\alpha,\beta}(i\omega_\nu) = \frac{1}{Z}\sum_{i,j} \frac{e^{-\beta K_i} + e^{-\beta K_j}}{i\omega_\nu - \frac{1}{\hbar}(K_j - K_i)} \, \langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle. \tag{9}$$

This so-called *Lehmann representation* of the Green function is exact but not really helpful for practical computations because it requires knowledge of all eigenstates and energies of H. It can be used, however, for establishing certain properties of the Green function as will be seen in the following.

We proceed to the definition of the real-time Green function. Defining the real-time Heisenberg operator $\hat{O}(\tau) = e^{itK/\hbar}\,\hat{O}\,e^{-itK/\hbar}$ the *retarded real-time Green function* is

$$\begin{aligned} G^R_{\alpha,\beta}(t,t') &= -i\Theta(t-t')\Big(\big\langle c_\alpha(t)c_\beta^\dagger(t')\big\rangle_{th} + \big\langle c_\beta^\dagger(t')c_\alpha(t)\big\rangle_{th}\Big), \\ &= -i\Theta(t-t')\frac{1}{Z}\Bigg(\sum_{i,j} e^{-\beta K_i}\, e^{i\frac{t-t'}{\hbar}(K_i-K_j)}\, \langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle \\ &\qquad + \sum_{i,j} e^{-\beta K_i}\, e^{i\frac{t-t'}{\hbar}(K_j-K_i)}\, \langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle\Bigg). \end{aligned} \tag{10}$$

Again this is a function of $t-t'$ only and, using the formula derived in Appendix A,

$$-i\Theta(t)\,e^{-iEt} = \lim_{\eta\to 0^+}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega t}}{\omega - E + i\eta}$$

we find its Fourier transform

$$G^R_{\alpha,\beta}(\omega) = \frac{1}{Z}\lim_{\eta\to 0^+}\sum_{i,j}\frac{e^{-\beta K_i} + e^{-\beta K_j}}{\omega + i\eta - \frac{1}{\hbar}(K_j - K_i)}\,\langle i|c_\alpha|j\rangle\,\langle j|c_\beta^\dagger|i\rangle. \tag{11}$$

Comparison with Eq. (9) shows that $G^R_{\alpha,\beta}(\omega)$ can be obtained from $G_{\alpha,\beta}(i\omega_\nu)$ by replacing $i\omega_\nu \to \omega + i\eta$. In other words, there is one function $G_{\alpha,\beta}(z)$ of the complex variable z, often called *the* Green function, which gives $G_{\alpha,\beta}(i\omega_\nu)$ when evaluated for the Matsubara frequencies, and $G^R_{\alpha,\beta}(\omega)$ when evaluated on a line infinitesimally above the real axis. The existence of such a function is the very reason why the imaginary time Green function is introduced in the first place. In principle, the quantities of interest, of course, are the real-time Green functions. For example, the single-particle Green function (11) contains information about the photoemission and inverse photoemission spectrum of the system. On the other hand, the imaginary-time Green function (9) can be evaluated approximately by using the powerful technique of expansion in Feynman diagrams [7–9], which is *not* possible for the real-time Green function. The standard way to obtain the real-time Green functions, which is used again and again in the literature, is to first obtain an approximate $G_{\alpha,\beta}(i\omega_\nu)$ by doing an expansion in Feynman diagrams and then obtain the real-time Green function by continuing it analytically to a line infinitesimally above the real axis. If one has an analytical expression for $G_{\alpha,\beta}(i\omega_\nu)$ this can be done by simply replacing $i\omega_\nu \to \omega + i\eta$.

We now discuss some properties of *the* Green function. In Eq. (11) the product of matrix elements $\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle$ can differ from zero only if $N_j = N_i{+}1$, whence $K_j{-}K_i = E_j{-}E_i{-}\mu$. $G_{\alpha,\beta}(z)$ therefore has poles on the real axis, which correspond to differences of energies of states whose electron number differ by one. Next, we rewrite the Green function as

$$\mathbf{G}(z) = \int_{-\infty}^{\infty} d\omega\, \frac{\boldsymbol{\rho}(\omega)}{z{-}\omega}, \tag{12}$$

where the elements of the *spectral density matrix* $\boldsymbol{\rho}(\omega)$ can be read off from (9)

$$\rho_{\alpha,\beta}(\omega) = \frac{1}{Z}\,\sum_{i,j}\left(e^{-\beta K_i}{+}e^{-\beta K_j}\right)\,\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle\,\delta\!\left(\omega - \frac{K_i{-}K_j}{\hbar}\right). \tag{13}$$

Since ω is real we find $\rho^*_{\alpha,\beta}(\omega) = \rho_{\beta,\alpha}(\omega)$, i.e., $\boldsymbol{\rho}(\omega)$ is Hermitian for any ω. Next consider any vector $\mathbf{v}$ of length N_α and define the linear combination $c^\dagger_{\mathbf{v}} = \sum\, v_\alpha c^\dagger_\alpha$. Then

$$\sum_{\alpha,\beta} v^*_\alpha\,\rho_{\alpha,\beta}(\omega)\,v_\beta = \frac{1}{Z}\sum_{i,j}\left(e^{-\beta K_i}{+}e^{-\beta K_j}\right)\left|\langle j|c^\dagger_{\mathbf{v}}|i\rangle\right|^2\delta\!\left(\omega - \frac{K_i{-}K_j}{\hbar}\right) > 0$$

i.e., $\boldsymbol{\rho}(\omega)$ is positive definite for each ω. It then follows from (12) that $\big(\mathbf{G}(z)\big)^+ = \mathbf{G}(z^*)$ so that $\mathbf{G}(z)$ is *not* Hermitian for complex z. Next consider

$$f(z) = \sum_{\alpha,\beta} v^*_\alpha\,G_{\alpha,\beta}(z)\,v_\beta = \frac{1}{Z}\,\sum_{i,j}\,\frac{e^{-\beta K_i} + e^{-\beta K_j}}{z - \frac{K_i-K_j}{\hbar}}\,\left|\langle j|c^\dagger_{\mathbf{v}}|i\rangle\right|^2. \tag{14}$$

We write $z = x{+}iy$ and find the imaginary part of this to be

$$\Im f(z) = -\frac{y}{Z}\,\sum_{i,j}\,\frac{e^{-\beta K_i} + e^{-\beta K_j}}{\left(x - \frac{K_i-K_j}{\hbar}\right)^2 + y^2}\,\left|\langle j|c^\dagger_{\mathbf{v}}|i\rangle\right|^2. \tag{15}$$

This expression cannot vanish unless $y = 0$, so that for z away from the real axis all eigenvalues of $\mathbf{G}(z)$ must have a nonvanishing imaginary part, otherwise we could choose $\mathbf{v}$ to be the normalized right-hand eigenvector belonging to a purely real eigenvalue λ and find that $f(z){=}\lambda$, in contradiction to (15). This implies in particular that for z away from the real axis all eigenvalues of $\mathbf{G}(z)$ are different from zero so that the determinant of $\mathbf{G}(z)$ is different from zero [11] and its inverse $\mathbf{G}^{-1}(z)$ does exist. Using Cramer's rule we find the elements of the inverse Green function

$$G^{-1}_{\alpha,\beta}(z) \;\;=\;\; \frac{(-1)^{\alpha+\beta}\,\det\,\mathbf{M}_{\alpha,\beta}(z)}{\det\,\mathbf{G}(z)}$$

where $\mathbf{M}_{\alpha,\beta}(z)$ is the respective minor of $\mathbf{G}(z)$, i.e. the matrix $\mathbf{G}(z)$ with line α and column β discarded. Since for z away from the real axis all elements of $\mathbf{G}(z)$ are finite (see Eq. (9)) and the determinant of $\mathbf{G}(z)$ is different from zero it moreover follows that away from the real axis all elements of $\mathbf{G}^{-1}(z)$ are analytical functions of z.

We proceed to a discussion of the behavior of $\mathbf{G}(z)$ for large $|z|$. We assume that the range of ω where the elements of $\boldsymbol{\rho}(\omega)$ are different from zero is finite, which simply means that the change

in energy upon adding or removing an electron is bounded. To discuss the limit $|z| \to \infty$ we rewrite $\mathbf{G}(z)$ as

$$G_{\alpha,\beta}(z) = \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\left(\frac{\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle}{z-\frac{K_j-K_i}{\hbar}} + \frac{\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle}{z+\frac{K_j-K_i}{\hbar}}\right), \tag{16}$$

and expand

$$\frac{1}{z\pm\frac{K_j-K_i}{\hbar}} \to \frac{1}{z} \mp \frac{K_j-K_i}{\hbar z^2} + \mathcal{O}\left(\frac{1}{z^3}\right).$$

Next use $(K_j-K_i)\langle j|c_\alpha|i\rangle = \langle j|Kc_\alpha|i\rangle - \langle j|c_\alpha K|i\rangle = \langle j|[K,\, c_\alpha]|i\rangle$ and find

$$G_{\alpha,\beta}(z) \to \frac{\delta_{\alpha,\beta}}{z} + \frac{\left\langle\left\{c_\beta^\dagger,\, [c_\alpha,\, K]\right\}\right\rangle_{th}}{\hbar z^2} + \mathcal{O}\left(\frac{1}{z^3}\right).$$

Using (2) we obtain

$$\left\langle\left\{c_\beta^\dagger,\, [c_\alpha, K]\right\}\right\rangle_{th} = t_{\alpha,\beta}-\mu\delta_{\alpha,\beta} + \sum_{\gamma,\delta}\left(V_{\alpha,\gamma,\beta,\delta}-V_{\alpha,\gamma,\delta,\beta}\right)\left\langle c_\gamma^\dagger c_\delta\right\rangle_{th}. \tag{17}$$

The term involving V looks like the Hartree-Fock potential $V_{\alpha,\beta}^{(HF)}$, however, whereas for the true Hartree-Fock potential the thermal average has to be taken using the Hartree-Fock wave functions and energies, the thermal average in (17) has to be taken using the fully interacting eigenstates and energies. Keeping this subtle difference in mind we still call the third term the Hartree-Fock potential $V_{\alpha,\beta}^{(HF)}$ so that

$$\mathbf{G}(z) \to \frac{1}{z} + \frac{\mathbf{t}-\mu+\mathbf{V}^{(HF)}}{\hbar z^2} + \mathcal{O}\left(\frac{1}{z^3}\right). \tag{18}$$

Eq. (16) also highlights the physical content of the Green function. We consider a single band of *non*-interacting electrons where $\alpha = (\mathbf{k},\sigma)$, and $K = \sum_{\mathbf{k}}\left(\varepsilon_{\mathbf{k}}-\mu\right) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}$. All eigenstates can then be characterized by the occupation numbers of the states $(\mathbf{k},\sigma)$ being either 0 or 1. In

$$G_{\mathbf{k},\mathbf{k}}(z) = \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\left(\frac{\langle i|c_{\mathbf{k},\sigma}^\dagger|j\rangle\langle j|c_{\mathbf{k},\sigma}|i\rangle}{z+\frac{K_j-K_i}{\hbar}} + \frac{\langle i|c_{\mathbf{k},\sigma}|j\rangle\langle j|c_{\mathbf{k},\sigma}^\dagger|i\rangle}{z-\frac{K_j-K_i}{\hbar}}\right)$$

the matrix element $\langle j|c_{\mathbf{k},\sigma}|i\rangle$ in the first term is then different from zero only if $|i\rangle$ has an electron in the single-electron state $(\mathbf{k},\sigma)$, whereas $|j\rangle$ has none, while all other momenta have identical occupation. It follows that $E_i = E_j+\varepsilon_{\mathbf{k}}$, whence $K_j-K_i = -\varepsilon_{\mathbf{k}}+\mu$. The first term therefore describes the removal of an electron with momentum $\mathbf{k}$ and spin σ. By analogous reasoning, in the second term $K_j-K_i = \varepsilon_{\mathbf{k}}-\mu$ and this term describes addition of an electron. In both terms K_j-K_i is independent of both, $|i\rangle$ and $|j\rangle$, so that we can use $\sum_j |j\rangle\langle j| = 1$ and find

$$G_{\mathbf{k},\mathbf{k}}(z) = \frac{1}{Z}\sum_i e^{-\beta K_i}\left(\frac{\langle i|c_{\mathbf{k},\sigma}^\dagger\, c_{\mathbf{k},\sigma}|i\rangle}{z-\frac{\varepsilon_{\mathbf{k}}-\mu}{\hbar}} + \frac{\langle i|c_{\mathbf{k},\sigma}\, c_{\mathbf{k},\sigma}^\dagger|i\rangle}{z-\frac{\varepsilon_{\mathbf{k}}-\mu}{\hbar}}\right) = \frac{\langle n_{\mathbf{k},\sigma}\rangle_{th}}{z-\frac{\varepsilon_{\mathbf{k}}-\mu}{\hbar}} + \frac{\langle 1-n_{\mathbf{k},\sigma}\rangle_{th}}{z-\frac{\varepsilon_{\mathbf{k}}-\mu}{\hbar}}.$$

Both terms have poles which trace the electrons' dispersion relation $\varepsilon_{\mathbf{k}}-\mu$, but the first term describes only the occupied part of the band, the second term the unoccupied part. The Green function is the combined photoemission and inverse photoemission spectrum and this holds true also for the interacting case.

2.2 The self-energy and its analytical properties

We proceed to the definition of another key quantity, the *self-energy*, and start by discussing the *equation of motion* of the imaginary time Green function Eq. (5). We set $G_{\alpha,\beta}(\tau,0)\to G_{\alpha,\beta}(\tau)$. It follows readily from the definition of the imaginary-time Heisenberg operator $\hat{O}(\tau)$ that $-\hbar\partial_\tau\hat{O}(\tau) = [\hat{O}(\tau), K]$. Moreover, using, e.g., the representation $\Theta(\tau) = \int_{-\infty}^{\tau} dx\, \delta(x)$ one finds $\partial_\tau\Theta(\pm\tau) = \pm\delta(\tau)$. Combining everything we get the equation of motion of the Green function

$$\begin{aligned} -\hbar\partial_\tau G_{\alpha,\beta}(\tau) &= \hbar\,\delta(\tau)\,\left\langle\{c_\alpha,\, c_\beta^\dagger\}\right\rangle_{th} + \left\langle T\,\left[c_\alpha(\tau),\, K\right]\, c_\beta^\dagger(0)\right\rangle_{th} \\ &= \hbar\,\delta(\tau)\,\delta_{\alpha,\beta} + \sum_\nu \left(t_{\alpha,\nu} - \mu\delta_{\alpha,\nu}\right) G_{\nu,\beta}(\tau) + F_{\alpha,\beta}(\tau), \qquad (19) \\ F_{\alpha,\beta}(\tau) &= -\sum_{\nu,\kappa,\lambda} V_{\alpha,\nu,\kappa,\lambda} \left\langle T\,\left[(c_\nu^\dagger c_\lambda c_\kappa)(\tau) c_\beta^\dagger(0)\right]\right\rangle_{th}, \qquad (20) \end{aligned}$$

where (2) was used. In the *noninteracting case*, i.e., all $V_{\alpha,\nu,\kappa,\lambda}{=}0$ we have $F_{\alpha,\beta}(\tau){=}0$ and the equation closes. Using the representation of the δ-function in terms of Matsubara-frequencies [8]

$$\delta(\tau) = \frac{1}{\hbar\beta}\sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu\tau}$$

straightforward Fourier transform gives the noninteracting Green function

$$\left(i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}\right)\mathbf{G}_0(i\omega_\nu) = 1. \qquad (21)$$

We return to the case $V \neq 0$. We recall that $G(\tau)$ fulfills $G(\tau{+}\beta\hbar) = -G(\tau)$ for $\tau \in [-\beta\hbar, 0]$, which established its Fourier expansion (7). It follows that $\partial_\tau G(\tau{+}\beta\hbar) = -\partial_\tau G(\tau)$ whence $F(\tau)$ must obey the same boundary condition: $F(\tau{+}\beta\hbar) = -F(\tau)$. Accordingly, $F(\tau)$ has the same Fourier expansion (7) as $G(\tau)$ itself and we find

$$\left(i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}\right)\mathbf{G}(i\omega_\nu) - \frac{1}{\hbar}\boldsymbol{F}(i\omega_\nu) = 1.$$

Now we define the *self-energy* $\boldsymbol{\Sigma}(i\omega_\nu)$ by $\boldsymbol{F}(i\omega_\nu) = \hbar\boldsymbol{\Sigma}(i\omega_\nu)\,\mathbf{G}(i\omega_\nu)$ (recall that $\mathbf{G}^{-1}(z)$ exists for all z away from the real axis so that $\boldsymbol{\Sigma}(i\omega_\nu)$ is well defined) whence

$$\left(i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar} - \boldsymbol{\Sigma}(i\omega_\nu)\right)\mathbf{G}(i\omega_\nu) = 1. \qquad (22)$$

By analytical continuation, $i\omega_\nu \to z$, this equation defines $\boldsymbol{\Sigma}(z)$ for all z away from the real axis. Next, notice that the brackets on the left-hand side of (21) and (22) are $\mathbf{G}_0^{-1}(z)$ and $\mathbf{G}^{-1}(z)$, respectively, so that we immediately read off the famous *Dyson equation*

$$\mathbf{G}^{-1}(z) = \mathbf{G}_0^{-1}(z) - \boldsymbol{\Sigma}(z) = z - \frac{\mathbf{t}-\mu}{\hbar} - \boldsymbol{\Sigma}(z). \qquad (23)$$

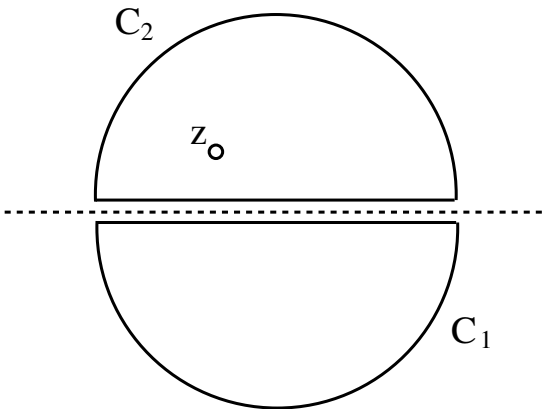

Fig. 1: *Integration contours for the proof of the spectral representation of $\boldsymbol{\Sigma}$. The dashed line is the real z' axis.*

We discuss some properties of $\boldsymbol{\Sigma}(z)$ which follow from its definition. Since both $\mathbf{G}^{-1}(z)$ and $\mathbf{G}_0^{-1}(z)$ are analytical in the complex z-plane except for the real axis, the same must hold true for $\boldsymbol{\Sigma}(z)$. Next, it follows from (18) that

$$\mathbf{G}^{-1}(z) \to z - \frac{\mathbf{t}-\mu}{\hbar} - \frac{\mathbf{V}^{(HF)}}{\hbar} + \mathcal{O}\left(\frac{1}{z}\right) \Rightarrow \boldsymbol{\Sigma}(z) \to \frac{\mathbf{V}^{(HF)}}{\hbar} + \mathcal{O}\left(\frac{1}{z}\right).$$

The shifted function $\bar{\boldsymbol{\Sigma}}(z) = \boldsymbol{\Sigma}(z) - \frac{\mathbf{V}^{(HF)}}{\hbar}$ therefore vanishes as $1/z$ for large $|z|$. Now consider the equation $\mathbf{G}^{-1}(z)\,\mathbf{G}(z) = 1$, take the Hermitian conjugate and use $[\mathbf{G}(z)]^+ = \mathbf{G}(z^*)$. It follows that $[\mathbf{G}^{-1}(z)]^+ = \mathbf{G}^{-1}(z^*)$. Since trivially $[\mathbf{G}_0^{-1}(z)]^+ = \mathbf{G}_0^{-1}(z^*)$ and $\mathbf{V}^{HF}$ is Hermitian it follows that $\bar{\boldsymbol{\Sigma}}(z^*) = \bar{\boldsymbol{\Sigma}}^+(z)$. Next, for real ω, define the real matrices $\mathbf{K}(\omega)$ and $\mathbf{J}(\omega)$ by

$$\bar{\boldsymbol{\Sigma}}(\omega+i0^+) = \mathbf{K}(\omega) + i\mathbf{J}(\omega) \quad \Rightarrow \quad \bar{\boldsymbol{\Sigma}}(\omega-i0^+) = \mathbf{K}^T(\omega) - i\mathbf{J}^T(\omega). \tag{24}$$

We introduce the symmetrized/antisymmetrized linear combinations $\mathbf{K}^{(\pm)} = (\mathbf{K} \pm \mathbf{K}^T)/2$ and $\mathbf{J}^{(\pm)} = (\mathbf{J} \pm \mathbf{J}^T)/2$ whence

$$\bar{\boldsymbol{\Sigma}}^{(+)}(z) = \frac{1}{2}\Big(\bar{\boldsymbol{\Sigma}}(z) + \bar{\boldsymbol{\Sigma}}^T(z)\Big), \qquad \bar{\boldsymbol{\Sigma}}^{(-)}(z) = \frac{i}{2}\Big(\bar{\boldsymbol{\Sigma}}(z) - \bar{\boldsymbol{\Sigma}}^T(z)\Big). \tag{25}$$

The latter can be expressed in terms of $\mathbf{K}^{(\pm)}(z)$ and $\mathbf{J}^{(\pm)}(z)$ as

$$\begin{aligned} \bar{\boldsymbol{\Sigma}}^{(+)}(\omega \pm i0^+) &= \ \mathbf{K}^{(+)}(\omega) \pm i\mathbf{J}^{(+)}(\omega), \\ \bar{\boldsymbol{\Sigma}}^{(-)}(\omega \pm i0^+) &= -\mathbf{J}^{(-)}(\omega) \pm i\mathbf{K}^{(-)}(\omega). \end{aligned} \tag{26}$$

Now consider the integration contours in figure 1 which consist of lines infinitesimally above and below the real axis and semicircles at infinity. Since $\bar{\boldsymbol{\Sigma}}(z)$ is analytic away from the real axis we have for any z in the upper half-plane

$$\oint_{C_1} dz' \, \frac{\bar{\boldsymbol{\Sigma}}^{(\pm)}(z')}{z'-z} = 0 \quad \Rightarrow \quad \int_{-\infty}^{\infty} d\omega \, \frac{\bar{\boldsymbol{\Sigma}}^{(\pm)}(\omega - i0^+)}{\omega - z} = 0\,. \tag{27}$$

The second equation follows because the integrand is $\propto 1/z'^2$ for large $|z'|$ so that the contribution from the arc vanishes and only the line infinitesimally below the real axis contributes,

where $z = \omega - i0^+$, and $\omega - i0^+ - z = \omega - z$ whenever z has a finite imaginary part. We can now use (26) and obtain

$$\int_{-\infty}^{\infty} d\omega \, \frac{\mathbf{K}^{(\pm)}(\omega)}{\omega - z} = i \int_{-\infty}^{\infty} d\omega \, \frac{\mathbf{J}^{(\pm)}(\omega)}{\omega - z} \,. \tag{28}$$

Next we apply Cauchy's theorem to the contour C_2 in figure 1 and find

$$\bar{\mathbf{\Sigma}}^{(\pm)}(z) = \frac{1}{2\pi i} \oint_{C_2} dz' \, \frac{\bar{\mathbf{\Sigma}}^{(\pm)}(z')}{z' - z} \,.$$

Again the contribution from the arc vanishes. We use (28) to eliminate the integrals over $\mathbf{K}^{(+)}$ and $\mathbf{J}^{(-)}$, revert (25) to obtain $\bar{\mathbf{\Sigma}}(z)$ and arrive at the spectral representation of the self-energy, as derived by Luttinger [12]

$$\mathbf{\Sigma}(z) = \frac{\mathbf{V}^{(HF)}}{\hbar} + \int_{-\infty}^{\infty} d\omega \, \frac{\boldsymbol{\sigma}(\omega)}{\omega - z}. \tag{29}$$

Here, the Hermitian matrix $\boldsymbol{\sigma}(\omega) = \mathbf{J}^{(+)}(\omega) - i\mathbf{K}^{(-)}(\omega)$.

Lastly, we notice a property of the self-energy that will be of some importance later on: we will often be concerned with systems which contain both, 'correlated orbitals' and 'uncorrelated orbitals'. A given orbital α is 'uncorrelated' if all interaction matrix elements $V_{\kappa\lambda\mu\nu} = 0$ if at least one of the four indices equals α. In other words, electrons in an uncorrelated orbital do not interact with the other electrons. An example is the well-known Anderson model where one usually has correlated 'f-orbitals' hybridizing with uncorrelated 'conduction electrons'. It then follows from the definition (20) that $F_{\alpha,\beta}(z) = 0$ whenever α or β are uncorrelated, and the same holds true for $\Sigma_{\alpha,\beta}(z)$: *matrix elements of the self-energy involving uncorrelated orbitals are zero!*

2.3 Physical significance of the self-energy

We briefly recall the key results of our discussion so far: The Green function and self-energy are related by the Dyson equation (23), they are analytical functions on the complex frequency plane except for the real axis, and they have the spectral representations (12) and (29). The poles of the Green function on real axis give the ionization and affinity energies of the system, i.e., the energies it takes to remove or add an electron. We now want to discuss the physical consequences of this formal structure. For the remainder of this subsection we consider the case of a single band, set $\hbar = 1$ and call $t_{\mathbf{k}} - V_{\mathbf{k}}^{(HF)} - \mu = \varepsilon_{\mathbf{k}}$. Moreover, we drop the dependence on $\mathbf{k}$ and replace $\varepsilon_{\mathbf{k}} \to \varepsilon$, $G(\mathbf{k}, \omega) \to G(\omega)$ and so on. To begin with, we consider a system with finite N, where the spacing between eigenvalues K_i and hence between the poles of $G(\omega)$ is finite. We have

$$G(\omega) = \frac{1}{\omega - \varepsilon - \bar{\Sigma}(\omega)} = \sum_{i=1}^{n+1} \frac{Z_i}{\omega - \omega_i} \tag{30}$$

$$\bar{\Sigma}(\omega) = \sum_{i=1}^{n} \frac{\sigma_i}{\omega - \zeta_i} \tag{31}$$

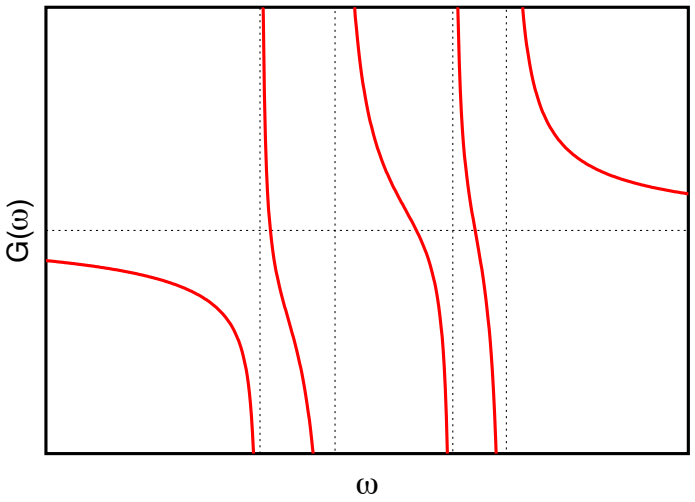

Fig. 2: *The Green function $G(\omega)$ for real ω. The dashed vertical lines give the poles, ω_i.*

where $Z_i > 0$ and ω_i, ζ_i real. On the real axis, $G(\omega)$ crosses zero precisely once in each interval $[\omega_i, \omega_{i+1}]$ with negative slope, see figure 2. It follows from (30) that $G(\zeta) = 0$ implies $\Sigma(\zeta) \to \infty$ so that the ζ_i in (31) must be the zeroes of $G(\omega)$. Moreover, the ζ_i are 'sandwiched' in between the poles ω_i and their number is indeed one less than the ω_i, see figure 2. Since $G^{-1}(\omega_i) = 0$ we find for ω close to ω_i

$$G^{-1}(\omega) = \left(1 - \frac{\partial\Sigma}{\partial\omega}\bigg|_{\omega_i}\right)(\omega - \omega_i) \quad \Rightarrow \quad Z_i = \left(1 - \frac{\partial\Sigma}{\partial\omega}\bigg|_{\omega_i}\right)^{-1}. \tag{32}$$

The residue Z_i, which equals the weight observed in photoemission/inverse photoemission, therefore is related to the slope of the self-energy, which is a well-known result.
We consider a situation where the self-energy has a single pole, $\sigma(\omega) = \sigma_0\delta(\omega - \zeta)$, and reinsert the k-dependence

$$G^{-1}(\mathbf{k}, z) = z - \varepsilon_{\mathbf{k}} - \frac{\sigma_0}{z - \zeta} \quad \Rightarrow \quad G(\mathbf{k}, z) = \frac{Z_+}{z - \omega_{+,\mathbf{k}}} + \frac{Z_-}{z - \omega_{-,\mathbf{k}}} \tag{33}$$

where we have introduced

$$\omega_{\pm,\mathbf{k}} = \frac{1}{2}\left((\varepsilon_{\mathbf{k}} + \zeta) \pm \sqrt{(\varepsilon_{\mathbf{k}} - \zeta)^2 + 4\sigma_0}\right), \qquad Z_\pm = \pm\frac{\omega_\pm - \zeta}{\omega_+ - \omega_-}.$$

It is easy to see that $Z_\pm > 0$ and $Z_+ + Z_- = 1$ as it has to be. We can see from this that the single pole of the noninteracting Green function at $\omega = \varepsilon_{\mathbf{k}}$ is split into two poles at $\omega_{\pm,\mathbf{k}}$, i.e., the single band with dispersion $\varepsilon_{\mathbf{k}}$ becomes two bands with dispersions $\omega_{\pm,\mathbf{k}}$. Note that irrespective of the value of $\varepsilon_{\mathbf{k}}$ we find $\omega_{+,\mathbf{k}} - \omega_{-,\mathbf{k}} \geq 2\sqrt{\sigma_0}$ so that the two resulting bands are separated by a gap of width $\geq 2\sqrt{\sigma_0}$. Thus, a single pole of the self-energy with macroscopic residuum σ_0 'pushes open' a gap in the band structure around its position ζ. In fact, this is exactly the situation encountered in a Mott insulator, where the self-energy has a single dominant pole of strength $\approx U^2/4$ which 'pushes open' the Mott gap of width $\approx U$.

3 The Luttinger-Ward functional

3.1 The Green function as a functional integral

We start from the representation of the Green function in terms of a functional integral over *Grassmann variables*. An excellent introduction to Grassmann variables and their use in quantum field theory can be found in the textbook by Negele/Orland [9]. We give a brief summary for readers unfamiliar with Grassmann variables, but it should be noted that this is nowhere near sufficient to fully understand their use. Grassmann variables are objects (here we write them as φ_i^* or φ_j, where i and j distinguish different Grassmann variables) which anticommute: $\varphi_i^*\varphi_j^* = -\varphi_j^*\varphi_i^*$, $\varphi_i\varphi_j^* = -\varphi_j^*\varphi_i$, and $\varphi_i\varphi_j = -\varphi_j\varphi_i$. It follows immediately that the square of any Grassmann variable is zero. While we will be using Grassmann variables with (φ_i^*) and without (φ_j) an asterisk, it should be noted that there is no such thing as the complex conjugate of a Grassmann variable – just as the index, the asterisk is simply a part of the name of the Grassmann variable. Once we have defined a set of Grassmann variables, the corresponding *Grassmann algebra* consists of all possible sums of products of Grassmann variables with complex coefficients. For example, if we have the two Grassmann variables φ^* and φ, the corresponding algebra consists of all expressions $a_0{+}a_1\varphi{+}a_2\varphi^*{+}a_3\varphi\varphi^*$ with complex a_0, a_1, a_2, and a_3 (note that all higher powers of Grassmann variables vanish). The key property of the Grassmann variables, which is used in field theory, is the rule for 'integration' over Grassmann variables, which is

$$\int d\varphi\, \varphi = 1, \qquad \int d\varphi\, 1 = 0\,.$$

In other words, integration over Grassmann variables is the same as differentiation for ordinary numbers, the only difference being that there are just two 'functions' of a Grassmann variable. When we integrate over several Grassmann variables it has to be kept in mind that the differentials $d\varphi_i^*$ and $d\varphi_j$ anticommute as well. Transcendental functions of elements of the Grassmann variables are defined via their power series expansion. To illustrate the above, we evaluate

$$\begin{aligned}
&\int d\varphi^* d\varphi\, e^{a_0+a_1\varphi+a_2\varphi^*+a_3\varphi\varphi^*} \\
&\quad = \int d\varphi^* d\varphi \left(1 + \big(a_0 + a_1\varphi + a_2\varphi^* + a_3\varphi\varphi^*\big) + \frac{1}{2}\big(a_0a_3\varphi\varphi^* + a_1a_2(\varphi\varphi^*{+}\varphi^*\varphi)\big)\right) \\
&\quad = a_3\left(1{+}\frac{a_0}{2}\right).
\end{aligned}$$

Note that the power series expansion of the exponential terminates very quickly due to the fact that all powers of Grassmann variables higher than the first vanish. Moreover, there is a nonvanishing contribution to the integral only from those terms in the integrand where each Grassmann variable to be integrated over appears precisely once.

After these preliminaries, we turn to the representation of the imaginary-time Green function as functional integral over Grassmann variables. The full derivation is too lengthy to present here but it is explained in a very understandable way by Negele/Orland [9]. Let the imaginary time interval $[0, \hbar\beta]$ be divided into M intervals of length $\varepsilon = \hbar\beta/M$, whereby we assume for

convenience that M is even. Define the imaginary time grid points $\tau_k = k{\cdot}\varepsilon$, $k = 1 \ldots M$. Then introduce Grassmann variables $\varphi^*_{\alpha,k}$ and $\varphi_{\alpha,k}$ where α is the 'compound index' that labels the Fermion operators $c^\dagger_\alpha$ and c_α, whereas $k = 1 \ldots M$ denotes the position in the imaginary time grid. Then, the partition function can be written as $Z = \lim_{M\to\infty} Z_M$, whereby [9]

$$Z_M = \prod_{k=1}^{M} \prod_{\gamma} \int d\varphi^*_{\gamma,k} d\varphi_{\gamma,k}\, e^{-S(\varphi^*,\varphi)}$$

$$S = \varepsilon \sum_{k=1}^{M} \left(\sum_{\gamma} \varphi^*_{\gamma,k} \, \frac{\varphi_{\gamma,k} - \varphi_{\gamma,k-1}}{\varepsilon} + \frac{1}{\hbar} K(\varphi^*_k, \varphi_{k-1}) \right). \tag{34}$$

Here the 'Grassmann Hamiltonian' $K(\varphi^*_k, \varphi_{k-1})$ is obtained from the Fermionic Hamiltonian (1) by replacing $c^\dagger_\gamma \to \varphi^*_{\gamma,k}$ and $c_\gamma \to \varphi_{\gamma,k-1}$. The imaginary time Green function (5) reads [9]

$$G_{\alpha,\beta}(\tau,\tau') = -\lim_{M\to\infty} \frac{1}{Z_M} \prod_{k=1}^{M} \prod_{\gamma} \int d\varphi^*_{\gamma,k}\; d\varphi_{\gamma,k}\; \varphi_{\alpha,k(\tau)} \varphi^*_{\beta,k(\tau')}\; e^{-S(\varphi^*,\varphi)}\,. \tag{35}$$

The symbols $k(\tau)$ and $k(\tau')$ denote those points on the imaginary-time grid which are closest to τ and τ'. Note that in the definition of S the term with $k = 1$ also involves the variable $\varphi_{\gamma,0}$, which is *not* included in the set of integration variables. Rather one has to set $\varphi_{\gamma,0} = -\varphi_{\gamma,M}$ to account for Fermi statistics [9]. If we let $M \to \infty$ so that $\varepsilon \to 0$, S appears to become an integral whereas $(\varphi_{\gamma,k} - \varphi_{\gamma,k-1})/\varepsilon$ appears to become a derivative whence, apparently,

$$S \to \int_0^{\hbar\beta} d\tau \left(\sum_{\gamma} \varphi^*_\gamma \, \frac{\partial \varphi_\gamma}{\partial \tau} + \frac{1}{\hbar}\, K(\varphi^*, \varphi) \right).$$

This notation can often be found in the literature but, as stressed by Negele/Orland, this can be misleading because the 'trajectories' $\varphi(\tau)$ over which the functional integral is performed may not at all be expected to be 'smooth'.

Doing all calculations at finite M and taking the limit $M \to \infty$ in the end is quite unwieldy but fortunately there is an easy way to circumvent this. Namely we may always switch to the Fourier transforms $\tilde\varphi_{\gamma,\nu}$ and $\tilde\varphi^*_{\gamma,\nu}$, defined as

$$\tilde\varphi^*_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{-i\omega_\nu \tau_k}\, \varphi^*_{\gamma,k}\,, \qquad \tilde\varphi_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{i\omega_\nu \tau_k}\, \varphi_{\gamma,k}\,, \tag{36}$$

whereby the frequencies $\omega_\nu = (2\nu{+}1)\pi/\hbar\beta$ are the Fermionic Matsubara frequencies defined above. The second equation looks like the Hermitian conjugate of the first one but recall that there is no such thing as the Hermitian conjugate of a Grassmann variable, so this is actually a *definition*. If we restrict ν to $-M/2 + 1 \le \nu \le M/2$, so that the number of ω_ν equals the number of τ_k, the above transformations are unitary as shown in Appendix B, and can be reverted to give

$$\varphi^*_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu} e^{i\omega_\nu \tau_k}\, \tilde\varphi^*_{\gamma,\nu}\,, \qquad \varphi_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu} e^{-i\omega_\nu \tau_k} \tilde\varphi_{\gamma,\nu}\,. \tag{37}$$

Note that $e^{i\omega_\nu \tau_M} = e^{i(2\nu+1)\pi} = -1$. Accordingly, if we *define* $\varphi_{\gamma,0}$ to be (37) evaluated for $k = 0$ we automatically have $\varphi_{\gamma,0} = -\varphi_{\gamma,M}$ which was implicit in the definition of S. Since the transformation from the $\varphi_{\gamma,k}$ to the $\tilde{\varphi}_{\gamma,\nu}$ is unitary the Jacobian is unity and

$$\prod_{k=1}^{M} \prod_{\gamma} \int d\varphi^*_{\gamma,k}\, d\varphi_{\gamma,k} \quad \to \quad \prod_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} \prod_{\gamma} \int d\tilde{\varphi}^*_{\gamma,\nu}\, d\tilde{\varphi}_{\gamma,\nu}\,.$$

We proceed to rewrite S in terms of the $\tilde{\varphi}^*$ and $\tilde{\varphi}$. First, consider the 'derivative term'

$$\varepsilon \sum_{k=1}^{M} \varphi^*_{\gamma,k}\, \frac{\varphi_{\gamma,k} - \varphi_{\gamma,k-1}}{\varepsilon} = \sum_{\nu,\nu'} \frac{\varepsilon}{M} \sum_{k=1}^{M} e^{i(\omega_\nu - \omega_{\nu'})\tau_k} \left(\frac{1 - e^{i\omega_{\nu'}\varepsilon}}{\varepsilon} \right) \tilde{\varphi}^*_\nu \tilde{\varphi}_{\nu'} = \varepsilon \sum_{\nu} \left(\frac{1 - e^{i\omega_\nu \varepsilon}}{\varepsilon} \right) \tilde{\varphi}^*_\nu \tilde{\varphi}_\nu .$$

In the limit of small ε (i.e. $M \to \infty$) the square bracket can be written as

$$-e^{i\omega_\nu \varepsilon/2}\, \frac{e^{i\omega_\nu \varepsilon/2} - e^{-i\omega_\nu \varepsilon/2}}{\varepsilon} = -e^{i\omega_\nu \varepsilon/2} \left(\left. \frac{de^{i\omega_\nu x}}{dx} \right|_{x=0} + \mathcal{O}(\varepsilon^2) \right) \to -i\omega_\nu\, e^{i\omega_\nu \varepsilon/2}$$

whence we obtain the final expression

$$\varepsilon \sum_{k=1}^{M} \varphi^*_{\gamma,k}\, \frac{\varphi_{\gamma,k} - \varphi_{\gamma,k-1}}{\varepsilon} = -\varepsilon \sum_{\nu} i\omega_\nu\, e^{i\omega_\nu \varepsilon/2}\, \tilde{\varphi}^*_\nu \tilde{\varphi}_\nu\,.$$

A typical term in K_0 becomes

$$\varepsilon \sum_{k=1}^{M} \big(t_{\alpha,\beta} - \mu\delta_{\alpha,\beta} \big) \varphi^*_{\alpha,k} \varphi_{\beta,k-1} = \varepsilon \sum_{\nu} e^{i\omega_\nu \varepsilon} \big(t_{\alpha,\beta} - \mu\delta_{\alpha,\beta} \big) \tilde{\varphi}^*_{\alpha,\nu} \tilde{\varphi}_{\beta,\nu}$$

whereas the products of 4 Grassmann variables in K_1 become

$$\varepsilon \sum_{k=1}^{M} \varphi^*_{\alpha,k}\, \varphi^*_{\beta,k}\, \varphi_{\gamma,k-1}\, \varphi_{\delta,k-1} = \frac{\varepsilon^2}{\hbar\beta} \sum_{\nu_1,\nu_2,\nu_3,\nu_4} \delta_{\nu_1+\nu_2,\,\nu_3+\nu_4}\, e^{i(\omega_{\nu_3}+\omega_{\nu_4})\varepsilon}\, \tilde{\varphi}^*_{\alpha,\nu_1}\, \tilde{\varphi}^*_{\beta,\nu_2}\, \tilde{\varphi}_{\gamma,\nu_3}\, \tilde{\varphi}_{\delta,\nu_4}\,.$$

The various powers of ε which show up as prefactors can be eliminated by introducing the rescaled Fourier transform $\varphi_{\gamma,\nu} = \sqrt{\varepsilon}\, \tilde{\varphi}_{\gamma,\nu}$. This transformation is no longer unitary, rather the Jacobian is ε^M which does not have a well-defined limit as $M \to \infty$. However, for any finite M the Jacobian is the same in both numerator and denominator in (35) and simply cancels out so that the limit $M \to \infty$ can be taken without problem. Having rewritten S in terms of the (rescaled) Fourier amplitudes the limit $M \to \infty$ becomes trivial: since we had $-M/2 + 1 \leq \nu \leq M/2$, we simply let each ν range over all integers. Our final result then becomes

$$\begin{aligned} -S[\varphi^*, \varphi] = \quad & \sum_{\nu} \varphi^*_{\alpha,\nu}\, e^{i\omega_\nu \varepsilon}\, G^{-1}_{0,\alpha,\beta}(i\omega_\nu)\, \varphi_{\beta,\nu} \\ & - \frac{1}{2\hbar^2\beta} \sum_{\substack{\alpha,\beta,\gamma,\delta \\ \nu_1,\nu_2,\nu_3,\nu_4}} V_{\alpha\beta,\delta,\gamma}\, \delta_{\nu_1+\nu_2,\,\nu_3+\nu_4}\, e^{2i(\omega_{\nu_3}+\omega_{\nu_4})\varepsilon}\, \varphi^*_{\alpha,\nu_1}\, \varphi^*_{\beta,\nu_2}\, \varphi_{\gamma,\nu_3}\, \varphi_{\delta,\nu_4}\,, \end{aligned} \tag{38}$$

whereby the limit $\varepsilon \to 0^+$ has to be taken and the matrix $\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}$ is the inverse noninteracting Green function, see (21). Keeping the explicit factors of $e^{i\omega_\nu\varepsilon}$ and $e^{2i(\omega_{\nu_3}+\omega_{\nu_4})\varepsilon}$ while $\varepsilon \to 0$ may seem awkward, however, these factors are in fact crucial in some cases to obtain meaningful results (see Appendix C) whereas they may be safely replaced by unity in other cases. Next, using Eqs. (7) and (8) it is easy to show that

$$\frac{1}{\hbar\beta}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, e^{i\omega_\nu\tau}\, e^{-i\omega_{\nu'}\tau'}\, G(\tau,\tau') = \delta_{\nu,\nu'}\, G(i\omega_\nu)\,,$$

the 'finite-M-version' of which is

$$\begin{aligned} G_{\alpha,\beta}(i\omega_\nu) &= \lim_{M\to\infty} \frac{\varepsilon^2}{\hbar\beta} \sum_{k,k'=1}^{M} e^{i\omega_\nu\tau_k}\, e^{-i\omega_\nu\tau_{k'}}\, G_{\alpha,\beta}(\tau_k,\tau_{k'}) \\ &= -\frac{\prod_{\mu=-\infty}^{\infty}\prod_\gamma \int d\varphi^*_{\gamma,\mu}\, d\varphi_{\gamma,\mu}\; \varphi_{\alpha,\nu}\, \varphi^*_{\beta,\nu}\, e^{-S(\varphi^*,\varphi)}}{\prod_{\mu=-\infty}^{\infty}\prod_\gamma \int d\varphi^*_{\gamma,\mu}\, d\varphi_{\gamma,\mu}\, e^{-S(\varphi^*,\varphi)}}, \end{aligned} \tag{39}$$

because $\frac{\varepsilon^2}{\hbar\beta} = \left(\frac{\sqrt{\varepsilon}}{\sqrt{M}}\right)^2$. This expression readily lends itself to a perturbation expansion in K_1 which leads to the known representation of the Green function in terms of Feynman diagrams. However, we do not pursue this here but switch to our central objective, namely the construction of the Luttinger-Ward functional, thereby closely following Potthoff [5, 6].

3.2 Construction of the Luttinger-Ward functional

We start by slightly changing our point of view. We note that the various objects that we are concerned with (the noninteracting Green function $\mathbf{G}_0$, the full Green function $\mathbf{G}$ and the self-energy $\mathbf{\Sigma}$) all are just sets of complex numbers: $F_{\alpha,\beta}(i\omega_\nu)$, $F \in \{G_0, G, \Sigma\}$. Then, we may consider (39) with (38) as the definition of a functional $\mathcal{G}[\mathbf{G}_0^{-1}]$, which maps one such set, $\mathbf{G}_0^{-1}(i\omega_\nu)$, to another one: $\mathbf{G}(i\omega_\nu)$. If the initial set happens to be a noninteracting Green function of the form $\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - (\mathbf{t}-\mu)/\hbar$ with some physical set of single particle elements $\mathbf{t}$, $\mathcal{G}[\mathbf{G}_0^{-1}]$ yields the corresponding interacting Green function, with interaction part K_1. Accordingly, K_1 in (38) may be viewed as an implicit parameter of the functional and we consider K_1 fixed from now on. One may wonder if the functional $\mathcal{G}[\mathbf{G}_0^{-1}]$ gives a well-defined result for any choice of $\mathbf{G}_0^{-1}$. This is probably not the case, but we simply restrict its domain those $\mathbf{G}_0^{-1}$ which give a well-defined result. Next consider the functional

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta}\,\ln\left(\prod_{\mu=-\infty}^{\infty}\prod_\gamma \int d\varphi^*_{\gamma,\mu}\, d\varphi_{\gamma,\mu}\, e^{-S(\varphi^*,\varphi)}\right),$$

which is the grand canonical potential for a physical $\mathbf{G}_0^{-1}$ because the bracket is Z in this case, see (34). Its variation with respect to $\mathbf{G}_0^{-1}$ is

$$\beta\,\frac{\partial\,\Omega[\mathbf{G}_0^{-1}]}{\partial\, G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} = -e^{i\omega_\nu\varepsilon}\,\mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)\,. \tag{40}$$

Note the 'inverted' order of indices of G on the right hand side, which follows by a comparison of (38) and (39). Next, for a given 'self energy' $\mathbf{\Sigma}$ and a given 'Green function' $\mathbf{G}$ consider

$$\mathbf{D}[\mathbf{G}, \mathbf{\Sigma}] = \mathcal{G}[\mathbf{G}^{-1}+\mathbf{\Sigma}] - \mathbf{G}\,.$$

Assume $\mathbf{\Sigma}$ is a true self-energy corresponding to some $\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - (\mathbf{t}-\mu)/\hbar$ (and interaction K_1) and $\mathbf{G}$ the corresponding interacting Green function. By the Dyson equation $\mathbf{G}^{-1}+\mathbf{\Sigma} = \mathbf{G}_0^{-1}$, and since $\mathcal{G}[\mathbf{G}_0^{-1}] = \mathbf{G}$ we find $\mathbf{D}[\mathbf{G}, \mathbf{\Sigma}] = 0$. Next, for a given 'Green function' $\mathbf{G}$ define the functional $\mathcal{S}[\mathbf{G}]$ to be the 'self energy' which minimizes the norm of $\mathbf{D}[\mathbf{G}, \mathbf{\Sigma}]$, defined as

$$\big|\mathbf{D}\big| = \frac{1}{N}\sum_{\alpha,\beta}\sum_{\nu}\big|D_{\alpha,\beta}(i\omega_\nu)\big|^2.$$

For a physical Green function $\mathbf{G}$ and the corresponding self-energy $\mathbf{\Sigma}$ we found $\mathbf{D} = 0$, which gives the minimal value of $|\mathbf{D}|$, whence $\mathcal{S}[\mathbf{G}] = \mathbf{\Sigma}$ and $\mathcal{S}$ simply maps the Green function to the self-energy. If $\mathbf{G}$ is not a physical Green function, but sufficiently 'reasonable' such that the above functionals can be defined, we expect

$$\mathcal{G}\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right] = \mathbf{G} + \delta\mathbf{G} \tag{41}$$

where $\delta\mathbf{G} \to 0$ whenever $\mathbf{G}$ approaches a physical Green function. We are now in the position to define the *Luttinger-Ward functional*, which is the following complex valued functional of a Green function

$$\Phi[\mathbf{G}] = \Omega\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda\varepsilon}\Big(-\ln\det\mathbf{G}(i\omega_\lambda) + \operatorname{Tr}\mathbf{G}(i\omega_\lambda)\mathbf{\Sigma}[\mathbf{G}](i\omega_\lambda)\Big). \tag{42}$$

The logarithm of the determinant is the sum of the logarithms of the $2Nn_{orb}$ eigenvalues of $\mathbf{G}(i\omega_\lambda)$ and the limit $\varepsilon \to 0^+$ is understood (to shorten the notation we henceforth omit factors like $e^{i\omega_\lambda\varepsilon}$ and reinsert them only in the final result). Consider the variation of this functional under a change of $\mathbf{G}$: Using (40), (41) and the chain rule we find the variation of the first term

$$\begin{aligned}\beta\,\frac{\partial\Omega\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right]}{\partial G_{\alpha,\beta}(i\omega_\nu)} &= -\sum_{\lambda}\sum_{\delta,\gamma}\mathcal{G}\left[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]\right]_{\delta,\gamma}(i\omega_\lambda)\,\frac{\partial(G^{-1}+\mathcal{S}[\mathbf{G}])_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} \\ &= -\sum_{\lambda}\sum_{\delta,\gamma}(G_{\delta,\gamma}+\delta G_{\delta,\gamma})(i\omega_\lambda)\,\frac{\partial(G^{-1}+\mathcal{S}[\mathbf{G}])_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}\end{aligned} \tag{43}$$

Next, notice that for each λ

$$\sum_{\gamma,\delta} G_{\delta,\gamma}(i\omega_\lambda)\,G^{-1}_{\gamma,\delta}(i\omega_\lambda) = 2Nn_{orb}\,, \tag{44}$$

and since the $G_{\alpha,\beta}(i\omega_\nu)$ for different α, β and ν must be considered as independent variables

$$\frac{\partial G_{\delta,\gamma}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)} = \delta_{\nu,\lambda}\,\delta_{\alpha,\delta}\,\delta_{\beta,\gamma}\,.$$

Differentiating (44) with respect to $G_{\alpha,\beta}(i\omega_\nu)$ we therefore obtain

$$\sum_{\gamma,\delta}\left(\delta_{\nu,\lambda}\delta_{\alpha,\delta}\,\delta_{\beta,\gamma}\,G^{-1}_{\gamma,\delta}(i\omega_\nu)+G_{\delta,\gamma}(i\omega_\lambda)\,\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}\right)=0$$

$$\Rightarrow\quad -\sum_{\gamma,\delta}G_{\delta,\gamma}(i\omega_\lambda)\,\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}=\delta_{\nu,\lambda}\,G^{-1}_{\beta,\alpha}(i\omega_\nu)\,,$$

and inserting this into (43) we find

$$\beta\,\frac{\partial\Omega\,[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]]}{\partial G_{\alpha,\beta}(i\omega_\nu)}=G^{-1}_{\beta,\alpha}(i\omega_\nu)-\sum_\lambda\sum_{\delta,\gamma}G_{\delta,\gamma}(i\omega_\lambda)\,\frac{\partial\mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}+\mathcal{O}(\delta G). \tag{45}$$

Using Appendix D the derivative of the second term on the right hand side of (42) becomes

$$\beta\,\frac{\partial}{\partial G_{\alpha,\beta}(i\omega_\nu)}\left(-\frac{1}{\beta}\sum_\lambda\ln\det\mathbf{G}(i\omega_\lambda)\right)=-G^{-1}_{\beta,\alpha}(i\omega_\nu)\,, \tag{46}$$

whereas the derivative of the third term (multiplied by β) is

$$\mathcal{S}[\mathbf{G}]_{\beta,\alpha}(i\omega_\nu)+\sum_\lambda\sum_{\delta,\gamma}G_{\delta,\gamma}(i\omega_\lambda)\frac{\partial\mathcal{S}[\mathbf{G}]_{\gamma,\delta}(i\omega_\lambda)}{\partial G_{\alpha,\beta}(i\omega_\nu)}\,. \tag{47}$$

Adding up (45), (46), and (47) and reinserting the exponential of $e^{i\omega_\nu\varepsilon}$ we obtain

$$\beta\,\frac{\partial\Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)}=e^{i\omega_\nu\varepsilon}\mathcal{S}[\mathbf{G}]_{\beta,\alpha}(i\omega_\nu)+\mathcal{O}(\delta G). \tag{48}$$

If we now let $\mathbf{G}$ become the physical Green function for some noninteracting Green function (and the fixed interaction K_1) $\mathcal{S}[\mathbf{G}]$ becomes the physical self-energy and δG vanishes. We arrive at the key result that the self-energy is the functional derivative of the Luttinger-Ward functional Φ with respect to the Green function (but note the inverted matrix indices on the right hand side). For a physical $\mathbf{G}$, $\Omega\,[\mathbf{G}^{-1}+\mathcal{S}[\mathbf{G}]]$ becomes the grand canonical potential and we arrive at the expression for Ω first derived by Luttinger and Ward

$$\Omega=-\lim_{\varepsilon\to0}\frac{1}{\beta}\sum_\lambda e^{i\omega_\lambda\varepsilon}\Big(\ln\det\mathbf{G}^{-1}(i\omega_\lambda)+\mathrm{Tr}\,\mathbf{G}(i\omega_\lambda)\,\mathbf{\Sigma}(i\omega_\lambda)\Big)+\Phi[\mathbf{G}]\,. \tag{49}$$

As it stands this expression is not really helpful for evaluating Ω, because if one wanted to use the definition (42) to evaluate $\Phi[\mathbf{G}]$ one would have to know Ω in the first place. However, Luttinger and Ward have shown that $\Phi[\mathbf{G}]$ can be represented as a sum over infinitely many suitably chosen Feynman diagrams [1], so that for example a partial summation over a subset of diagrams gives an explicit (approximate) expression for $\Phi[\mathbf{G}]$. The expression (49) gives Ω as a functional of $\mathbf{G}$ (the self-energy $\mathbf{\Sigma}$ can be eliminated using the Dyson equation) and in the

next step we want to write Ω as a functional of $\mathbf{\Sigma}$. Since the self-energy is the derivative of Φ with respect to $\mathbf{G}$

$$\frac{1}{\beta} e^{i\omega_\nu \varepsilon} \, \mathbf{\Sigma}_{\beta,\alpha}(i\omega_\nu) = \frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(i\omega_\nu)} \,, \tag{50}$$

this can be done by Legendre transform. Assuming that the functional $\mathcal{S}[\mathbf{G}]$ can be inverted to yield $\mathbf{G}[\mathbf{\Sigma}]$, define the Legendre transform

$$\begin{aligned} F[\mathbf{\Sigma}] &= \Phi\left[\mathbf{G}[\mathbf{\Sigma}]\right] - \sum_\lambda \sum_{\gamma,\delta} G[\mathbf{\Sigma}]_{\delta,\gamma}(i\omega_\lambda) \, \frac{\partial \Phi[\mathbf{G}]}{\partial G_{\delta,\gamma}(i\omega_\lambda)} \\ &= \Phi\left[\mathbf{G}[\mathbf{\Sigma}]\right] - \frac{1}{\beta} \sum_\lambda \sum_{\gamma,\delta} e^{i\omega_\lambda \varepsilon} \, G[\mathbf{\Sigma}]_{\delta,\gamma}(i\omega_\lambda) \, \mathbf{\Sigma}_{\gamma,\delta}(i\omega_\lambda) \end{aligned}$$

and inserting this into (49) we find

$$\Omega = -\lim_{\varepsilon \to 0} \frac{1}{\beta} \sum_\lambda e^{i\omega_\lambda \varepsilon} \ln \det \Big(\mathbf{G}_0^{-1}(i\omega_\lambda) - \mathbf{\Sigma}(i\omega_\lambda) \Big) + F[\mathbf{\Sigma}] \,. \tag{51}$$

By virtue of being a Legendre transform this functional obeys

$$\beta \, \frac{\partial F[\mathbf{\Sigma}]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = -e^{i\omega_\nu \varepsilon} \, G_{\beta,\alpha}(i\omega_\nu), \tag{52}$$

which is easily verified directly. Using this and again the theorem from Appendix D we arrive at the key result

$$\frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = 0 \,. \tag{53}$$

Let us summarize what we found. First, there exists a functional $\Phi[\mathbf{G}]$ such that the grand potential Ω is given by (49). By itself this is not really spectacular because one could always define $\Phi[\mathbf{G}]$ via (49). What is highly nontrivial, however, is the fact that the self-energy can be obtained as the functional derivative of $\Phi[\mathbf{G}]$ at the exact $\mathbf{G}$, see (50). Similarly, there exists a functional $F[\mathbf{\Sigma}]$ such that Ω is given by (51) and the Green function is obtained as the derivative of $F[\mathbf{\Sigma}]$, see (52). Moreover, when expressed as a functional of the self-energy, Ω is stationary with respect to variations of $\mathbf{\Sigma}$, see (53), *at the exact self-energy*. Moreover, the functionals $\Phi[\mathbf{G}]$ and $F[\mathbf{\Sigma}]$ have an additional important property: they depend only on the interaction part K_1 in the Hamiltonian, but are completely independent of the noninteracting term K_0 or, equivalently, the noninteracting Green function $\mathbf{G}_0$. To see this, let us carefully go through our above construction of the Luttinger-Ward functional. The functionals $\mathcal{G}[\mathbf{G}_0^{-1}]$ and $\Omega[\mathbf{G}_0^{-1}]$ have the noninteracting Green function as their argument while there is no further 'intrinsic' dependence on $\mathbf{G}_0$ (these functional do depend on K_1, however!). It follows that the functional $\mathcal{S}[G]$, which is defined using only the functional $\mathcal{G}$, does not have any implicit dependence on $\mathbf{G}_0$ either, i.e., it can in principle be evaluated without knowledge of $\mathbf{G}_0$. Accordingly, $\Phi[\mathbf{G}]$ is a functional only of the $G_{\alpha,\beta}(i\omega_\lambda)$ with no implicit dependence on $\mathfrak{t}$ and μ, so that the same holds true for its Legendre-transform $F[\mathbf{\Sigma}]$.

4 Self-energy functional theories

4.1 Dynamical mean-field theory

In the preceding section we have seen that the grand potential Ω of an interacting Fermi system can be represented as a functional of its self-energy, see Eq. (51), and that this functional is stationary at the true self-energy, see Eq. (53). This is a promising result: Such stationarity principles are put to use in almost every area of physics. In fact, one might come up with the following variational determination of the self-energy: choose a trial self-energy of the form (29), whence Ω ultimately becomes a functional of the spectral density $\boldsymbol{\sigma}(\omega)$ ($\mathbf{V}^{(HF)}$ is itself a functional of the Green function and hence the self-energy) and then use (53) to derive an Euler-Lagrange equation for $\boldsymbol{\sigma}(\omega)$. The problem is that the definition of the functional $\Phi[\mathbf{G}]$, Eq. (42), allowed to prove some of its properties, such as (50), but that it is completely impossible to actually evaluate it for a given 'trial $\mathbf{G}$' (this would, for example, necessitate knowledge of Ω). Accordingly, it is equally impossible to give an explicit expression for its Legendre transform $F[\boldsymbol{\Sigma}]$ and evaluate this for a given 'trial $\boldsymbol{\Sigma}$'.

However, we can circumvent this problem by making use of the fact that the functional $F[\boldsymbol{\Sigma}]$ does not depend on the noninteracting part of the Hamiltonian K_0, but only on the interaction part K_1. To illustrate the idea we consider the well-known Hubbard model on a lattice with N sites and periodic boundary conditions

$$H = \sum_{i,j} \sum_{\sigma} t_{i,j}\, c^\dagger_{i,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i\downarrow} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_i n_{i,\uparrow} n_{i\downarrow}\,.$$

Thereby $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$ and $\varepsilon_{\mathbf{k}}$ is the Fourier transform of $t_{i,j}$. In addition we consider an artificial system, called the *reference system*, with Hamiltonian $\tilde{H} = \sum_i \tilde{H}_i$, where all H_i have the identical form of an Anderson impurity model

$$\tilde{H}_i = \sum_{\nu} \varepsilon_\nu\, l^\dagger_{i,\nu,\sigma} l_{i,\nu,\sigma} + \sum_{\nu} \Big(V_\nu\, l^\dagger_{i,\nu,\sigma} c_{i,\sigma} + H.c. \Big) + U\, n_{i,\uparrow} n_{i\downarrow} \tag{54}$$

where again $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$. This describes a single 'Hubbard-site' (described by $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$) coupled to a number of 'ligand' sites (described by $l^\dagger_{i,\nu,\sigma}$ and $l_{i,\nu,\sigma}$). We assume that the impurity system can be solved, and denote the Green function and self-energy for this system by $\tilde{G}$ and $\tilde{\Sigma}$. We have seen above that all matrix elements of the self-energy involving uncorrelated sites vanish. Since the ligands in the Hamiltonian (54) are uncorrelated, the only nonvanishing element is $\tilde{\Sigma}_{c,c}(z)$.

After these preliminaries we come to the crucial point: since H and $\tilde{H}$ have the same interaction, namely $K_1 = U \sum_i n_{i,\uparrow} n_{i,\downarrow}$, the functional $F[\tilde{\boldsymbol{\Sigma}}]$ is the same for the Hubbard model and the reference system. We now make use of this fact by taking the self-energy $\tilde{\Sigma}$ of the impurity model to be the 'trial self-energy' for the lattice system. Since the reference system consists of disconnected clusters its self-energy is diagonal in real space: $\tilde{\Sigma}_{(i,c),(j,c)}(z) = \delta_{i,j}\, \tilde{\Sigma}_{c,c}(z)$, whence its Fourier transform is k-independent: $\tilde{\Sigma}(\mathbf{k}, z) = \tilde{\Sigma}_{c,c}(z)$. The resulting Green function of the lattice therefore is $G^{-1}(\mathbf{k}, z) = z - (\varepsilon_{\mathbf{k}} - \mu)/\hbar - \tilde{\Sigma}_{c,c}(z)$. Using (51) we thus obtain

an approximate Ω_{latt} for the Hubbard model (the factor of 2 is for spin)

$$\Omega_{latt} = F[\tilde{\Sigma}] - \lim_{\varepsilon\to 0}\frac{2}{\beta}\sum_{\mathbf{k}}\sum_{\lambda} e^{i\omega_\lambda\varepsilon}\,\ln\left(i\omega_\lambda - \frac{\varepsilon_{\mathbf{k}}-\mu}{\hbar} - \tilde{\Sigma}_{c,c}(i\omega_\lambda)\right). \tag{55}$$

Now we know that Ω is stationary under variations of the self-energy, see Eq. (53). We cannot perform a variation of the self-energy over *all* possible self-energies but we may restrict the domain to 'impurity model representable' ones, that means those self-energies which can be obtained by solution of the impurity model for some set of parameters $\{\varepsilon_\nu, V_\nu\}$. The variation of $\tilde{\Sigma}$ then amounts to a variation of the parameters ε_ν and V_ν in (54). Let us discuss how the value of $F[\tilde{\Sigma}]$ changes with the parameters of the impurity model, $t \in \{\varepsilon_\nu, V_\nu\}$. Using the chain rule and (52) we find

$$\begin{aligned}
\frac{\partial F[\tilde{\mathbf{\Sigma}}]}{\partial t} &= \sum_{\alpha,\beta}\sum_{\lambda}\frac{\partial F[\tilde{\mathbf{\Sigma}}]}{\partial\tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}\,\frac{\partial\tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}\\
&= -\frac{1}{\beta}\sum_{\alpha,\beta}\sum_{\lambda} e^{i\omega_\lambda\varepsilon}\,\tilde{G}_{\beta,\alpha}(i\omega_\lambda)\,\frac{\partial\tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}\\
&= -\frac{2N}{\beta}\sum_{\lambda} e^{i\omega_\lambda\varepsilon}\,\tilde{G}_{c,c}(i\omega_\lambda)\,\frac{\partial\tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t}\,.
\end{aligned}$$

The last equation follows from the fact that there are N lattice sites i and the two spin directions for each site. It follows that

$$\frac{\partial\Omega_{latt}}{\partial t} = -\frac{2}{\beta}\sum_{\mathbf{k},\lambda} e^{i\omega_\lambda\varepsilon}\left[\tilde{G}_{c,c}(i\omega_\lambda) - G(\mathbf{k},i\omega_\lambda)\right]\frac{\partial\tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t} = 0\,. \tag{56}$$

We may now perform a limiting procedure by sending the number of ligands $\to\infty$ that means considering a continuum of ligands which hybridize with the correlated c-orbital. Then the number of parameters t for which (56) must be fulfilled becomes a continuum. The simplest way to fulfill all of these conditions at once is to set the square bracket equal to zero for each λ, that means

$$\tilde{G}_{c,c}(i\omega_\lambda) = \frac{1}{N}\sum_{\mathbf{k}} G(\mathbf{k},i\omega_\lambda) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{i\omega_\lambda - (\varepsilon_{\mathbf{k}}-\mu)/\hbar - \tilde{\Sigma}_{c,c}(i\omega_\lambda)}\,. \tag{57}$$

This equation must be solved simultaneously for each ω_λ by adjusting the hybridization function $V(E)$ and the density of states $\rho(E)$ for the ligands in the impurity model, and in fact is nothing but the well-known self-consistency equation for dynamical mean-field theory (DMFT) [13] . The derivation above shows that DMFT can be understood as approximate minimization of the grand potential as functional of the self-energy. The impurity model thereby acts as the 'self-energy preparation lab' to generate trial Green functions and the associated exact self-energy.
So far we have partitioned the lattice into single sites and each site was 'decorated' with a 'bath' of ligands. However, we also could have partitioned the lattice into small but finite clusters and decorated each cluster with a bath of noninteracting ligand sites. Going through similar steps as above one can easily derive the self-consistency equations for various cluster-generalizations of DMFT [6]. The variational principle for the grand potential as a functional of the self-energy thus provides a unifying principle to derive all of these theories.

4.2 Metal-insulator-transition in a dimer

We have seen that DMFT can be derived from the variational principle for the grand potential by restricting the domain of self-energies to those which are derivable from an impurity model. However, self-energy functional theory as outlined above allows for even simpler approaches and as an example we now study Potthoff's re-derivation of the phase diagram for the metal-insulator transition in the Hubbard model [14]. We again consider the single-band Hubbard model on a simple cubic N-site lattice with periodic boundary condition, but focus on the case of *particle-hole symmetry*. To develop this idea we first note that the simple cubic lattice can be divided into two *sublattices*, A and B, such that all neighbors of a site on the A sublattice are on the B-sublattice and vice versa. Also, we rewrite the Hubbard model as

$$\begin{aligned} K = H - \mu &= \sum_{i,j} \sum_{\sigma} t_{i,j}\, c^\dagger_{i,\sigma} c_{i,\sigma} + \frac{U}{2} \sum_{i=1}^{N} \big(n_i - 1\big)\big(n_i - 1\big) - N\,\frac{U}{2} \\ &= \sum_{\mathbf{k},\sigma} \left(\varepsilon_{\mathbf{k}} - \frac{U}{2}\right) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i=1}^{N} n_{i,\uparrow}\, n_{i,\downarrow}\,, \end{aligned}$$

where $n_i = c^\dagger_{i,\uparrow} c_{i,\uparrow} + c^\dagger_{i,\downarrow} c_{i,\downarrow}$ and we assume that all $t_{i,j}$ are real so that $t_{i,j} = t_{j,i}$. Under the transformation $c^\dagger \leftrightarrow c$ we have $n_i - 1 \to 1 - n_i$ so that the interaction part is invariant, whereas the hopping term changes sign. If the hopping integral $t_{i,j}$ is different from zero only if the sites i and j belong to different sublattices, which is what we assume, this sign change can be compensated by the gauge transformation $c^\dagger_{i,\sigma} \to -c^\dagger_{i,\sigma}$ for all sites i of, say, sublattice B. It is straightforward to show that this transformation exchanges photoemission and inverse photoemission spectrum and implies $\mu = U/2$. We will now use particle-hole symmetry to construct a simplified reference system.

Namely for the reference system we follow Potthoff and choose N dimers with one 'Hubbard-site' hybridizing with one bath-site, i.e., the Hamiltonian for one dimer reads

$$\tilde{K} = \tilde{H} - \mu N = -V \sum_{\sigma} \Big(c^\dagger_\sigma l_\sigma + l^\dagger_\sigma c_\sigma \Big) + \Big(\varepsilon_l - \frac{U}{2}\Big) \sum_{\sigma} l^\dagger_\sigma l_\sigma + \frac{U}{2}\big(n_c - 1\big)\big(n_c - 1\big) - \frac{U}{2}\,. \quad (58)$$

Here $l^\dagger_\sigma$ creates an electron in the ligand site and $n_c = c^\dagger_\uparrow c_\uparrow + c^\dagger_\downarrow c_\downarrow$. Compared to the reference system (54) for DMFT that was discussed in the previous section, this amounts to retaining only a single ligand. We have to write $\varepsilon_l - U/2$ because $\mu = U/2$. Since we want to generate particle-hole symmetric self-energies we have to impose particle-hole symmetry also in the reference system. The transformation $c^\dagger \leftrightarrow c$, $l^\dagger \leftrightarrow -l$ indeed converts the Hamiltonian into itself *except* for the second term. Setting $\varepsilon_l = U/2$, however, eliminates this term and particle-hole symmetry is restored. The Hamiltonian thus becomes

$$\tilde{K} = -V \sum_{\sigma} \Big(c^\dagger_\sigma l_\sigma + l^\dagger_\sigma c_\sigma \Big) + \frac{U}{2}\big(n_c - 1\big)\big(n_c - 1\big) - \frac{U}{2}\,. \quad (59)$$

and the only remaining parameter to be varied therefore is V, the ligand energy ε_l having been eliminated by the requirement of particle-hole symmetry. The Fock space of the dimer has a

dimension of $2^4 = 16$ so that all eigenstates $|i\rangle$ and corresponding eigenenergies K_i can be obtained by numerical diagonalization of the matrix for $\tilde{K}$. If we construct basis functions with fixed particle number, spin and z-component of the spin, the problem in fact can be broken down to diagonalizing 2×2 matrices. We therefore can calculate the grand potential $\tilde{\Omega}$ by numerical evaluation of the grand partition function (4), the Green function $\tilde{G}_{\alpha,\beta}(z)$ by using the Lehmann representation (9) and the self-energy $\tilde{\Sigma}_{\alpha,\beta}(z)$ from the Dyson equation (23). Again, only the entry $\tilde{\Sigma}_{c,c}(z)$ may differ from zero for any z, which is a good check for the computer program. For concreteness, at $T = 0$ the self-energy of the dimer becomes [15]

$$\tilde{\Sigma}(z) = \frac{U}{2} + \frac{U^2}{8}\left(\frac{1}{z+3V} + \frac{1}{z-3V}\right). \tag{60}$$

Note that this has exactly the form (29), in particular the first term is indeed the Hartree-Fock potential $\langle n_\sigma\rangle\, U$ because $\langle n_\sigma\rangle = 1/2$ due to particle-hole symmetry. Reverting Eq. (51) we can now calculate the numerical value of the functional $F[\tilde{\Sigma}]$

$$F[\tilde{\Sigma}] = \tilde{\Omega} + \lim_{\varepsilon\to0}\frac{1}{\beta}\sum_\lambda e^{i\omega_\lambda\varepsilon}\ln\det\tilde{\mathbf{G}}^{-1}(i\omega_\lambda).$$

Notice that this is possible *only* because we could obtain the numerical value of $\tilde{\Omega}$ by full exact diagonalization of $\tilde{K}$. This procedure gives us a self-energy $\tilde{\Sigma}(z)$ and the corresponding numerical value of the functional $F[\tilde{\Sigma}]$ and we recall that both of these are functions of the hybridization matrix element V in (59). Next, we proceed as above: we use the self-energy $\tilde{\Sigma}(z)$ as a trial self-energy for the lattice model and write

$$\Omega_{latt} = -\frac{2}{\beta}\sum_\lambda e^{i\omega_\lambda\varepsilon}\int d\varepsilon\,\rho_0(\varepsilon)\,\ln\Big(i\omega_\lambda - \varepsilon + \mu - \tilde{\Sigma}_{c,c}(i\omega_\lambda)\Big) + F[\tilde{\Sigma}]\,,$$

where $\rho_0(\varepsilon)$ is the density of states for the conduction band. Following Potthoff [14] we use a semi-elliptical density of states of width $W = 4$

$$\rho_0(\varepsilon) = \frac{1}{2\pi}\sqrt{4-\varepsilon^2}.$$

In this approximation Ω becomes a function of V and figure 3(a) shows $\Omega(V)$ at $T = 0$ for different U. For smaller U there are two stationary points: a maximum at $V = 0$ and a minimum at finite V, which is the physical solution. At $U_c \approx 5.82$ the two extrema coalesce into a single minimum at $V = 0$, which is the only stationary point for larger U. This change from finite V to $V = 0$ precisely corresponds to the metal-insulator transition. To see this we recall equation (60) for $\tilde{\Sigma}(z)$ and insert it into the **k**-integrated Green function

$$G(z) = 2\int_{-2}^{2} d\varepsilon\,\frac{\rho_0(\varepsilon)}{z + U/2 - \varepsilon - \tilde{\Sigma}(z)}\,. \tag{61}$$

This is shown in figure 4 together with $\Im\tilde{\Sigma}(z)$ for $z = \omega - i\eta$. The self-energy has two poles at $\zeta_1 = -3V$ and $\zeta_2 = 3V$ which give the two Lorentzian peaks in $\Im\tilde{\Sigma}(z)$. As discussed above

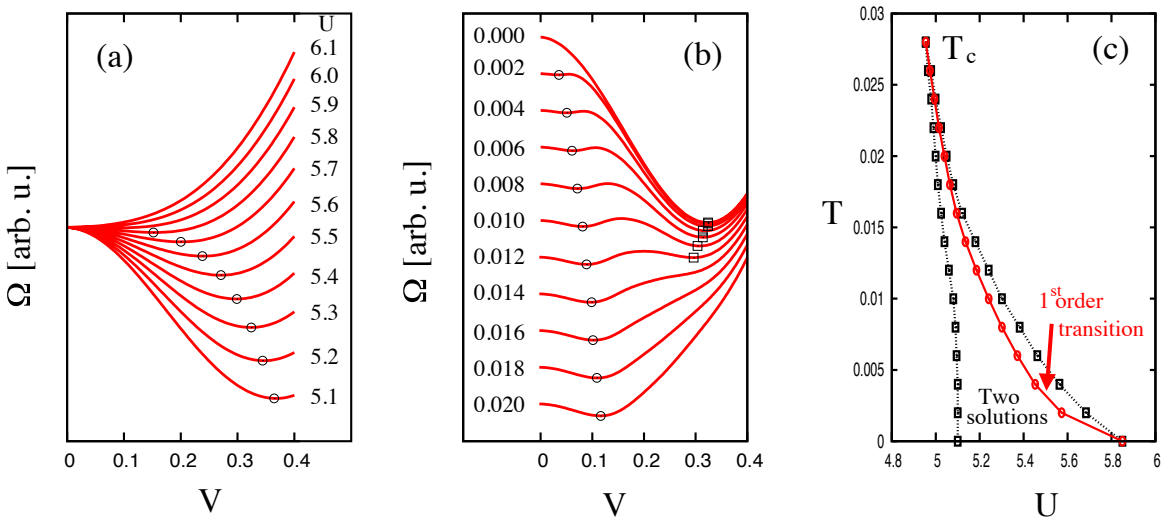

Fig. 3: *(a): $\Omega(V)$ versus V at $T = 0$, variation with U, (b): Ω versus V at $U = 5.2$, variation with T, (c): the resulting phase diagram.*

these two poles 'push open' gaps in the density of states around themselves, see the top panel of Fig. 4. There is still a finite spectral weight at the Fermi level, $\omega = 0$, i.e., the system is a metal. As V becomes smaller, see the center panel of Fig. 4, the slope of $\tilde{\Sigma}(z)$ in the energy range between ζ_1 and ζ_2 (which is $\frac{\partial \Sigma}{\partial \omega} = -\left(\frac{U}{6V}\right)^2$ at $\omega = 0$) becomes steeper and steeper so that according to (32) the spectral weight at the Fermi level becomes smaller and smaller. Finally, as $V \to 0$ the two poles coalesce, see the bottom panel of Fig. 4, and there remains only a single pole at $\omega = 0$ which pushes open a gap of order U and the spectral density at $\omega = 0$ vanishes – the system has turned into a Mott-insulator! This is precisely the scenario predicted by DMFT [13], whereby DMFT calculations find $U_c \approx 5.84$ [13] as compared to $U_c \approx 5.82$ from the simple dimer calculation.

Next, figure 3(b) shows $\Omega(V)$ for the fixed value of $U = 5.2$ and different temperatures T. For most temperatures there are three stationary points whereby the local maximum can be discarded. It follows, that there are actually two possible solutions for each temperature which cross in between $T = 0.10$ and $T = 0.12$. This implies that there is a first order phase transition between these two temperatures. Repeating the procedure for various U gives the phase diagram in figure 3(c). There is only a metallic solution for small U, at a first U_{c1} a second insulating solution starts to appear, at U_c there is a first order metal-insulator transition and on from U_{c2} there is only an insulating solution. The results obtained in this way by the solution of a dimer are qualitatively very similar to those obtained by extensive numerical renormalization group [16] and quantum Monte Carlo [17] calculations in the framework of DMFT. The main deficiency of the dimer calculation is the underestimation of the critical temperature T_c in figure 3(c) by a factor of ≈ 2.

This application of self-energy functional theory, whereby trial self-energies $\mathbf{\Sigma}(z)$ and the numerical value of Ω and hence $F[\mathbf{\Sigma}]$ are obtained by exact diagonalization of a suitably chosen reference system is called the *Variational Cluster Approximation*. This was first proposed by Potthoff and successfully applied to a large number of problems.

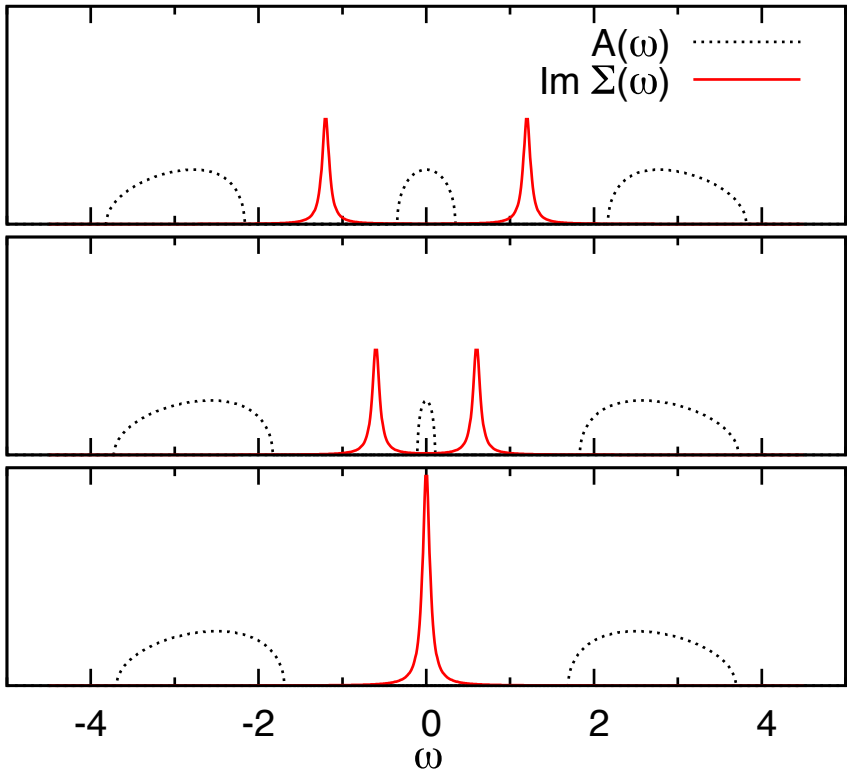

Fig. 4: *Single particle spectral function and imaginary part of the self-energy (calculated with an imaginary part of* 0.05 *for the frequency) obtained from the angle integrated Green function (61) with self-energy (60). Parameter values are* $U=5$ *and* $V=0.4$ *(top),* $V=0.2$ *(center) and* $V=0$ *(bottom).*

5 Summary and conclusion

We have discussed the single-particle Green function $\mathbf{G}(z)$ which describes the propagation of a particle added to a system of interacting fermions. It is a function of the complex frequency variable z which is analytical throughout the complex z-plane except for the real axis. On the real axis it has poles which give the energies needed to add or remove a particle. Via the Dyson equation it can be related to the self-energy $\mathbf{\Sigma}(z)$ which describes the effects of the interaction with the propagating particle with the other particles in the system. We have derived the spectral representations Eq. (12) and Eq. (29) for these quantities. We have then given a nonperturbative derivation of the results of Luttinger and Ward: the grand canonical potential Ω is a functional of the Green function and self-energy (see Eq. (49), the self-energy is the derivative of the Luttinger-Ward functional with respect to the Green function (see Eq. (50)) and Ω is stationary with respect to variations of the self-energy (see Eq. (53)). We have then seen that Ω can also be expressed as a functional of the self-energy alone (see Eq. (51)) which is stationary with respect to variations of the self-energy. This then is the basis of self-energy functional theory which provides a simple unifying framework for Dynamical Mean-Field Theory and its cluster generalizations and which also can be applied directly in the framework of the Variational Cluster Approximation.

Appendix A

We want to prove the formula

$$-i\Theta(t)\,e^{-iEt} = \lim_{\eta\to 0^+}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\frac{e^{-i\omega t}}{\omega - E + i\eta}\,. \tag{62}$$

We consider the integral on the right-hand-side as a contour integral in the complex ω-plane along the real axis. We initially limit the range of integration to be $\int_{-R}^{R} d\omega\cdots$ and take the limit $R\to\infty$ in the end. We augment this contour by a semicircle of radius R around the origin so that the resulting contour is closed. For any ω on the semicircle we have

$$e^{-i\omega t} \;=\; e^{\sin(\varphi)Rt}\;e^{-i\cos(\varphi)Rt}$$

where φ is the phase of ω. Assume that $t\sin(\varphi) < 0$. Then, for any $\varepsilon > 0$ we can find an R such that $R\;e^{\sin(\varphi)Rt} < \varepsilon$. It follows that the contour integral over the part of the semicircle where $t\sin(\varphi) < 0$ vanishes in the limit $R\to 0$. For $t > 0$ this means that the integral over the semicircle in the lower half-plane $\pi < \varphi < 2\pi$ vanishes, whereas it is the semicircle in the upper half-plane $0 < \varphi < \pi$ which gives vanishing contribution for $t < 0$. We can thus replace the integral on the right-hand-side by an integral along a *closed* contour which consists of the real axis and an infinitely large semicircle in the lower (upper) half-plane for $t > 0$ ($t < 0$). But this means we can invoke the *theorem of residues* which tells us that the integral is $\pm 2\pi i$ times the sum of residues of all poles within the integration contour. The integrand has one pole at $\omega_0 = E - i\eta$ with residuum $e^{-i\omega_0 t}$. This is in the lower half-plane so that we know immediately that for $t < 0$ the integral vanishes i.e., it is $\propto \Theta(t)$. For $t > 0$ we readily find that the integral is $-2\pi i\;e^{-i\omega_0 t}$ and inserting this into (62) and taking the limit $\eta\to 0$ proves (62), which shows that the Fourier transform of the left-hand side is $(\omega - E + i\eta)^{-1}$.

Appendix B

Call $\lambda = e^{i\frac{2m\pi}{M}}$ where m and M are integers. Then

$$\sum_{k=1}^{M}\lambda^k = \lambda\sum_{k=0}^{M-1}\lambda^k = \lambda\,\frac{\lambda^M - 1}{\lambda - 1}\,,$$

but since $\lambda^M = (e^{2\pi i})^m$ this is zero. Defining M-component vectors $\vec{\varphi}^* = (\varphi_1^*, \varphi_2^*, \ldots, \varphi_M^*)$ and $\vec{v}_\nu = \frac{1}{\sqrt{M}}(e^{-i\omega_\nu\tau_1}, e^{-i\omega_\nu\tau_2}, \ldots e^{-i\omega_\nu\tau_M})$ the first one of Equations (36) can be written as $\varphi^*_{\gamma,\nu} = \vec{v}^*_\nu\cdot\vec{\varphi}^*$. Introducing $\lambda = e^{2i\frac{\mu-\nu}{M}\pi}$ one has, using $\omega_\nu = (2\nu{+}1)\pi/\hbar\beta$ and $\tau_k = \hbar\beta k/M$,

$$\vec{v}^*_\nu\cdot\vec{v}_\mu = \frac{1}{M}\sum_{k=1}^{M} e^{i(\omega_\mu-\omega_\nu)\tau_k} = \frac{1}{M}\sum_{k=1}^{M}\lambda^k = \begin{cases} 1 \quad \text{for } \mu{-}\nu = nM, \\ \\ \lambda\,\frac{\lambda^M-1}{\lambda-1} = 0 \quad \text{for } \mu{-}\nu \neq nM. \end{cases} \tag{63}$$

with integer n. The M vectors $\vec{v}_\nu$ with $-M/2+1 \le \nu \le M/2$ therefore are orthonormal. The matrix T, which transforms the M variables φ_k^* into the M variables, $\vec{\varphi}^*_\nu = T\;\vec{\varphi}^*_k$, therefore has the $\vec{v}_\mu$ as its lines, whence $T^+ = T^{-1}$ and the transformation is unitary. Eq. (37) follows immediately.

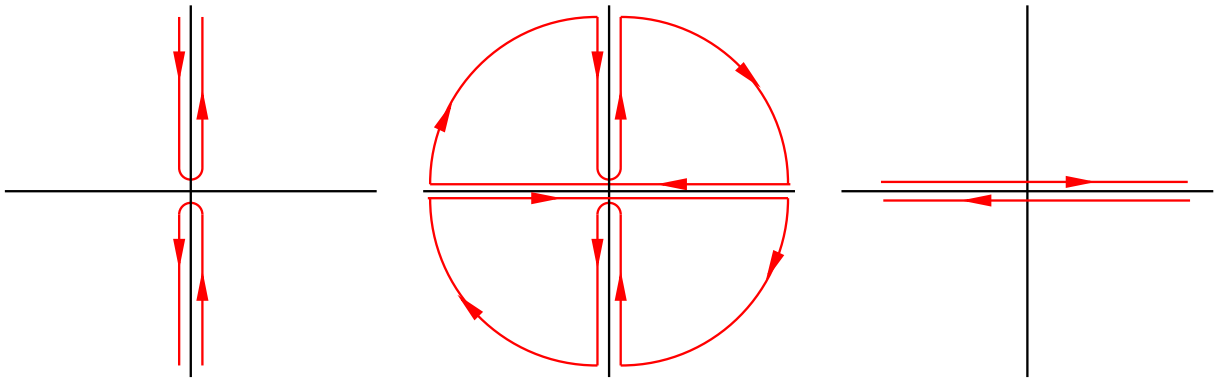

Fig. 5: *Integration contours for sums over Matsubara frequencies.*

Appendix C

In this Appendix we want to highlight the importance of the factors of $e^{i\omega_\lambda \varepsilon}$ and discuss the evaluation of sums of the form

$$S = -\lim_{\varepsilon\to 0} \frac{1}{\beta} \sum_\lambda e^{i\omega_\lambda \varepsilon}\, g(i\omega_\lambda)\,,$$

whereby we assume that $g(z)$ is an analytic function except for the real axis. Since $i\hbar\beta\omega_\lambda = (2\lambda{+}1)i\pi$ the Fermi function $f(z) = (e^{\beta\hbar z}+1)^{-1}$ has poles at the Matsubara frequencies $i\omega_\lambda$. Straightforward calculation shows that for $z = i\omega_\lambda + \zeta$ we have $f(z) = -1/\beta\hbar\zeta$ so that the residuum is $-1/\beta\hbar$. Invoking the theorem of residues we can rewrite

$$S = \lim_{\varepsilon\to 0} \frac{\hbar}{2\pi i} \oint_{\mathcal{C}} dz\, f(z)\, e^{\varepsilon z}\, g(z)\,,$$

where $\mathcal{C}$ encircles the imaginary axis in counterclockwise fashion, see figure 5(a). Next we note that the integrals along the two clover-shaped contours in figure 5(b) are zero, *provided* the integrand is analytic in the interior of the two curves. Since the Fermi function has all of its poles along the imaginary axis, which is outside of the curves in figure 5(b), and since we assumed that $g(z)$ is analytic except on the real axis this is certainly true. The Fermi function $f(z)$ guarantees that the contribution from the semicircle with $\Re(z) > 0$ vanishes, whereas the factor $e^{z\varepsilon}$ does the same for the semicircle with $\Re(z) < 0$, see the discussion in Appendix A. It follows that the integral along the contour $\mathcal{C}$ in figure 5(a) is equal to that along the contour $\mathcal{C}'$ in figure 5(c) (note the inverted direction of the curves in figure 5(c) as compared to figure 5(b)!). We could thus convert the sum over Matsubara frequencies to an integral over a contour which runs counterclockwise around the real axis, which can again be evaluated using the theorem of residues whereby we pick up contributions from the singularities of $g(z)$. In particular, the limit $T \to 0$ can be taken without problem for this expression. Notice that the seemingly unimportant factor of $e^{i\omega_\lambda \varepsilon}$ was instrumental for this construction because it was only due to this factor that the arc with $\Re(z) < 0$ could be neglected. This is the reason why these factors have to be followed carefully in all calculations.

Appendix D

Here we prove the identity

$$\frac{\partial \ln \det A}{\partial A_{ij}} = A^{-1}_{ji}$$

We use Laplace's formula and expand $\det A$ in terms of minors

$$\det A = \sum_{l=1,n} (-1)^{i+l}\ A_{il} M_{il}$$

Since none of the minors M_{il} contains the element A_{ij} we find

$$\frac{\partial \ln \det A}{\partial A_{ij}} = \frac{(-1)^{i+j} M_{ij}}{\det A}$$

Next, the i^{th} column of A^{-1} is the solution of the system of equations

$$Ac = E_i$$

where E_i is the i^{th} column of the unit matrix. It has all elements equal to zero, except for the i^{th}, which is one. We use Cramer's rule and find for the j^{th} element of the i^{th} column

$$A^{-1}_{ji} = \frac{\det \bar{A}_j}{\det A}$$

where $\bar{A}_j$ is the matrix where the j^{th} column has been replaced by E_i. Now we use again Laplace's formula for $\det \bar{A}_j$ and obtain

$$A^{-1}_{ji} = \frac{(-1)^{i+j} M_{ij}}{\det A}$$

which proves the theorem.
As an application we assume that the matrix elements of A are functions of some parameter α. Then we find

$$\frac{\partial \ln \det A}{\partial \alpha} = \sum_{i,j} \frac{\partial \ln \det A}{\partial A_{ij}} \frac{\partial A_{ij}}{\partial \alpha} = \sum_{i,j} A^{-1}_{ji} \frac{\partial A_{ij}}{\partial \alpha} = \mathrm{Tr}\, A^{-1} \frac{\partial A}{\partial \alpha}\,.$$

References

[1] J.M. Luttinger and J.C. Ward, Phys. Rev. **118**, 1417 (1960)

[2] J.M. Luttinger, Phys. Rev. **119**, 1153 (1960)

[3] G. Baym and L.P. Kadanoff, Phys. Rev. **124**, 287 (1961)

[4] G. Baym, Phys. Rev. **127**, 1391 (1962)

[5] M. Potthoff, Condens. Mat. Phys. **9**, 557 (2006)

[6] M. Potthoff in A. Avella and F. Mancini (eds.): *Theoretical Methods for Strongly Correlated Systems*, (Springer, 2011); see also preprint arXiv:11082183

[7] A.A. Abrikosov, L.P. Gorkov, and I.E. Dzyaloshinksi: *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, New Jersey 1964)

[8] A.L. Fetter and J.D. Walecka: *Quantum Theory of Many-Particle Systems* (McGraw-Hill, San Francisco, 1971)

[9] J.W. Negele and H. Orland: *Quantum Many-Particle Systems* (Addison-Wesley, Redwood, 1988)

[10] G. Baym and N.D. Mermin, J. Math. Phys. **2**,232 (1961)

[11] I. Dzyaloshinskii, Phys. Rev. B **68**, 085113 (2003)

[12] J.M. Luttinger, Phys. Rev. **121**, 942 (1961)

[13] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

[14] M. Potthoff, Eur. Phys. J. B**36**, 335 (2003)

[15] E. Lange, Mod. Phys. Lett.B **12**, 915 (1998)

[16] R. Bulla, T.A. Costi, and D. Vollhardt, Phys. Rev. B **64** 045103 (2001)

[17] J. Joo and V. Oudovenko, Phys. Rev. B **64** 103102 (2001)