

# 6 Linear Response Functions

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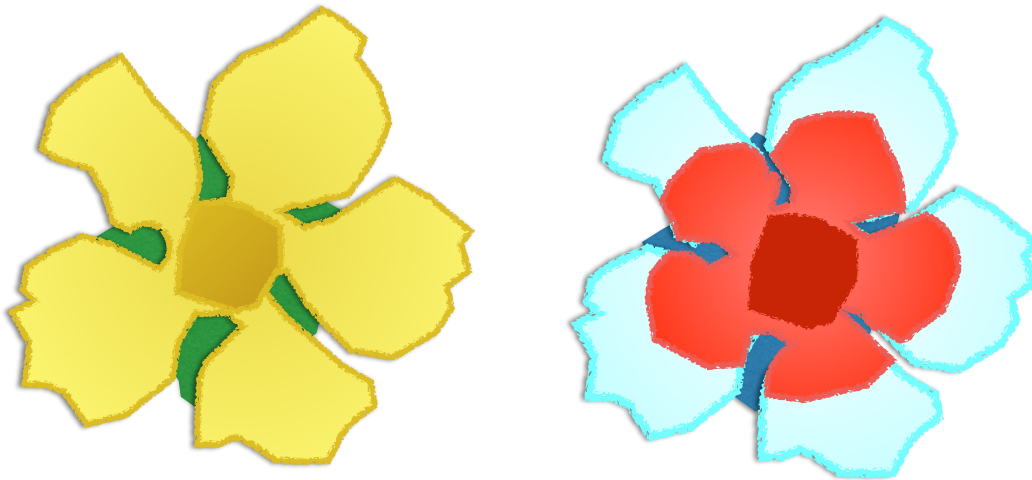
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# 1 Introduction

All we know about a physical system stems either from its effects on other physical systems or from its response to external forces [1–3]. Making sense out of this information is a very difficult task. First of all, what do we actually mean by physical system? Typically we are interested in crystals. A sample of a crystal is an object with unique characteristics, a specific number of atoms or defects, a certain surface, a given weight. What we are interested in, however, are its general properties, i.e., those common to all possible samples. This idealized crystal is the one we have in mind [4, 5] with the word *system* or *material*. How do we unravel the mechanisms behind its properties? The first step is constructing the Hamiltonian. The latter should be abstract enough to indeed describe the ideal crystal only, but it should retain enough details to actually distinguish it from other systems, i.e., it should be *material-specific*. At a first glance, constructing such a material-specific Hamiltonian appears straightforward. All of solid-state physics stems from the Coulomb interaction, attractive between nuclei and electrons and repulsive between electrons; we can therefore, in principle, just choose a complete one-electron basis and, in the Born-Oppenheimer approximation, write down in second quantization the electronic Hamiltonian for a given ideal crystal  $\hat{H}_e$ . To make progress, we then have to solve the eigenvalue problem  $\hat{H}_e\Psi = E\Psi$ . Here trouble starts, since the Schrödinger equation defined by  $\hat{H}_e$  cannot, in general, be solved exactly, and even if we knew the exact solution, with  $N_e \rightarrow \infty$  electrons, it would be very hard to make sense out of it. For the ground state, a very powerful tool to attack such a many-body problem is density-functional theory (DFT), which shifts the focus from finding the ground-state wavefunction to finding the ground-state electronic density. Remarkably, this can be achieved via the solution of a reference auxiliary one-electron problem, a much simpler task than solving the original problem. Although DFT is an exact ground-state theory, in practice only approximated forms of the DFT universal functional are known, the most popular of which is perhaps the local-density approximation (LDA). DFT, in the LDA or its simple extensions, is very successful in describing and even predicting the properties of various classes of materials, to the extent that it can be considered the standard model of solid-state physics [5–7]. For strongly correlated systems, those on which we focus in this lecture, the LDA and its simple extension fail even qualitatively, however. Thus, if we want to understand correlated materials we have to revisit the first step, the Hamiltonian. We can change the perspective; if the full many-body problem cannot be solved, the best approach is perhaps to reduce the number of degrees of freedom to the essential by integrating out high-energy ones in the spirit of the Wilson renormalization group. Hence, we have to construct low-energy *minimal* material-specific models. Systematically downfolding the high-energy states of the full many-body problem, although desirable in theory, is basically impossible in practice [8]. It turns out, however, that we can exploit the successes of DFT to build *ab-initio* Wannier functions spanning the low-energy bands [9, 10]; via these Wannier functions, we can construct effective many-body models, minimal and materials-specific, suited to describe the low-energy part of the spectrum. But we are still not at the end of the story; with few exceptions, even these minimal models cannot be solved exactly, and finding powerful and flexible solution techniques



**Fig. 1:** A silverweed: Schematic view of color patterns as seen by the human eye (left) and as might be seen by the eyes of a bee (right, false colors).

is therefore crucial. Typically this involves making a series of approximations, which, together with the model, have at the end to be put to a test. To this end a big step forward was the development, started 25 years ago, of the dynamical mean-field theory (DMFT) [11–15] and shortly after of the LDA+DMFT method [16, 17], which combines density-functional theory and dynamical mean-field theory. The LDA+DMFT technique quickly proved very successful. Through this method, we have learned that details do matter; for example we understood that a crystal-field splitting much smaller than the band-width can play an important role in the metal-insulator transition of correlated transition-metal oxides [10]. The LDA+DMFT approach was key in identifying the nature of important phenomena such as, e.g., the origin of orbital ordering in paradigmatic correlated transition-metal systems [18]. Various of the striking LDA+DMFT success stories are told in the lecture notes in this book. Thanks to its successes, LDA+DMFT is nowadays the method of choice for strongly-correlated materials.

A central issue remains to be discussed at this point. Once we have built a material specific model and solved it within a given set of approximations, e.g., using the LDA+DMFT approach, how do we actually test our theory against experiments? To make this connection we have to calculate the quantity actually measured, the response of the system to external perturbations. This is a challenge on its own. Methods or approximations that work well for the ground state can, e.g., perform badly for the excitation spectrum, the knowledge of which is crucial for obtaining response functions – examples are the Hartree-Fock or static mean-field approximation or the LDA itself. Furthermore, experiments let us see a system only through a distorting glass, and our task is to reconstruct the original image. Perhaps some part of the energy spectrum is invisible to us, because the transition probability from the ground state to certain excited states is forbidden by symmetry. If the response of a system to a given perturbation is zero in a certain energy window, e.g., filtered away, we have no chance of seeing what is there. Our eyes filter the ultraviolet, and thus we cannot see the beautiful color patterns that attract insects to flowers

such as silverweeds, for us monochromatic (Fig. 1). Response theory therefore plays a crucial role in our comprehension of Nature. Typically, the external force used in experiments is small with respect to the internal ones in a crystal, so that the system is weakly perturbed. Thus, the dominant term is the *linear response function*. If we are able to disentangle it, the linear-response function returns us information on the ground state and the excitation spectrum, their symmetry properties, the strength of correlations. In this lecture, I will present the basics of linear response theory [1–3] together with some representative examples for strongly correlated materials, using for the latter LDA+DMFT as theoretical approach.

To set the stage, let us introduce the basics of the LDA+DMFT method, different aspects of which will be used in the whole lecture. Let us start with the electronic Hamiltonian. In the Born-Oppenheimer approximation, the non-relativistic electronic Hamiltonian for an ideal crystal  $\hat{H}_e$  can then be written as the sum of a one-electron part  $\hat{H}_0$  and an interaction part  $\hat{H}_U$

$$\hat{H}_e = \hat{H}_0 + \hat{H}_U. \quad (1)$$

In a complete basis of Wannier functions  $\psi_{in\sigma}(\mathbf{r})$ , the one-electron term is given by

$$\hat{H}_0 = - \sum_{\sigma} \sum_{ii'} \sum_{nn'} t_{n,n'}^{i,i'} c_{in\sigma}^{\dagger} c_{i'n'\sigma},$$

where  $c_{in\sigma}^{\dagger}$  ( $c_{in\sigma}$ ) creates (destroys) an electron with spin  $\sigma$  in orbital  $n$  at site  $i$ . The on-site ( $i = i'$ ) terms yield the crystal-field matrix while the  $i \neq i'$  contributions are the hopping integrals. This part of the Hamiltonian describes the attraction between electrons and nuclei, the latter forming an ideal lattice. The electron-electron repulsion  $\hat{H}_U$  is instead given by

$$\hat{H}_U = \frac{1}{2} \sum_{ii'jj'} \sum_{\sigma\sigma'} \sum_{nn'pp'} U_{np\ n'p'}^{ij\ i'j'} c_{in\sigma}^{\dagger} c_{jp\sigma'}^{\dagger} c_{j'p'\sigma'} c_{i'n'\sigma}.$$

Although the Hamiltonian (1) is very general, for a given system, the *material-specific* hopping and crystal-field parameters can be obtained *ab-initio* using, e.g., Wannier functions constructed from first principles via density-functional theory [19, 20]. Then

$$t_{n,n'}^{i,i'} = - \int d\mathbf{r} \overline{\psi_{in\sigma}(\mathbf{r})} \left[ -\frac{1}{2} \nabla^2 + v_R(\mathbf{r}) \right] \psi_{i'n'\sigma}(\mathbf{r}),$$

where  $v_R(\mathbf{r})$  is the self-consistent one-electron LDA reference potential. The *bare* Coulomb integrals can be expressed in terms of Wannier functions as well

$$U_{np\ n'p'}^{ij\ i'j'} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \overline{\psi_{in\sigma}(\mathbf{r}_1)} \overline{\psi_{jp\sigma'}(\mathbf{r}_2)} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{j'p'\sigma'}(\mathbf{r}_2) \psi_{i'n'\sigma}(\mathbf{r}_1).$$

Here we have to be careful, however. The LDA includes in  $v_R(\mathbf{r})$  also Coulomb effects, via the long-range Hartree term and the exchange-correlation contribution; if we use LDA Wannier functions as one-electron basis, to avoid double counting we have to subtract from  $\hat{H}_U$  the effects already included in the LDA. This means that we have to replace

$$\hat{H}_U \rightarrow \Delta\hat{H}_U = \hat{H}_U - \hat{H}_{DC},$$

where  $\hat{H}_{\text{DC}}$  is the double-counting correction. Unfortunately we do not know which correlation effects are exactly included in the LDA, and therefore the exact expression of  $\hat{H}_{\text{DC}}$  is also unknown.<sup>1</sup> The remarkable successes of the LDA suggest, however, that in many materials the LDA is overall a good approximation, and therefore, in those systems at least, the term  $\Delta\hat{H}_U$  can be neglected. What about strongly correlated materials? Even in correlated systems, most likely the LDA works rather well for the delocalized electrons or in describing the average or the long-range Coulomb effects. Thus one can think of separating the electrons into *uncorrelated* and *correlated*; only for the latter we do take the correction  $\Delta\hat{H}_U$  into account explicitly, assuming furthermore that  $\Delta\hat{H}_U$  is local or almost local [19]. Typically, correlated electrons are those that partially retain their atomic character, e.g., those that originate from localized  $d$  and  $f$  shells; for convenience in this lecture we assume that in a given system they stem from a single atomic shell  $l$  (e.g.,  $d$  for transition-metal oxides or  $f$  for heavy-fermion systems) and label their states with the atomic quantum numbers  $l$  and  $m = -l, \dots, l$  of that shell. Thus

$$U_{np,n'p'}^{ijj'j'} \sim \begin{cases} U_{m_\alpha m_\beta m'_\alpha m'_\beta}^l & ijj'j' = iiii \quad npn'p' \in l \\ 0 & ijj'j' \neq iiii \quad npn'p' \notin l \end{cases}$$

and  $\Delta\hat{H}_U$  is replaced by  $\Delta\hat{H}_U^l = \hat{H}_U^l - \hat{H}_{\text{DC}}^l$ , where  $\hat{H}_{\text{DC}}^l$  is, e.g., given by the static mean-field contribution of  $\hat{H}_U^l$ . There is a drawback in this procedure, however. By splitting electrons into correlated and uncorrelated we implicitly assume that the main effect of the latter is the renormalization or *screening* of parameters for the former, in particular of the Coulomb interaction. The calculation of screening effects remains, unfortunately, a challenge to date. Approximate schemes are the constrained LDA and the constrained random-phase approximation (RPA) methods [6]. Nevertheless, we have now identified the general class of models for strongly-correlated systems, namely the generalized Hubbard model

$$\hat{H}_e = \hat{H}^{\text{LDA}} + \hat{H}_U^l - \hat{H}_{\text{DC}}^l. \quad (2)$$

It is often convenient to integrate out or downfold empty and occupied states and work directly with a set of Wannier functions spanning the correlated bands only. The LDA term in  $\hat{H}_e$  is then given by

$$\hat{H}^{\text{LDA}} = - \sum_{ii'} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} t_{m_\alpha, m'_\alpha}^{i, i'} c_{im_\alpha\sigma}^\dagger c_{i'm'_\alpha\sigma} = \sum_{\mathbf{k}} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} [H_{\mathbf{k}}^{\text{LDA}}]_{m_\alpha, m'_\alpha} c_{\mathbf{k}m_\alpha\sigma}^\dagger c_{\mathbf{k}m'_\alpha\sigma},$$

where the right-hand side is rewritten using as a one-electron basis Bloch functions  $\psi_{\mathbf{k}m_\alpha\sigma}$  constructed from the Wannier functions  $\psi_{im_\alpha\sigma}$ . The local *screened* Coulomb interaction is instead given by

$$\hat{H}_U^l = \frac{1}{2} \sum_i \sum_{\sigma\sigma'} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c_{im_\alpha\sigma}^\dagger c_{im_\beta\sigma'}^\dagger c_{im'_\beta\sigma'} c_{im'_\alpha\sigma}.$$

<sup>1</sup>A more detailed discussion of the double-counting correction can be found in the lectures of Tim Wehling and Alexander Lichtenstein.

More details on building realistic models can be found, e.g., in the lecture notes of previous schools [5–7], in particular in the chapters listed in Refs. [19–22]. The simplest version of Hamiltonian (2) is the one-band Hubbard model

$$\hat{H}_{\text{Hubbard}} = \underbrace{-\sum_{ii'} \sum_{\sigma} t_{1,1}^{i,i'} c_{i\sigma}^{\dagger} c_{i'\sigma}}_{\hat{H}_0} + \underbrace{\varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}}_{\hat{H}_U}, \quad (3)$$

where  $\varepsilon_d$  is the crystal-field level,  $t_{1,1}^{i,i'}$  is the hopping integral between electrons at site  $i$  and  $i'$ ,  $U$  the on-site Coulomb repulsion, and  $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ . Since in this model only the correlated orbital ( $m_{\alpha} = 1$ ) appears, the double-counting correction amounts to a mere shift of the chemical potential, and therefore does not have to be included explicitly. The one-band Hubbard model describes, at least in first approximation, the low-energy states of high-temperature superconducting cuprates (HTSCs), characterized by a partially filled Cu  $d x^2 - y^2$ -like band at the Fermi level. In these systems the most relevant hopping integrals are the one between nearest neighbors,  $t$ , and the one between next-nearest neighbors,  $t'$ ; the ratio  $t'/t$  ranges from 0.1 to 0.4 [9]. At half-filling, the one-band Hubbard model describes the physics of the Mott metal-insulator transition. In the atomic limit ( $U/t \rightarrow \infty$ ), it is a collection of decoupled one-electron atoms

$$\hat{H}_{\text{Hubbard}} \sim \hat{H}_U = \varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (4)$$

In the non-interacting limit ( $U/t \rightarrow 0$ ) it describes instead a metallic half-filled band

$$\hat{H}_{\text{Hubbard}} \sim \hat{H}_0 = -\sum_{ii'} \sum_{\sigma} t_{1,1}^{i,i'} c_{i\sigma}^{\dagger} c_{i'\sigma} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}. \quad (5)$$

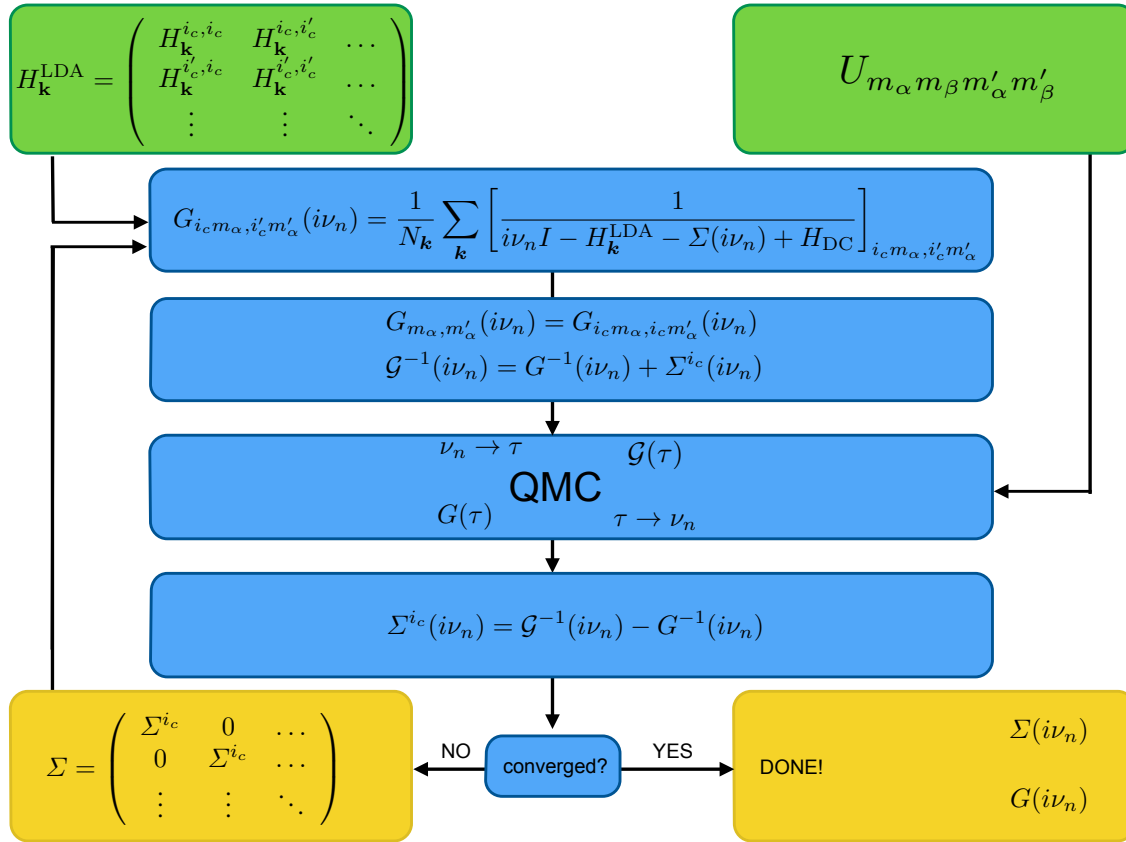
In this lecture we will use the half-filled Hubbard model (3) for most examples. In particular, we will discuss its magnetic linear-response function; the microscopic mechanisms leading to magnetism in the Hubbard model – and in correlated systems in general – are discussed in detail in my lecture of last year's school [22], which is complementary to the present one.

Although apparently simple, even Hamiltonian (3) cannot be solved exactly except than in special cases. The state-of-the art method for solving Hubbard-like models is, as discussed, dynamical mean-field theory. The latter maps the correlated *lattice* problem described by the Hubbard model onto a correlated single-impurity problem [14, 15], i.e., onto an effective model describing a correlated site  $i_c$  coupled via hybridization to a bath of non-correlated electrons. This effective single impurity model has to be solved self-consistently in the spirit of mean-field theories. The DMFT self-consistency loop is shown in Fig. 2. The impurity Green function  $G(\omega)$ , in general a matrix in spin-orbital space, is obtained by solving the quantum-impurity problem for a given bath. Next, the Dyson equation yields the self-energy

$$\Sigma(\omega) = \mathcal{G}^{-1}(\omega) - G^{-1}(\omega),$$

where  $\mathcal{G}(\omega)$  is the bath Green-function matrix; the self-energy matrix  $\Sigma(\omega)$  is then used to calculate the local Green-function matrix

$$G_{i_c, i_c}(\omega) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} [\omega - H_{\mathbf{k}}^{\text{LDA}} - \Sigma(\omega)]_{i_c, i_c}^{-1},$$



**Fig. 2:** The LDA+DMFT self-consistency loop. The LDA Hamiltonian  $H_{\mathbf{k}}^{\text{LDA}}$  is built in the basis of Bloch states obtained from localized Wannier functions. The set  $\{i_c\}$  labels the equivalent correlated sites inside the unit cell. The local Green-function matrix is at first calculated using an initial guess for the self-energy matrix. The bath Green-function matrix is then obtained via the Dyson equation and used to build an effective quantum-impurity model. The latter is solved via a quantum-impurity solver, here quantum Monte Carlo (QMC), yielding the impurity Green-function matrix. Through the Dyson equation the self-energy is then obtained, and the procedure is repeated till self-consistency is reached.

where  $N_{\mathbf{k}}$  is the number of  $\mathbf{k}$  points. Self-consistency is reached when the impurity Green function  $G(\omega)$  equals the actual local Green function  $G_{i_c, i_c}(\omega)$  of the system. The main approximation adopted is that the self-energy is local; the self-energy becomes indeed local in the infinite-coordination-number limit [11, 12]. The combination of DMFT with density-functional theory, just described above in short, defines the LDA+DMFT approach [17]. In this lecture we will not further discuss this technique, except for the specific aspects related to the calculation of linear-response functions. These include the local-vertex approximation, used to obtain from DMFT calculations the  $\mathbf{q}$ -dependent linear-response function  $\chi(\mathbf{q}; \omega)$  and the quantum-impurity model and its solution; the latter yields the local impurity Green-function matrix and the local linear response function  $\chi(\omega)$ . A more detailed description of the DMFT and LDA+DMFT methods and their development can be found in the lecture notes of Dieter Vollhardt, Gabriel Kotliar, Antoine Georges, and Alexander Lichtenstein.

## 2 Linear response theory

### 2.1 The linear susceptibility $\chi(\mathbf{r}, \mathbf{r}'; t, t')$

Let us consider a system described by the Hamiltonian  $\hat{H}$  and a space- and time-dependent perturbation  $\mathbf{h}(\mathbf{r}, t)$ , for example a magnetic field. How does the system react to the external perturbation? If the perturbation is weak and we can calculate the change in the Hamiltonian to linear order, the response of the system can be given in terms of retarded correlation functions calculated at equilibrium, even if the perturbation has brought the sample out of equilibrium. The linear correction to the Hamiltonian can be expressed as

$$\begin{aligned}\hat{H} &\rightarrow \hat{H} + \int d\mathbf{r} \hat{H}_1(\mathbf{r}; t) + \dots \\ \hat{H}_1(\mathbf{r}; t) &= - \sum_{\nu} \hat{O}_{\nu}(\mathbf{r}; t) h_{\nu}(\mathbf{r}; t),\end{aligned}\tag{6}$$

where  $\hat{O}(\mathbf{r}; t)$  is an operator that describes the system property affected by the perturbation; often this operator is a vector, thus we indicate with  $\nu = x, y, z$  its components along the Cartesian axes. If the perturbation is an external magnetic field,  $\hat{O}(\mathbf{r}; t)$  could be the magnetic moment density,  $\hat{M}(\mathbf{r}; t)$ . It is convenient to express  $\hat{O}(\mathbf{r}; t)$  in the Heisenberg representation

$$\hat{O}_{\nu}(\mathbf{r}; t) = e^{i(\hat{H} - \mu\hat{N})t} \hat{O}_{\nu}(\mathbf{r}) e^{-i(\hat{H} - \mu\hat{N})t},$$

where  $\mu$  is the chemical potential and  $\hat{N}$  the electron number operator. The perturbation  $\mathbf{h}(\mathbf{r}; t)$  can display very different forms, depending on the experiment. It could have been, e.g., initially switched on adiabatically at  $t = -\infty$ ; this can be expressed mathematically by multiplying the perturbation by the prefactor  $e^{\epsilon t}$ , where here  $\epsilon$  is an infinitesimally small positive number,  $\mathbf{h}(\mathbf{r}; t) \rightarrow e^{\epsilon t} \mathbf{h}(\mathbf{r}; t)$ , and taking later the limit  $\epsilon \rightarrow 0$ . The perturbation could also be a sharp impulse at  $t = t_0$  and therefore have the form  $\mathbf{h}(\mathbf{r}; t) = \mathbf{h}(\mathbf{r}) \delta(t - t_0)$ , or have been switched on or off suddenly at a certain time  $t = t_0$ .

Whatever its form, let us consider the effect of the time-dependent perturbation  $\mathbf{h}(\mathbf{r}; t)$  on a specific system property, described by the operator  $\hat{P}(\mathbf{r}; t)$ , also expressed in the Heisenberg representation; in general  $\hat{P}(\mathbf{r}; t)$  can be a different operator than  $\hat{O}(\mathbf{r}; t)$ , but in many common cases it is proportional to it. To linear order in the perturbation, at a given temperature the expectation value of  $\hat{P}(\mathbf{r}; t)$  is modified as follows

$$\begin{aligned}\langle \hat{P}_{\nu}(\mathbf{r}; t) \rangle &= \langle \hat{P}_{\nu}(\mathbf{r}) \rangle_0 + \langle \delta \hat{P}_{\nu}(\mathbf{r}; t) \rangle_0, \\ \langle \delta \hat{P}_{\nu}(\mathbf{r}; t) \rangle_0 &= -i \int d\mathbf{r}' \int_{-\infty}^t dt' \left\langle \left[ \Delta \hat{P}_{\nu}(\mathbf{r}; t), \Delta \hat{H}_1(\mathbf{r}'; t') \right] \right\rangle_0.\end{aligned}$$

Here  $\langle \hat{P}_{\nu}(\mathbf{r}) \rangle_0$  is the (equilibrium) thermal average in the absence of the perturbation. For a given operator  $\hat{A}$ , the latter is defined as

$$\langle \hat{A} \rangle_0 = \frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H} - \mu\hat{N})} \hat{A} \right],$$



where  $\beta = 1/k_B T$ , and  $Z$  is the partition function

$$Z = \text{Tr} e^{-\beta(\hat{H}-\mu\hat{N})}.$$

The difference

$$\Delta\hat{A}(\mathbf{r}; t) = \hat{A}(\mathbf{r}; t) - \langle\hat{A}(\mathbf{r})\rangle_0,$$

measures the deviation with respect to the thermal average in the absence of perturbation; in most common cases  $\langle\hat{A}(\mathbf{r})\rangle_0 = 0$ . Let us consider as an example the case in which the perturbation is a magnetic field and  $\hat{P}_\nu(\mathbf{r}; t)$  the  $\nu$ -component of the magnetic density operator  $\hat{M}_\nu(\mathbf{r}; t)$ ; for a paramagnetic system the equilibrium expectation value  $\langle\hat{M}_\nu(\mathbf{r})\rangle_0$  is zero and  $\Delta\hat{M}_\nu(\mathbf{r}; t) = \hat{M}_\nu(\mathbf{r}; t)$ . Finally, for a given operator  $\hat{A}(\mathbf{r})$ , the expectation value  $\langle\Delta\hat{A}^2(\mathbf{r})\rangle_0$  yields the mean-square fluctuation of the quantity  $\hat{A}(\mathbf{r})$ .

By replacing the operator  $\Delta\hat{H}_1(\mathbf{r}'; t')$  in the commutator with its expression obtained from Eq. (6), we can express the linear correction to  $\langle\hat{P}_\nu(\mathbf{r}; t)\rangle_0$  as

$$\langle\delta\hat{P}_\nu(\mathbf{r}; t)\rangle_0 = i \sum_{\nu'} \int d\mathbf{r}' \int_{-\infty}^t dt' \left\langle \left[ \Delta\hat{P}_\nu(\mathbf{r}; t), \Delta\hat{O}_{\nu'}(\mathbf{r}'; t') \right] \right\rangle_0 h_{\nu'}(\mathbf{r}'; t').$$

The linear response function or *linear susceptibility* is then given by

$$\chi_{\hat{P}_\nu\hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t, t') \equiv \lim_{h_{\nu'} \rightarrow 0} \frac{\partial\langle\hat{P}_\nu(\mathbf{r}; t)\rangle}{\partial h_{\nu'}(\mathbf{r}'; t')}.$$

The equation

$$\chi_{\hat{P}_\nu\hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t, t') = i \left\langle \left[ \Delta\hat{P}_\nu(\mathbf{r}; t), \Delta\hat{O}_{\nu'}(\mathbf{r}'; t') \right] \right\rangle_0 \Theta(t - t'), \quad (7)$$

is known as the *Kubo formula*. In order to respect causality, a perturbation can only modify the system *after* it has been switched on. Thus, if the perturbation is switched on at time  $t'$ , the linear response function can only have finite value for  $t > t'$ , and it has to vanish for  $t < t'$ ; in other words, the response function is *retarded*. This cause-and-effect principle is included in Eq. (7) through the Heaviside step function  $\Theta(t - t')$ , defined as

$$\Theta(t - t') = \begin{cases} 1 & \text{if } t - t' > 0 \\ 0 & \text{if } t - t' < 0. \end{cases}$$

It is worth pointing out that the Kubo formula Eq. (7) yields the response function in terms of the *correlation function*

$$\mathcal{S}_{\hat{P}_\nu\hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t, t') = \langle\Delta\hat{P}_\nu(\mathbf{r}; t)\Delta\hat{O}_{\nu'}(\mathbf{r}'; t')\rangle_0. \quad (8)$$

The latter expresses the joint probability of having a finite  $\Delta\hat{P}_\nu$  at position  $\mathbf{r}$  and time  $t$  if there was a finite  $\Delta\hat{O}_{\nu'}$  at position  $\mathbf{r}'$  and time  $t'$ . This relation between linear response function and correlation function will turn out to be very important, as we will see in Sec. 2.5.

## 2.2 The Fourier transform $\chi(\mathbf{q}; \omega)$

Let us consider the case in which the Hamiltonian  $\hat{H}$  of the system is time-independent and thus also invariant under time translations. Then the linear response function depends only on time differences,  $t - t'$ , and we can rewrite it as follows

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t, t') = \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t - t').$$

Thus the linear correction to the expectation value of  $\hat{P}_\nu(\mathbf{r}; t)$  becomes

$$\langle \delta \hat{P}_\nu(\mathbf{r}; t) \rangle_0 = i \sum_{\nu'} \int d\mathbf{r}' \int_{-\infty}^{+\infty} dt' \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t - t') h_{\nu'}(\mathbf{r}'; t'). \quad (9)$$

Many perturbations are periodic in time after they have been switched on. It is therefore convenient to Fourier transform Eq. (9) with respect to time (see Appendix for definitions and conventions on Fourier transforms adopted in this lecture), obtaining

$$\langle \delta \hat{P}_\nu(\mathbf{r}; \omega) \rangle_0 = \sum_{\nu'} \int d\mathbf{r}' \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; \omega) h_{\nu'}(\mathbf{r}'; \omega),$$

where  $\mathbf{h}(\mathbf{r}'; \omega)$  is the Fourier transform of the perturbation and  $\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; \omega)$  the Fourier transform of the susceptibility. The latter is given by

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; \omega) = \int_{-\infty}^{\infty} dt \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t) e^{i\omega t} = \int_0^{\infty} dt \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; t) e^{i\omega t}.$$

It is also convenient to Fourier transform Eq. (9) with respect to  $\mathbf{r}$ ; for a system with full spatial translational invariance symmetry, i.e., for which the momentum is conserved,

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; \omega) = \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r} - \mathbf{r}'; \omega),$$

and thus we have

$$\begin{aligned} \langle \delta \hat{P}_\nu(\mathbf{q}; \omega) \rangle_0 &= \sum_{\nu'} \int \frac{d\mathbf{q}'}{(2\pi)^3} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}, -\mathbf{q}'; \omega) h_{\nu'}(\mathbf{q}'; \omega) \\ &= \sum_{\nu'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) h_{\nu'}(\mathbf{q}; \omega), \end{aligned} \quad (10)$$

where

$$\begin{aligned} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}, -\mathbf{q}'; \omega) &= \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \int d\mathbf{r}' e^{-i\mathbf{q}'\cdot\mathbf{r}'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}, \mathbf{r}'; \omega) \\ &= \int d\mathbf{r}' \left[ \int d\mathbf{r} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r} - \mathbf{r}'; \omega) \right] e^{-i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{r}'} \\ &= (2\pi)^3 \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) \delta(\mathbf{q} - \mathbf{q}'), \end{aligned}$$

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = \int d\mathbf{r}'' e^{i\mathbf{q}\cdot\mathbf{r}''} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}''; \omega).$$

An ideal crystal has only lattice translational invariance, however. How does relation (10) change in this case? It turns out that it is still valid, but we have to express  $\chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}, -\mathbf{q}'; \omega)$  differently. Let us see how. For simplicity, we consider a lattice of Bravais type (one atom per unit cell); we define as  $\mathbf{T}_i$  the lattice vector which identifies site  $i$ . Let us assume that  $\Delta\hat{P}_\nu(\mathbf{r})$  is the one-body operator  $\Phi^\dagger(\mathbf{r})\Delta\hat{P}_\nu\Phi(\mathbf{r})$ , where  $\Phi^\dagger(\mathbf{r})$  is the fermionic field creation operator. The term  $\Delta\hat{P}_\nu(\mathbf{r})$  can then be expressed as follows

$$\Delta\hat{P}_\nu(\mathbf{r}) = \sum_{ii'} \sum_{\alpha\alpha'} \underbrace{\overline{\psi_{i\alpha'}(\mathbf{r})}\psi_{i'\alpha}(\mathbf{r})}_{\rho_{\alpha'\alpha}^{i,i'}(\mathbf{r})} \underbrace{c_{i\alpha'}^\dagger [\Delta\hat{P}_\nu]_{\alpha\alpha'} c_{i'\alpha}}_{\Delta\hat{P}_{\nu,\alpha\alpha'}^{i,i'}} = \sum_{ii'} \sum_{\alpha\alpha'} \rho_{\alpha'\alpha}^{i,i'}(\mathbf{r}) \Delta\hat{P}_{\nu,\alpha\alpha'}^{i,i'}$$

where  $\{\psi_{i\alpha}(\mathbf{r})\}$  is a complete set of orthonormal one-electron wavefunctions and  $\alpha$  a collective index for its quantum numbers (for example  $\alpha = m_\alpha\sigma$ ). If we now choose for  $\{\psi_{i\alpha}(\mathbf{r})\}$  a set of localized Wannier functions, to first approximation the overlap of two  $\psi_{i\alpha}(\mathbf{r})$  centered at different sites is small and can be neglected; this means that  $\rho_{\alpha'\alpha}^{i,i'}(\mathbf{r})$  is only sizeable for  $i = i'$ , and therefore

$$\Delta\hat{P}_\nu(\mathbf{r}) \sim \sum_i \sum_{\alpha\alpha'} \rho_{\alpha'\alpha}^{i,i}(\mathbf{r}) \Delta\hat{P}_{\nu,\alpha\alpha'}^i$$

i.e.,  $\Delta\hat{P}_\nu(\mathbf{r})$  is approximatively a weighted sum of the site operators  $\Delta\hat{P}_{\nu,\alpha\alpha'}^i$ . A similar approximation holds for  $\Delta\hat{O}_\nu(\mathbf{r})$ ,

$$\Delta\hat{O}_\nu(\mathbf{r}) \sim \sum_i \sum_{\gamma'\gamma} \rho_{\gamma'\gamma}^{i,i}(\mathbf{r}) \Delta\hat{O}_{\nu,\gamma\gamma'}^i$$

Let us introduce the tensorial components of the linear-response function for the site operators

$$\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(t-t') = i \left\langle \left[ \Delta\hat{P}_{\nu,\alpha\alpha'}^i(t-t'), \Delta\hat{O}_{\nu',\gamma\gamma'}^{i'}(0) \right] \right\rangle_0 \Theta(t-t').$$

The Fourier transform of  $\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(t-t')$  in time is given by  $\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\omega)$ ; furthermore

$$\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\mathbf{q}, -\mathbf{q}'; \omega) = \sum_{ii'} e^{i\mathbf{q}\cdot\mathbf{T}_i - i\mathbf{q}'\cdot\mathbf{T}_{i'}} \chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\omega) = \underbrace{\sum_{i'} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{T}_{i'}}}_{N_s \sum_{\mathbf{G}} \delta_{\mathbf{q}', \mathbf{q}+\mathbf{G}}} \underbrace{\sum_i e^{i\mathbf{q}\cdot\mathbf{T}_i} \chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\omega)}_{\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\mathbf{q}; \omega)},$$

where  $N_s$  is the number of lattice sites. In terms of these components, the term  $\chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}, -\mathbf{q}'; \omega)$  in Eq. (10) is given by

$$\chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}, -\mathbf{q}'; \omega) = N_s \sum_{\alpha\alpha'\gamma\gamma'} \sum_{\mathbf{G}} \rho_{\alpha'\alpha}(\mathbf{q}) \rho_{\gamma'\gamma}(-\mathbf{q}') \delta_{\mathbf{q}', \mathbf{q}+\mathbf{G}} \chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}^{\alpha\alpha'\gamma\gamma'}(\mathbf{q}; \omega).$$

where  $\rho_{\alpha'\alpha}(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \rho_{\alpha'\alpha}^{i_0, i_0}(\mathbf{r})$ . Long-range order instabilities are typically at  $\mathbf{q}_C$  vectors that correspond to deformations commensurate with the lattice. To study them, one can, e.g., perturb the system at  $\mathbf{q}' = \mathbf{q}_C$ , or possibly use experimental techniques that have access to the  $\mathbf{q}$ -dependent response function.

Let us now consider as an example the case in which the perturbation is a magnetic field oriented along  $z$  and the operators  $\Delta\hat{P}_\nu(\mathbf{r})$  and  $\Delta\hat{O}_\nu(\mathbf{r})$  are both equal to  $\hat{M}_z(\mathbf{r}) = \Phi^\dagger(\mathbf{r})\hat{\sigma}_z\Phi(\mathbf{r})$ , the magnetic density at position  $\mathbf{r}$ ; the operator  $\hat{\sigma}_z$  is the  $z$  Pauli matrix. Let us derive the magnetic response for a strongly correlated system with a partially filled  $l$  shell; for simplicity, we focus on the  $l$  electrons and choose as a basis the set of Wannier functions  $\psi_{im_\alpha\sigma}(\mathbf{r})$  spanning the corresponding  $l$  bands. Then  $\hat{M}_z(\mathbf{r})$  can be expressed as follows

$$\hat{M}_z(\mathbf{r}) \sim -g\mu_B \sum_i \sum_{m_\alpha m'_\alpha} \rho_{m_\alpha m'_\alpha}(\mathbf{r}) \frac{1}{2} \sum_{\sigma\sigma'} c_{im_\alpha\sigma}^\dagger [\Delta\hat{M}_z]_{\sigma\sigma'} c_{im'_\alpha\sigma'},$$

where  $[\Delta\hat{M}_z]_{\sigma\sigma'} = \langle\sigma|\hat{\sigma}_z|\sigma'\rangle$ . If our low-energy model includes only a single orbital we can drop the indices  $\{m_\alpha\}$ ; in this case we obtain the simple expression

$$\hat{M}_z(\mathbf{r}) \sim -g\mu_B \rho(\mathbf{r}) \sum_i \hat{S}_z^i. \quad (11)$$

The Fourier transform of  $\hat{M}_z(\mathbf{r})$  is then given by  $\hat{M}_z(\mathbf{q}) \sim -g\mu_B \rho(\mathbf{q}) \hat{S}_z(\mathbf{q})$  with

$$\hat{S}_z(\mathbf{q}; 0) = \frac{1}{2} \sum_{\mathbf{k}} \sum_{\sigma} c_{\mathbf{k}\sigma}^\dagger \langle\sigma|\hat{\sigma}_z|\sigma\rangle c_{\mathbf{k}+\mathbf{q}\sigma}.$$

Finally, to linear order the change in  $\langle\hat{M}_z(\mathbf{q}; \omega)\rangle_0$  can be expressed as

$$\begin{aligned} \langle\delta\hat{M}_z(\mathbf{q}; \omega)\rangle_0 &\sim (g\mu_B)^2 |\rho(\mathbf{q})|^2 \sum_{ii'} e^{-i\mathbf{q}\cdot(\mathbf{T}_i - \mathbf{T}_{i'})} \sum_{\sigma\sigma'} \sigma\sigma' \chi_{\hat{S}_z^i \hat{S}_z^{i'}}^{\sigma\sigma\sigma'\sigma'}(\omega) h_z(\mathbf{q}; \omega) \\ &= (g\mu_B)^2 |\rho(\mathbf{q})|^2 \chi_{\hat{S}_z \hat{S}_z}(\mathbf{q}; \omega) h_z(\mathbf{q}; \omega), \end{aligned}$$

where  $\sigma = 1$  for spin up and  $\sigma = -1$  for spin down and

$$\chi_{\hat{S}_z \hat{S}_z}(\mathbf{q}; \omega) = i \int dt e^{i\omega t} \left\langle \left[ \hat{S}_z(\mathbf{q}; t), \hat{S}_z(-\mathbf{q}; 0) \right] \right\rangle_0 \Theta(t).$$

Later in the lecture we will discuss the case of the one-band Hubbard model; we will focus on the response function for site operators,  $\chi_{\hat{S}_z^i \hat{S}_z^{i'}}(\omega)$  and its Fourier transform  $\chi_{\hat{S}_z \hat{S}_z}(\mathbf{q}; \omega)$  and do not further discuss the prefactor  $\rho(\mathbf{q})$ . For multi-orbital systems with well-defined localized spins but quenching of the angular momentum, e.g.,  $3d$  transition-metal oxides that are Mott insulators [22], the magnetization density can still be expressed via Eq. (11). We have, however, to replace  $\rho(\mathbf{r})$  with the normalized spin density at the atomic site,  $\rho_s(\mathbf{r})$ , originating from the unpaired electrons in the  $l$  shell. Thus

$$\hat{M}_z(\mathbf{r}) \sim -g\mu_B \rho_s(\mathbf{r}) \sum_i \hat{S}_z^i.$$

Then we have

$$\begin{aligned} \langle\delta\hat{M}_z(\mathbf{q}; \omega)\rangle_0 &\sim (g\mu_B)^2 |\rho_s(\mathbf{q})|^2 \sum_{ii'} e^{-i\mathbf{q}\cdot(\mathbf{T}_i - \mathbf{T}_{i'})} \sum_{\sigma\sigma'} \sigma\sigma' \chi_{\hat{S}_z^i \hat{S}_z^{i'}}^{\sigma\sigma\sigma'\sigma'}(\omega) h_z(\mathbf{q}; \omega) \\ &= (g\mu_B)^2 |\rho_s(\mathbf{q})|^2 \chi_{\hat{S}_z \hat{S}_z}(\mathbf{q}; \omega) h_z(\mathbf{q}; \omega). \end{aligned}$$

The Fourier transform of the spin density  $\rho_s(\mathbf{q})$  is the so-called atomic form factor and can be probed via, e.g., neutron scattering experiments.

### 2.3 Analytic properties of $\chi(\mathbf{q}; \omega)$

The Fourier transform of  $\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{r}; t)$  to momentum space can be written as

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; t) = i \left\langle \left[ \Delta \hat{P}_\nu(\mathbf{q}; t), \Delta \hat{O}_{\nu'}(-\mathbf{q}; 0) \right] \right\rangle_0 \Theta(t).$$

Let us assume that  $\{\Psi_n^N\}$  is the full set of eigenvectors of the Hamiltonian  $\hat{H}$  for  $N$  electrons and that the corresponding eigenenergies are  $\{E_n^N\}$ . Let us also define the matrix elements

$$\begin{aligned} P_\nu^{nm}(\mathbf{q}) &= \langle \Psi_n^N | \Delta \hat{P}_\nu(\mathbf{q}; 0) | \Psi_m^N \rangle, \\ O_{\nu'}^{mn}(\mathbf{q}) &= \langle \Psi_m^N | \Delta \hat{O}_{\nu'}(\mathbf{q}; 0) | \Psi_n^N \rangle. \end{aligned}$$

We can then rewrite  $\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; t)$  as follows

$$\begin{aligned} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) &= \frac{i}{Z} \int_0^\infty dt e^{i\omega t} \text{Tr} \left\{ e^{-\beta(\hat{H} - \mu\hat{N})} \left[ \Delta \hat{P}_\nu(\mathbf{q}; t), \Delta \hat{O}_{\nu'}(-\mathbf{q}; 0) \right] \right\} \\ &= \frac{i}{Z} \sum_{nm} \int_0^\infty dt e^{-\beta(E_n^N - \mu N)} e^{i(\omega + E_n^N - E_m^N)t} P_\nu^{nm}(\mathbf{q}) O_{\nu'}^{mn}(-\mathbf{q}) \\ &\quad - \frac{i}{Z} \sum_{nm} \int_0^\infty dt e^{-\beta(E_n^N - \mu N)} e^{i(\omega + E_m^N - E_n^N)t} O_{\nu'}^{nm}(-\mathbf{q}) P_\nu^{mn}(\mathbf{q}) \\ &= \frac{i}{Z} \sum_{nm} F_{nm} \int_0^\infty dt e^{i(\omega - E_m^N + E_n^N)t} \hat{P}_\nu^{nm}(\mathbf{q}) \hat{O}_{\nu'}^{mn}(-\mathbf{q}), \end{aligned}$$

where  $F_{nm} = e^{-\beta(E_n^N - \mu N)} - e^{-\beta(E_m^N - \mu N)}$ . The time integral can be obtained from the formula

$$I(x) = \int_0^\infty e^{ixt} dt = \frac{i}{x + i\delta},$$

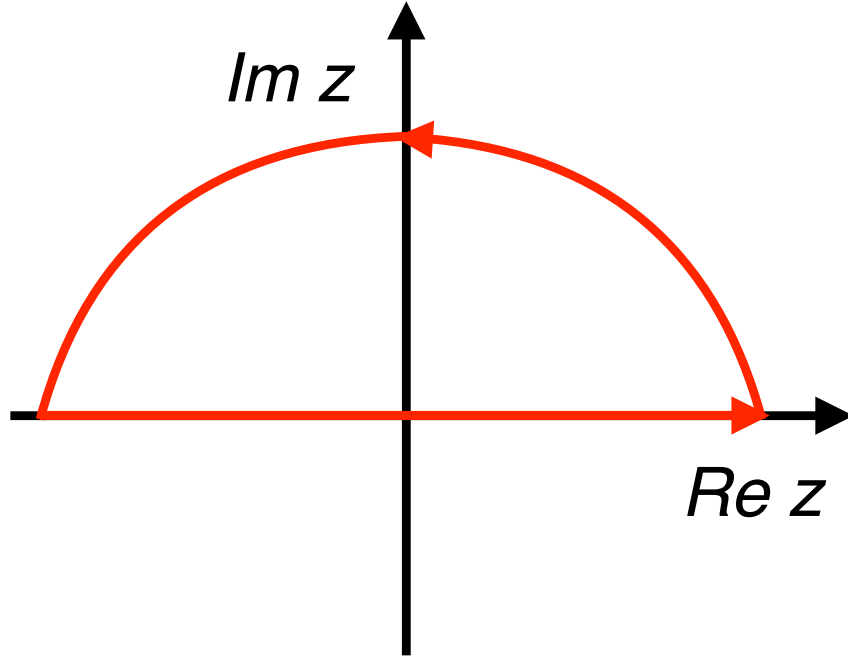
where  $\delta$  is a positive infinitesimal; we thus arrive to the final expression

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = \frac{1}{Z} \sum_{nm} \frac{e^{-\beta(E_n^N - \mu N)} - e^{-\beta(E_m^N - \mu N)}}{E_m^N - E_n^N - \omega - i\delta} P_\nu^{nm}(\mathbf{q}) O_{\nu'}^{mn}(-\mathbf{q}). \quad (12)$$

This equation shows that the complex function  $\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; z)$ , obtained from  $\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega)$  replacing  $\omega$  with the complex variable  $z$ , thanks to the positive infinitesimal  $\delta$ , is analytic in the upper half and has poles in the lower half of the complex plane. The fact that the response function is analytic is a direct consequence of causality; the fact that it is analytic in the upper instead than in the lower half of the complex plane is a consequence of our conventions on the signs of the exponents in the Fourier transform.

Up to now we did not make any assumption on the properties of the operators  $\hat{O}_\nu$  and  $\hat{P}_\nu$ ; if, however, they are Hermitian, one can show, starting from Eq. (12), that

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = \left[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(-\mathbf{q}; -\omega) \right]^*$$



**Fig. 3:** The semicircular contour  $\mathcal{C}$  in the upper complex plane.

Therefore if we split the response function into a real and an imaginary part,

$$\chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) = \text{Re} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) \right] + i \text{Im} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) \right],$$

the two components should satisfy the relations

$$\begin{aligned} \text{Re} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) \right] &= \text{Re} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(-\mathbf{q}; -\omega) \right], \\ \text{Im} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) \right] &= -\text{Im} \left[ \chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(-\mathbf{q}; -\omega) \right]. \end{aligned}$$

Thus the real part of the linear response function is even and the imaginary part is odd in  $\omega$ .

## 2.4 Kramers-Kronig relations and sum rules

The Kramers-Kronig relations are valid for any retarded response function  $\chi(\mathbf{q}; \omega)$ . They follow from the fact that the complex function  $\chi(\mathbf{q}; z)$  is analytic in the upper half of the complex plane, a property that we have just proved, and vanishes in the limit  $|z| \rightarrow \infty$ . Let us consider the integral on the real axis

$$I_{\mathcal{R}} = \int_{-\infty}^{+\infty} \frac{\chi(\mathbf{q}; \omega')}{\omega' - \omega + i\delta} d\omega',$$

where  $\delta$  is an infinitesimally small positive number. The integrand is a complex analytic function in the upper part of the complex plane, and therefore, because of the Cauchy integral theorem, the integral on any closed contour  $\mathcal{C}$  in that half-plane has to vanish

$$I_{\mathcal{C}} = \oint_{\mathcal{C}} \frac{\chi(\mathbf{q}; z)}{z - \omega + i\delta} dz = 0.$$

Let us take as contour  $\mathcal{C}$  the semicircle shown in Fig. 3. If  $\chi(\mathbf{q}; z)$  vanishes as  $1/|z|$  or faster for  $|z| \rightarrow \infty$ , from  $I_{\mathcal{C}} = 0$  it also follows that  $I_{\mathcal{R}} = 0$ . To ensure that indeed this condition is met, we subtract from the real part<sup>2</sup> of the susceptibility its infinite frequency limit  $\text{Re}[\chi(\mathbf{q}; \infty)]$ . Next, we rewrite  $I_{\mathcal{R}}$  by using the Sokhotski-Plemelj formula

$$\frac{1}{\omega + i\delta} = \mathcal{P} \frac{1}{\omega} - i\pi\delta(\omega)$$

where  $\mathcal{P}$  is the Cauchy principal value

$$\int_{-\infty}^{\infty} \mathcal{P} \frac{1}{\omega} d\omega = \int_{-\infty}^{-\varepsilon} \frac{1}{\omega} d\omega + \int_{\varepsilon}^{\infty} \frac{1}{\omega} d\omega,$$

and  $\delta(\omega)$  the Dirac delta function. Thus we obtain the Cauchy relation

$$I_{\mathcal{R}} = \mathcal{P} \int_{-\infty}^{+\infty} \frac{\chi(\mathbf{q}; \omega') - \text{Re}[\chi(\mathbf{q}; \infty)]}{\omega' - \omega} d\omega' - i\pi \{\chi(\mathbf{q}; \omega) - \text{Re}[\chi(\mathbf{q}; \infty)]\}$$

As a consequence the real and imaginary part of the susceptibility are the Hilbert transform of each other, hence they satisfy the so-called Kramers-Kronig relations

$$\begin{aligned} \text{Re}[\chi(\mathbf{q}; \omega)] - \text{Re}[\chi(\mathbf{q}; \infty)] &= \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Im}[\chi(\mathbf{q}; \omega')]}{\omega' - \omega} d\omega', \\ \text{Im}[\chi(\mathbf{q}; \omega)] &= -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Re}[\chi(\mathbf{q}; \omega')] - \text{Re}[\chi(\mathbf{q}; \infty)]}{\omega' - \omega} d\omega'. \end{aligned}$$

The first Kramers-Kronig relation yields the sum rule

$$\text{Re}[\chi(\mathbf{q}; \omega = 0)] - \text{Re}[\chi(\mathbf{q}; \infty)] = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Im}[\chi(\mathbf{q}; \omega')]}{\omega'} d\omega'. \quad (13)$$

In the  $\mathbf{q} = \mathbf{0}$  limit, Eq. (13) is known as *thermodynamic sum rule* and

$$\chi_{\nu\nu'}(\mathbf{0}; 0) = \lim_{h_{\nu'} \rightarrow 0} \frac{\partial \langle P_{\nu} \rangle}{\partial h_{\nu'}},$$

is the response to a static and uniform perturbation,  $h_{\nu'} = h_{\nu'}(\mathbf{0}; 0)$ .

Finally, if  $\hat{O}_{\nu'} \propto \hat{P}_{\nu'}^{\dagger}$  and thus the product  $P_{\nu}^{nm}(\mathbf{q})O_{\nu'}^{mn}(-\mathbf{q})$  is real, by using (12) for the left-hand side and the invariant properties of the trace under cyclic permutations for the right-hand side, one can show that

$$\frac{2}{\pi} \int_0^{\infty} \omega \text{Im} \left[ \chi_{\hat{P}_{\nu}, \hat{O}_{\nu'}}(\mathbf{q}; \omega) \right] d\omega = \left\langle \left[ [\hat{P}_{\nu}, \hat{H}], \hat{O}_{\nu'} \right] \right\rangle_0,$$

a relation known as Thomas-Reich-Kuhn or *f-sum rule*.

<sup>2</sup>For Hermitian operators the real part of the function  $\chi(\mathbf{q}; \omega)$  is even in  $\omega$ ; thus, the infinite frequency limit of  $\chi(\mathbf{q}; \omega)$  could, in principle, be a constant.

## 2.5 Fluctuation-dissipation theorem

The fluctuation-dissipation theorem is a relation between the correlation function  $\mathcal{S}(\mathbf{q}; \omega)$ , which essentially describes fluctuations at equilibrium, and the linear response function  $\chi(\mathbf{q}; \omega)$ , which describes dissipative effects or relaxation phenomena as well. To derive it, let us start from the spatial Fourier transform of the correlation function

$$\mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; t) = \left\langle \Delta \hat{P}_\nu(\mathbf{q}; t) \Delta \hat{O}_{\nu'}(-\mathbf{q}) \right\rangle_0.$$

This equation, together with the definition of the susceptibility, yields the relation

$$\chi_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; t) = i[\mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; t) - \mathcal{S}_{\hat{O}_{\nu'}, \hat{P}_\nu}(-\mathbf{q}; -t)]\Theta(t). \quad (14)$$

Let us now take the time Fourier transform of the correlation function and express it in term of a full set of eigenvectors of the Hamiltonian, as we have previously done for the susceptibility

$$\begin{aligned} \mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \Delta \hat{P}_\nu(\mathbf{q}; t) \Delta \hat{O}_{\nu'}(-\mathbf{q}; 0) \rangle_0 \\ &= \frac{1}{Z} \sum_{nm} \int_{-\infty}^{\infty} dt e^{i(\omega + E_n^N - E_m^N)t} e^{-\beta(E_n^N - \mu N)} P_\nu^{nm}(\mathbf{q}) O_{\nu'}^{mn}(-\mathbf{q}) \\ &= \frac{2\pi}{Z} \sum_{nm} e^{-\beta(E_n^N - \mu N)} P_\nu^{nm}(\mathbf{q}) O_{\nu'}^{mn}(-\mathbf{q}) \delta(\omega - E_m^N + E_n^N). \end{aligned}$$

If we exchange first the order of the operators and later the indices  $n$  and  $m$  in the sum, we find

$$\mathcal{S}_{\hat{O}_{\nu'}, \hat{P}_\nu}(\mathbf{q}; \omega) = \frac{2\pi}{Z} \sum_{nm} e^{-\beta(E_m^N - \mu N)} P_\nu^{nm}(-\mathbf{q}) O_{\nu'}^{mn}(\mathbf{q}) \delta(\omega - E_n^N + E_m^N).$$

The correlation function therefore satisfies the *principle of detailed balance*

$$\mathcal{S}_{\hat{O}_{\nu'}, \hat{P}_\nu}(-\mathbf{q}; -\omega) = e^{-\beta\omega} \mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega).$$

The relation above can be understood as follows. If  $\omega > 0$ , the correlation function  $\mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega)$  describes the probability  $P_{n \rightarrow m} \propto n(E_n)[1 - n(E_m)]$  that the system is excited from an initial state with energy  $E_n$  to a final state with higher energy  $E_m = E_n + \omega$ . Instead,  $\mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(-\mathbf{q}; -\omega)$ , describes the probability  $P_{m \rightarrow n} \propto n(E_m)[1 - n(E_n)]$  that the system goes from the initial state with energy  $E_m$  to a final state with lower energy  $E_n = E_m - \omega$ . The probability  $P_{m \rightarrow n}$  is lower than  $P_{n \rightarrow m}$  by the factor  $e^{-\beta\omega}$ .

We are now ready to Fourier transform Eq. (14). To do this, first we replace the step function with its Fourier representation

$$\Theta(t) = i \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} e^{-i\omega''t} \frac{1}{\omega'' + i\delta},$$

and do the same with the correlation function,

$$\mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; t) = \int \frac{d\omega'}{2\pi} e^{-i\omega't} \mathcal{S}_{\hat{P}_\nu, \hat{O}_{\nu'}}(\mathbf{q}; \omega');$$



next we Fourier transform in  $t$  the left- and right-hand side of Eq. (14), obtaining

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = - \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega') - \mathcal{S}_{\hat{O}_{\nu'} \hat{P}_\nu}(-\mathbf{q}; -\omega')}{\omega - \omega' + i\delta}.$$

Finally, via the principle of detailed balance we arrive at the expression

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = - \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega') \frac{1 - e^{-\beta\omega'}}{\omega - \omega' + i\delta}.$$

Thus, if  $\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega')$  is real, as happens when  $\hat{O}_{\nu'} \propto \hat{P}_\nu^\dagger$ , the following relation holds

$$\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega) = 2(1 + n_B) \text{Im}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega)], \quad n_B(\omega) = \frac{1}{e^{\beta\omega} - 1}.$$

This is the fluctuation-dissipation theorem. The left-hand side yields the spectrum of spontaneous fluctuations and the right-hand side the energy dissipation. When  $k_B T$  is large, it follows from the first Kramers-Kronig relation, Eq. (13), and the fluctuation-dissipation theorem that

$$\text{Re}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \omega = 0)] - \text{Re}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; \infty)] \sim \frac{1}{k_B T} \mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\mathbf{q}; t = 0).$$

## 2.6 Single-particle Green function

### 2.6.1 Definitions

In the non-interacting limit or within certain approximations, the susceptibility can be written in terms of single-particle Green functions. It is therefore important to introduce the latter and their properties. Let us first define the Green function or *propagator*

$$G_{\alpha\alpha'}(t, t') = -i \left\langle \mathcal{T} c_\alpha(t) c_{\alpha'}^\dagger(t') \right\rangle_0,$$

where  $\mathcal{T}$  is the time-ordering operator, which orders the operators in decreasing time from left to right. The indices  $\alpha$  and  $\alpha'$  are flavors, and  $c_\alpha^\dagger(c_\alpha)$  is a fermionic creation (annihilation) operator. When the Hamiltonian is time-independent,

$$G_{\alpha\alpha'}(t, t') = G_{\alpha\alpha'}(t - t').$$

It is useful to express the Green function using a full set of eigenvectors  $\{\Psi_n^N\}$  of the Hamiltonian, as we have done for the susceptibility and the correlation function. We obtain

$$G_{\alpha\alpha'}(t) = -\frac{i}{Z} \sum_{Nnm} e^{-\beta(E_n^N - \mu N)} \begin{cases} e^{i(E_n^N - E_m^{N+1} + \mu)t} \langle \Psi_n^N | c_\alpha | \Psi_m^{N+1} \rangle \langle \Psi_m^{N+1} | c_{\alpha'}^\dagger | \Psi_n^N \rangle & t > 0 \\ -e^{i(-E_n^N + E_m^{N-1} + \mu)t} \langle \Psi_n^N | c_{\alpha'}^\dagger | \Psi_m^{N-1} \rangle \langle \Psi_m^{N-1} | c_\alpha | \Psi_n^N \rangle & t < 0 \end{cases}$$

Let us define  $C_\alpha^{nm} = \langle \Psi_n^N | c_\alpha | \Psi_m^{N+1} \rangle$  and  $\overline{C}_{\alpha'}^{nm} = \langle \Psi_m^{N+1} | c_{\alpha'}^\dagger | \Psi_n^N \rangle$ . If, for negative times, we replace  $N$  with  $N + 1$  and exchange  $m$  and  $n$ , we obtain

$$G_{\alpha\alpha'}(t) = -\frac{i}{Z} \sum_{Nnm} e^{-\beta(E_n^N - \mu N)} \overline{C}_{\alpha'}^{nm} C_\alpha^{nm} e^{i(E_n^N - E_m^{N+1} + \mu)t} \left[ \Theta(t) - e^{-\beta(E_m^{N+1} - E_n^N - \mu)} \Theta(-t) \right].$$

The Fourier transform with respect to time yields

$$G_{\alpha\alpha'}(\omega) = \frac{1}{Z} \sum_{Nnm} e^{-\beta(E_n^N - \mu N)} \overline{C_{\alpha'}^{nm}} C_{\alpha}^{nm} \times \left\{ \frac{1}{\omega - E_m^{N+1} + E_n^N + \mu + i\delta} + \frac{e^{-\beta(E_m^{N+1} - E_n^N - \mu)}}{\omega - E_m^{N+1} + E_n^N + \mu - i\delta} \right\}.$$

Let us define the function

$$A_{\alpha\alpha'}(\omega) = \frac{2\pi}{Z} \sum_{Nnm} e^{-\beta(E_n^N - \mu N)} \overline{C_{\alpha'}^{nm}} C_{\alpha}^{nm} [1 + e^{-\beta\omega}] \delta(\omega - E_m^{N+1} + E_n^N + \mu).$$

In terms of  $A_{\alpha\beta}(\omega)$ , the Green function takes the simpler form

$$G_{\alpha\alpha'}(\omega) = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \left[ \frac{1 - n(\omega')}{\omega - \omega' + i\delta} + \frac{n(\omega')}{\omega - \omega' - i\delta} \right] A_{\alpha\alpha'}(\omega').$$

This expression is known as *Lehmann representation*, and  $A_{\alpha\beta}(\omega)$  is called *spectral function*. It is often useful to introduce the retarded and advanced Green functions  $G_{\alpha\alpha'}^R(t, t')$  and  $G_{\alpha\alpha'}^A(t, t')$ .

The first is given by

$$G_{\alpha\alpha'}^R(t, t') = -i\Theta(t - t') \left\langle \left[ c_{\alpha}(t), c_{\alpha'}^{\dagger}(t') \right] \right\rangle_0,$$

and the latter by

$$G_{\alpha\alpha'}^A(t, t') = i\Theta(t' - t) \left\langle \left[ c_{\alpha}(t), c_{\alpha'}^{\dagger}(t') \right] \right\rangle_0.$$

If we Fourier transform them in time we have

$$G_{\alpha\alpha'}^R(\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{1}{2\pi} \left[ \frac{1}{\omega - \omega' + i\delta} \right] A_{\alpha\alpha'}(\omega'),$$

$$G_{\alpha\alpha'}^A(\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{1}{2\pi} \left[ \frac{1}{\omega - \omega' - i\delta} \right] A_{\alpha\alpha'}(\omega'),$$

and therefore

$$A_{\alpha\alpha'}(\omega) = i [G_{\alpha\alpha'}^R(\omega) - G_{\alpha\alpha'}^A(\omega)].$$

## 2.6.2 Temperature Green function

To build a consistent many-body perturbation theory at finite temperature it is convenient to introduce an imaginary time variable,  $\tau$ . The imaginary-time Green function, given by

$$G_{\alpha\alpha'}(\boldsymbol{\tau}) = -\langle \mathcal{T} c_{\alpha}(\tau_1) c_{\alpha'}^{\dagger}(\tau_2) \rangle_0 = -\frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H} - \mu \hat{N})} \mathcal{T} c_{\alpha}(\tau_1) c_{\alpha'}^{\dagger}(\tau_2) \right],$$

is known as the temperature or Matsubara Green function. In this expression,  $\mathcal{T}$  is again the time-ordering operator; the imaginary time fermionic operators  $o(\tau) = c(\tau), c^{\dagger}(\tau)$  are given by

$$o(\tau) = e^{\tau(\hat{H} - \mu \hat{N})} o e^{-\tau(\hat{H} - \mu \hat{N})}.$$

The vector  $\boldsymbol{\tau}$  is defined as  $\boldsymbol{\tau} = (\tau_1, \tau_2)$ . Writing explicitly the action of  $\mathcal{T}$ , we obtain

$$G_{\alpha\alpha'}(\boldsymbol{\tau}) = -\Theta(\tau_1 - \tau_2)\langle c_\alpha(\tau_1)c_{\alpha'}^\dagger(\tau_2)\rangle + \Theta(\tau_2 - \tau_1)\langle c_{\alpha'}^\dagger(\tau_2)c_\alpha(\tau_1)\rangle.$$

If the Hamiltonian is time-independent,

$$G_{\alpha\alpha'}(\boldsymbol{\tau}) = G_{\alpha\alpha'}(\tau_1 - \tau_2).$$

The imaginary-time Green function is well defined only in the interval  $-\beta < \tau_1 - \tau_2 = \tau < \beta$ . This can be seen by writing it explicitly in a basis of eigenvectors of the Hamiltonian,  $\{\Psi_n^N\}$

$$G_{\alpha\alpha'}(\tau) = \frac{1}{Z} \sum_{Nnm} \langle \Psi_n^N | c_\alpha | \Psi_m^{N+1} \rangle \langle \Psi_m^{N+1} | c_{\alpha'}^\dagger | \Psi_n^N \rangle e^{-\beta(E_n^N - \mu N)} \begin{cases} -e^{(E_n^N - E_m^{N+1} + \mu)\tau} & \tau > 0 \\ e^{-(E_n^N - E_m^{N+1} + \mu)(-\beta - \tau)} & \tau < 0 \end{cases}$$

For imaginary times outside the interval  $-\beta < \tau < \beta$ , the high energy states would give divergent contributions. Either from the expression above or from the definition of  $G_{\alpha\alpha}(\tau)$  and the invariance of the trace under cyclic permutation of operators, one can show that  $G_{\alpha\alpha'}(\tau)$  has the following symmetry property

$$G_{\alpha\alpha'}(\tau) = -G_{\alpha\alpha'}(\tau + \beta) \quad \text{for } -\beta < \tau < 0.$$

Finally, if  $n_\alpha$  is the number of electrons for flavor  $\alpha$ , one can show that

$$G_{\alpha\alpha}(\tau \rightarrow 0^+) = -1 + n_\alpha, \quad G_{\alpha\alpha}(\tau \rightarrow \beta^-) = -n_\alpha.$$

For negative times, we have

$$G_{\alpha\alpha}(\tau \rightarrow 0^-) = n_\alpha, \quad G_{\alpha\alpha}(\tau \rightarrow -\beta^-) = 1 - n_\alpha.$$

Thus,  $G_{\alpha\alpha}(\tau)$  is discontinuous at  $\tau = 0$  because of time ordering. It is at this point convenient to introduce a generalized imaginary-time Green function  $\tilde{G}_{\alpha\alpha'}(\boldsymbol{\tau})$  defined for any  $\boldsymbol{\tau}$ ,

$$\tilde{G}_{\alpha\alpha'}(\tau_1 \pm n_1\beta, \tau_2 \pm n_2\beta) \equiv (-1)^{n_1+n_2} G_{\alpha\alpha'}(\tau_1, \tau_2),$$

where  $n_1$  and  $n_2$  are integers. The Green function  $\tilde{G}_{\alpha\alpha'}(\tau_1, \tau_2) = \tilde{G}_{\alpha\alpha'}(\tau_1 - \tau_2)$  is, by construction, antiperiodic with period  $\beta$  in both  $\tau_1$  and  $\tau_2$  and in the time difference  $\tau = \tau_1 - \tau_2$ . From now on we will work with  $\tilde{G}_{\alpha\alpha'}(\tau)$ , and therefore for simplicity we rename it  $G_{\alpha\alpha'}(\tau)$ . Thanks to its periodicity,  $G_{\alpha\alpha'}(\tau)$  can be written as the Fourier series

$$G_{\alpha\alpha'}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\nu_n\tau} G_{\alpha\alpha'}(i\nu_n),$$

where the frequency  $\nu_n$  is given by  $2\pi$  multiplied by an integer multiple of the inverse period,  $1/2\beta$ . For fermionic Green functions only the odd Matsubara frequencies,  $\nu_n = \pi(2n+1)/\beta$ , for which  $e^{\pm i\nu_n\beta} = -1$ , yield finite Fourier coefficients, given by

$$G_{\alpha\alpha'}(i\nu_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau) = \frac{1}{2} (1 - e^{-i\nu_n\beta}) \int_0^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau) = \int_0^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau).$$

$g_r(\tau; x)$	$g_r(\nu_n; x) = \int_0^\beta e^{i\nu_n\tau} g_r(\tau; x) d\tau$
$g_0(\tau; x) = e^{-x\tau}$	$[i\nu_n - x]^{-1} [n_\sigma(x) - 1]^{-1}$
$g_1(\tau; x) = \tau e^{-x\tau}$	$\beta n_\sigma(x) [i\nu_n - x]^{-1} [n_\sigma(x) - 1]^{-1} - [i\nu_n - x]^{-2} [n_\sigma(x) - 1]^{-1}$
$g_r(\tau; x) = \tau^r e^{-x\tau}$	$\beta^r n_\sigma(x) g_0(i\nu_n; x) - r [i\nu_n - x]^{-1} g_{r-1}(i\nu_n; x)$

**Table 1:** Some of the most common Matsubara Fourier transforms (fermionic case). The function  $n_\sigma(x)$  is the Fermi-Dirac distribution function  $n_\sigma(x) = 1/(1 + e^{x\beta})$ ; the parameter  $x$  is a real number. For fermionic Matsubara frequencies  $e^{i\nu_n\beta} = -1$ .

It is interesting to point out the relation between the imaginary-time Green function and the actual retarded and advanced Green functions. One can show that they correspond to different analytic continuations to the real axis

$$\begin{aligned} G_{\alpha\alpha'}^R(\omega) &= G_{\alpha\alpha'}(i\nu_n)|_{i\nu_n \rightarrow \omega + i\delta} \\ G_{\alpha\alpha'}^A(\omega) &= G_{\alpha\alpha'}(i\nu_n)|_{i\nu_n \rightarrow \omega - i\delta}. \end{aligned}$$

The odd or fermionic Matsubara frequencies  $i\nu_n$  are also the poles of the Fermi-Dirac distribution function. The even or bosonic Matsubara frequencies,  $i\omega_m = \pi(2m)/\beta$ , are, correspondingly, the poles of the Bose-Einstein distribution function.

### 2.6.3 One-band Hubbard model: Non-interacting limit

Let us now consider as a representative case the one-band Hubbard model. In the non-interacting limit the Hubbard Hamiltonian is given by Eq. (5), which we rewrite here for convenience

$$\hat{H}_0 = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}.$$

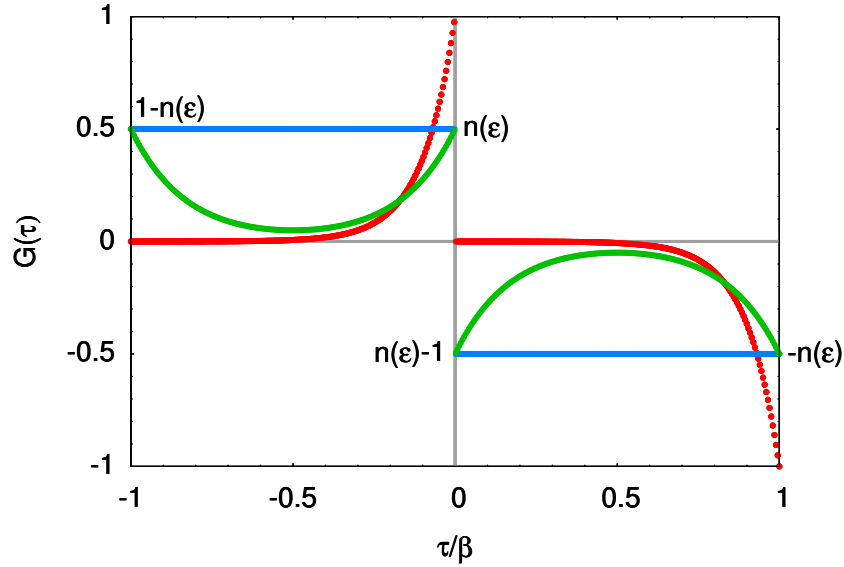
For high-temperature superconducting cuprates, the dispersion  $\varepsilon_{\mathbf{k}}$  describing the Cu  $d$   $x^2 - y^2$  band crossing the Fermi level is

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a + \dots, \quad (15)$$

where  $a$  is the lattice constant,  $t$  the nearest neighbor hopping integral and  $t'$  the next-nearest neighbor hopping integral [9].

The imaginary-time Green function for the Hamiltonian  $\hat{H}_0$  can be calculated analytically

$$\begin{aligned} \mathcal{G}_{\mathbf{k}\sigma}(\tau) &= -\left\langle \mathcal{T} \left[ c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger(0) \right] \right\rangle_0 \\ &= -\Theta(\tau) \frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H}_0 - \mu \hat{N})} c_{\mathbf{k}\sigma}(\tau) c_{\mathbf{k}\sigma}^\dagger(0) \right] + \Theta(-\tau) \frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H}_0 - \mu \hat{N})} c_{\mathbf{k}\sigma}^\dagger(0) c_{\mathbf{k}\sigma}(\tau) \right] \\ &= -[\Theta(\tau) (1 - n_\sigma(\varepsilon_{\mathbf{k}})) - \Theta(-\tau) n_\sigma(\varepsilon_{\mathbf{k}})] e^{-(\varepsilon_{\mathbf{k}} - \mu)\tau}, \end{aligned} \quad (16)$$



**Fig. 4:** The function  $\mathcal{G}_{k\sigma}(\tau)$  defined in Eq. (16) for a state well below the Fermi level (red) and at the Fermi level (blue) and  $\beta = 2 \text{ eV}^{-1}$ . The green line shows the atomic Green function  $G(\tau)$  from Eq. (19) calculated for  $U = 6 \text{ eV}$ .

where  $n_{\sigma}(\varepsilon_{\mathbf{k}})$  is the Fermi-Dirac distribution function

$$n_{\sigma}(\varepsilon_{\mathbf{k}}) = \frac{1}{1 + e^{\beta(\varepsilon_{\mathbf{k}} - \mu)}}.$$

The Matsubara Fourier transform of  $\mathcal{G}_{k\sigma}(\tau)$  is simple to obtain since

$$\int_0^{\beta} e^{(i\nu_n - x)\tau} d\tau = \frac{1}{i\nu_n - x} [e^{(i\nu_n - x)\beta} - 1] = -\frac{1}{i\nu_n - x} [e^{-x\beta} + 1] = \frac{1}{i\nu_n - x} \frac{1}{n_{\sigma}(x) - 1}.$$

This result, together with other useful Matsubara Fourier transforms, can be found in Tab. 1. Thus

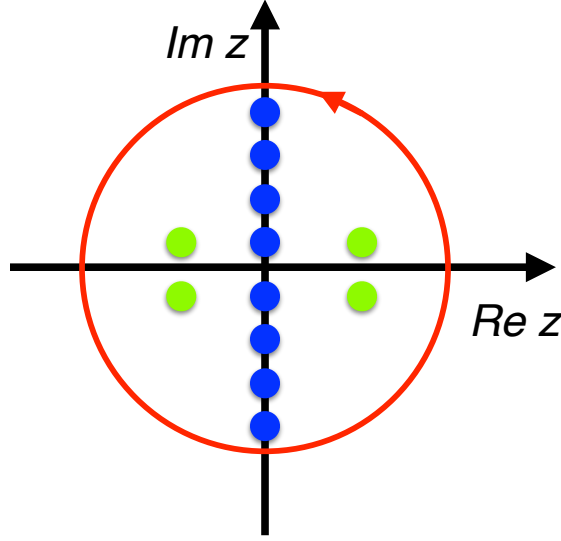
$$\mathcal{G}_{k\sigma}(i\nu_n) = \frac{1}{i\nu_n - \varepsilon_{\mathbf{k}} + \mu}.$$

It is often necessary to perform sums of Green functions or of product of Green functions over the Matsubara frequencies. To see how these can be calculated, let us consider the integral

$$I_C = \frac{1}{2\pi i} \oint_C \mathcal{F}_{k\sigma}(z) n_{\sigma}(z) e^{z\tau} dz, \quad (17)$$

where  $0 < \tau < \beta$  and  $n_{\sigma}(z)$  is the Fermi function, which has poles for  $z = i\nu_n$ . We assume that  $\mathcal{F}_{k\sigma}(z)$  is a complex function, analytic everywhere except at some poles  $\{z_p\}$ , which differ from the Fermionic Matsubara frequencies; for example,  $\mathcal{F}_{k\sigma}(z)$  could be the Green function  $\mathcal{G}_{k\sigma}(z)$ . We define the contour  $\mathcal{C}$  (see Fig. 5) as a circle in the full complex plane, centered at the origin and including the poles of the integrand. The integral  $I_C$  is zero because the integrand vanishes exponentially for  $|z| \rightarrow \infty$ . Using Cauchy's integral theorem we then have

$$\frac{1}{\beta} \sum_n e^{i\nu_n \tau} \mathcal{F}_{k\sigma}(i\nu_n) = \sum_{z_p} \text{Res} [\mathcal{F}_{k\sigma}(z_p)] n_{\sigma}(z_p) e^{z_p \tau}, \quad (18)$$



**Fig. 5:** The contour  $\mathcal{C}$  used to perform the integral  $I_{\mathcal{C}}$  defined by Eq. (17). The blue circles represent poles of the Fermi function, i.e., Matsubara frequencies, and the green circles are representative poles of the function  $\mathcal{F}_{\mathbf{k}\sigma}(z)$ . Since the integral vanishes for  $|z| \rightarrow \infty$ , the sum of the contributions from all the poles must add up to zero for an infinitely large contour  $\mathcal{C}$ .

where we used the fact that  $\text{Res}[n_{\sigma}(i\nu_n)] = -\frac{1}{\beta}$ . Let us now apply this result in some typical cases. If  $\mathcal{F}_{\mathbf{k}\sigma}(z) = \mathcal{G}_{\mathbf{k}\sigma}(z)$ , remembering that  $G_{\alpha\alpha}(0^-) = n_{\alpha}$  and  $G_{\alpha\alpha}(0^+) = n_{\alpha} - 1$ , we obtain

$$\begin{aligned} \frac{1}{\beta} \sum_n e^{-i\nu_n 0^-} \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) &= \mathcal{G}_{\mathbf{k}\sigma}(0^-) = n_{\sigma}(\varepsilon_{\mathbf{k}}), \\ \frac{1}{\beta} \sum_n e^{-i\nu_n 0^+} \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) &= \mathcal{G}_{\mathbf{k}\sigma}(0^+) = n_{\sigma}(\varepsilon_{\mathbf{k}}) - 1. \end{aligned}$$

In a similar way we can show that

$$\begin{aligned} \frac{1}{\beta} \sum_n e^{i\nu_n 0^+} \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) &= \frac{dn_{\sigma}(\varepsilon_{\mathbf{k}})}{d\varepsilon_{\mathbf{k}}} = \beta n_{\sigma}(\varepsilon_{\mathbf{k}}) [-1 + n_{\sigma}(\varepsilon_{\mathbf{k}})], \\ \frac{1}{\beta} \sum_n e^{i\nu_n 0^+} \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) \mathcal{G}_{\mathbf{k}+\mathbf{q}\sigma}(i\nu_n + i\omega_m) &= \frac{n(\varepsilon_{\mathbf{k}+\mathbf{q}}) - n(\varepsilon_{\mathbf{k}})}{i\omega_m + \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}}, \end{aligned}$$

where in the last relation  $\omega_m = 2m\pi/\beta$  is a bosonic Matsubara frequency. In Tab. 2 we display some of the inverse Fourier transforms involving one-particle Green functions for a non-interacting system.

It is important to point out that, using Matsubara frequencies, the Lehmann representation takes the simple form

$$\mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) = \int_{-\infty}^{+\infty} A_{\mathbf{k}\sigma}(\omega') \frac{1}{i\nu_n - \omega'} d\omega',$$

where the spectral function satisfies the relation

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} A_{\mathbf{k}\sigma}(\omega') d\omega' = 1.$$

$g_\alpha(\nu_n; x, y)$	$g_\alpha(\tau; x, y) = \frac{1}{\beta} \sum_n e^{-i\nu_n \tau} g_\alpha(\nu_n; x, y)$
$g_a(\nu_n; x, y) = [i\nu_n - x]^{-1}$	$[n_\sigma(x) - 1]e^{-x\tau}$
$g_b(\nu_n; x, y) = [i\nu_n - x]^{-2}$	$n_\sigma(x)(\tau - \beta n_\sigma(x))e^{-x(\tau-\beta)}$
$g_c(\nu_n; x, y) = [i\nu_n - x]^{-1} [i\nu_n - y]^{-1}$	$-[e^{-x(\tau-\beta)}n_\sigma(x) - e^{-y(\tau-\beta)}n_\sigma(y)] [x - y]^{-1}$
$g_d(\nu_n; x, y) = [i\nu_n - x]^{-1} [i\nu_n + x]^{-1}$	$[g_a(\tau; x, y) - g_a(\tau; -x, y)]/2x$

**Table 2:** Some of the most common Matsubara Fourier transforms (fermionic case), obtained from Eq. (18). The function  $n_\sigma(x)$  is the Fermi-Dirac distribution function  $n_\sigma(x) = 1/(1 + e^{x\beta})$ . The parameters  $x$  and  $y$  are real numbers. For  $\tau$  we consider the interval  $(0, \beta)$ .

Furthermore the normalized spectral function,  $\tilde{A}_{\mathbf{k}\sigma}(\varepsilon) = A_{\mathbf{k}\sigma}(\varepsilon)/2\pi = -\frac{1}{\pi} \text{Im} [\mathcal{G}_{\mathbf{k}\sigma}(\varepsilon)]$  is related to the density of states as follows

$$\rho_\sigma(\varepsilon) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \tilde{A}_{\mathbf{k}\sigma}(\varepsilon).$$

These relations between  $\tilde{A}_{\mathbf{k}\sigma}(\varepsilon)$  and the density of states or the Green function are also valid for the interacting Hubbard model. In the non-interacting case

$$\tilde{A}_{\mathbf{k}\sigma}(\varepsilon) = \delta(\omega - \varepsilon_{\mathbf{k}}).$$

#### 2.6.4 One-band Hubbard model: Atomic limit

Let us consider now the half-filled one-band Hubbard model in the atomic ( $t = 0$ ) limit. Since the lattice sites are decoupled, we can focus on a single site and rewrite the Coulomb interaction in terms of the spin operator  $\hat{S}_z = \frac{1}{2}[n_\uparrow - n_\downarrow]$  and the electron number operator  $\hat{N} = n_\uparrow + n_\downarrow$ . We obtain

$$\hat{H}_U = \varepsilon_d \sum_{\sigma} n_{\sigma} + U \left( \frac{\hat{N}^2}{4} - \hat{S}_z^2 \right).$$

This Hamiltonian describes an idealized single-level atom. This system has four states,  $|0\rangle$ ,  $c_{\uparrow}^{\dagger}|0\rangle$ ,  $c_{\downarrow}^{\dagger}|0\rangle$ ,  $c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}|0\rangle$ , with expectation values of the operator  $\hat{H}_U - \mu\hat{N}$  equal to  $0, -U/2, -U/2$  and  $0$  respectively. We can calculate the imaginary-time Green function for such a system analytically; it is sufficient to perform the calculation in the interval  $(0, \beta)$ , since we can reconstruct the Green function in the interval  $(-\beta, 0)$  by using the antiperiodic properties. For  $0 < \tau < \beta$

$$G_{\sigma}(\tau) = -\frac{1}{2} \frac{1}{1 + e^{\beta U/2}} [e^{\tau U/2} + e^{(\beta-\tau)U/2}]. \quad (19)$$

The Matsubara Fourier coefficients can be obtained via the integrals in Tab. 1. We find

$$G_\sigma(i\nu_n) = \frac{1}{2} \left[ \frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2} \right]. \quad (20)$$

Thus the atomic Green function, as the non-interacting Green function, is the sum of functions with first order poles; the corresponding retarded Green function on the real axis can be obtained by analytic continuation replacing  $i\nu_n$  with  $\omega + i\delta$ , with  $\delta > 0$ . To obtain  $G_\sigma(\tau)$  from  $G_\sigma(i\nu_n)$  one can use the Matsubara sums in Tab. 2.

## 2.7 Two-particle Green function

### 2.7.1 Generalized imaginary time Green function

The temperature Green function can also be defined for quadratic operators; this generalization is relevant for calculating the elements of the linear-response tensor. Let us consider the operators  $\Delta\hat{P}_{\alpha\alpha'}(\tau_1, \tau_2)$  and  $\Delta\hat{O}_{\gamma\gamma'}(\tau_3, \tau_4)$ , with

$$\begin{aligned} \Delta\hat{P}_{\alpha\alpha'}(\tau_1, \tau_2) &= c_{\alpha'}^\dagger(\tau_2)c_\alpha(\tau_1) - \langle \mathcal{T} c_{\alpha'}^\dagger(\tau_2)c_\alpha(\tau_1) \rangle, \\ \Delta\hat{O}_{\gamma\gamma'}(\tau_3, \tau_4) &= c_{\gamma'}^\dagger(\tau_4)c_\gamma(\tau_3) - \langle \mathcal{T} c_{\gamma'}^\dagger(\tau_4)c_\gamma(\tau_3) \rangle. \end{aligned}$$

where  $\alpha, \alpha'$  and  $\gamma, \gamma'$  are, as usual, flavors. We define the temperature Green function for these operators as the two-particle Green function

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \langle \mathcal{T} \Delta\hat{P}_{\alpha\alpha'}(\tau_1, \tau_2) \Delta\hat{O}_{\gamma\gamma'}(\tau_3, \tau_4) \rangle, \quad (21)$$

where  $\boldsymbol{\tau} = (\tau_1, \tau_2, \tau_3, \tau_4)$ . From the invariance of the trace under cyclic permutation of operators one can show that, for a time-independent Hamiltonian,

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0),$$

where  $\tau_{ji} = \tau_j - \tau_i$ . In analogy with what we have seen in the single-particle case, the two-particle Green function at negative times ( $-\beta < \tau_{j4} < 0$ ) can be obtained from the two-particle Green function at positive times ( $0 < \tau_{j4} < \beta$ ). For example, if  $-\beta < \tau_{14} < 0$

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14} + \beta, \tau_{24}, \tau_{34}, 0) = -\chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0),$$

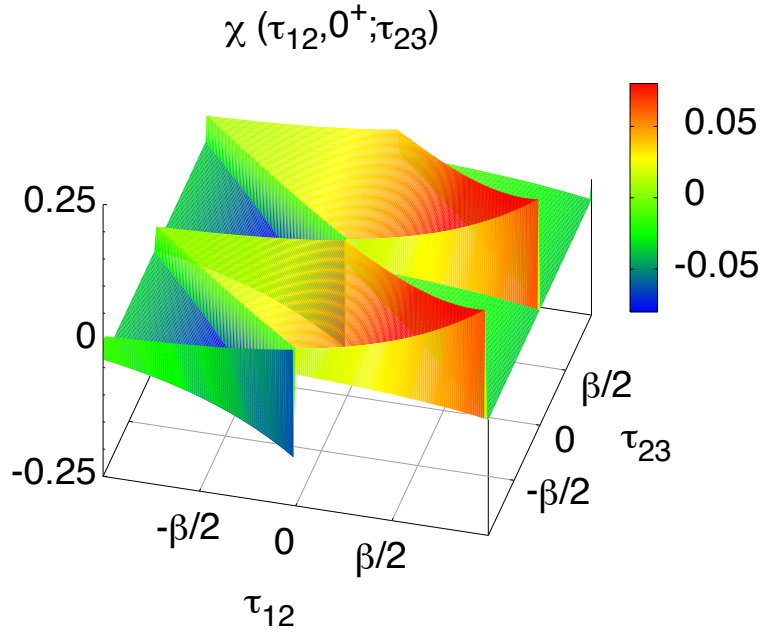
and similar relations hold for  $-\beta < \tau_{24} < 0$  or  $-\beta < \tau_{34} < 0$ . This can be shown using, once more, the invariance of the trace under cyclic permutation of the operators. As for the one-particle Green function, we can extend the two-particle Green function to any time interval by defining it periodic in each  $\tau_{j4}$  with period  $\beta$ .

It is often convenient to express  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau})$  as a function of the three independent variables  $\tau_{12}$ ,  $\tau_{23}$  and  $\tau_{34}$ . We then rewrite it as follows

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \mathcal{T} \text{Tr} \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathcal{Z}} \left[ e^{\tau_{14}(\hat{H}-\mu\hat{N})} c_\alpha e^{-\tau_{12}(\hat{H}-\mu\hat{N})} c_{\alpha'}^\dagger e^{-\tau_{23}(\hat{H}-\mu\hat{N})} c_\gamma e^{-\tau_{34}(\hat{H}-\mu\hat{N})} c_{\gamma'}^\dagger \right],$$

with  $\tau_{14} = \tau_{12} + \tau_{23} + \tau_{34}$ , and  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{12}, \tau_{34}; \tau_{23})$ . From this expression and the symmetry properties discussed above, it follows that the two-particle Green function is antiperiodic with period  $\beta$  in  $\tau_{12}$  and  $\tau_{34}$  and periodic with period  $\beta$  in  $\tau_{23}$  (see Fig. 6 as example).





**Fig. 6:** The function  $\chi(\tau_{12}, 0^+; \tau_{23}) = -G_{\alpha\alpha}(\tau_{12} + \tau_{23} + 0^+)G_{\alpha\alpha}(-\tau_{23})$  for a non-interacting system with  $n \sim 0.8$  electrons;  $\beta = 30 \text{ eV}^{-1}$ . It is antiperiodic in  $\tau_{12}$  and periodic in  $\tau_{23}$ .

### 2.7.2 The Fourier transform $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\nu})$ and its symmetry properties

The Fourier transform of the imaginary-time two-particle Green function is given by

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\nu}) = \frac{1}{16} \iiint d\boldsymbol{\tau} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\tau}} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}), \quad (22)$$

where the frequency vector is  $\boldsymbol{\nu} = (\nu_1, \nu_2, \nu_3, \nu_4)$ , and the imaginary times are chosen in the interval  $(-\beta, \beta)$ . From the fact that  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0)$  we obtain  $\nu_4 = -\nu_1 - \nu_2 - \nu_3$  (energy conservation), and thus only three frequencies are actually independent. Let us define  $\boldsymbol{\nu} = (\nu_n, -\nu_n - \omega_m, \nu_{n'} + \omega_m, -\nu_{n'})$  where  $\omega_m$  is a bosonic frequency. Then

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\nu}) = \chi_{n,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) = \frac{\beta}{8} \iiint d\boldsymbol{\tau} e^{i[-\omega_m\tau_{23} + \nu_n\tau_{12} + \nu_{n'}\tau_{34}]} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}),$$

where  $\boldsymbol{\tau} = (\tau_{14}, \tau_{24}, \tau_{34})$  and all integrals go from  $-\beta$  to  $\beta$ . By using the antiperiodicity of the two-particle Green function in imaginary times we can further simplify this expression, obtaining

$$\chi_{n,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) = \beta \int_0^\beta d\tau_{14} \int_0^\beta d\tau_{24} \int_0^\beta d\tau_{34} e^{i[-\omega_m\tau_{23} + \nu_n\tau_{12} + \nu_{n'}\tau_{34}]} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0).$$

Let us now analyze the symmetry properties of  $\chi_{n,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m)$ . For simplicity, we consider here only the case in which the one-electron basis can be chosen such that  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0)$  is real; indeed, this is the case for most strongly-correlated 3d transition metal-oxides, since their

Hamiltonian has typically time-reversal and even inversion symmetry and the spin-orbit interaction can be neglected. The complex conjugate is then given by

$$\left[ \chi_{n,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) \right]^* = \chi_{-n-1,-n'-1}^{\alpha\alpha'\gamma\gamma'}(-i\omega_m),$$

where  $\nu_{-n-1} = -\nu_n$ , and  $\nu_{-n'-1} = -\nu_{n'}$ . Furthermore, if in the integral (22) we replace  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau})$  with its complex conjugate and then exchange  $\tau_1 \leftrightarrow -\tau_4$  and  $\tau_2 \leftrightarrow -\tau_3$ , we find

$$\chi_{n,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) = \chi_{n',n}^{\gamma'\gamma\alpha'\alpha}(i\omega_m),$$

and hence, if  $\alpha = \gamma'$ ,  $\alpha' = \gamma$ ,  $\nu_n = \nu'_n$  is a reflection axis for the absolute value

$$\left| \chi_{n,n'}^{\alpha\alpha'\alpha'\alpha}(i\omega_m) \right| = \left| \chi_{n',n}^{\alpha\alpha'\alpha'\alpha}(i\omega_m) \right|.$$

An additional reflection axis can be found by first shifting the frequency  $\nu_n = \nu_l - \omega_m$

$$\chi_{l,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) = \frac{1}{16} \iiint d\boldsymbol{\tau} e^{i(-\omega_m\tau_{13} + \nu_l\tau_{12} + \nu_{n'}\tau_{34})} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}).$$

Since  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau})$  is invariant under particle exchange, if we exchange in the integrand  $\tau_1 \leftrightarrow \tau_3$  and  $\tau_2 \leftrightarrow \tau_4$ , we have

$$\chi_{l,n'}^{\alpha\alpha'\gamma\gamma'}(i\omega_m) = \chi_{n',l}^{\gamma'\gamma\alpha'\alpha}(-i\omega_m),$$

so that, if  $\alpha = \gamma$  and  $\alpha' = \gamma'$ ,  $\nu_{n+m} = -\nu_{n'}$  is a mirror line for the absolute value

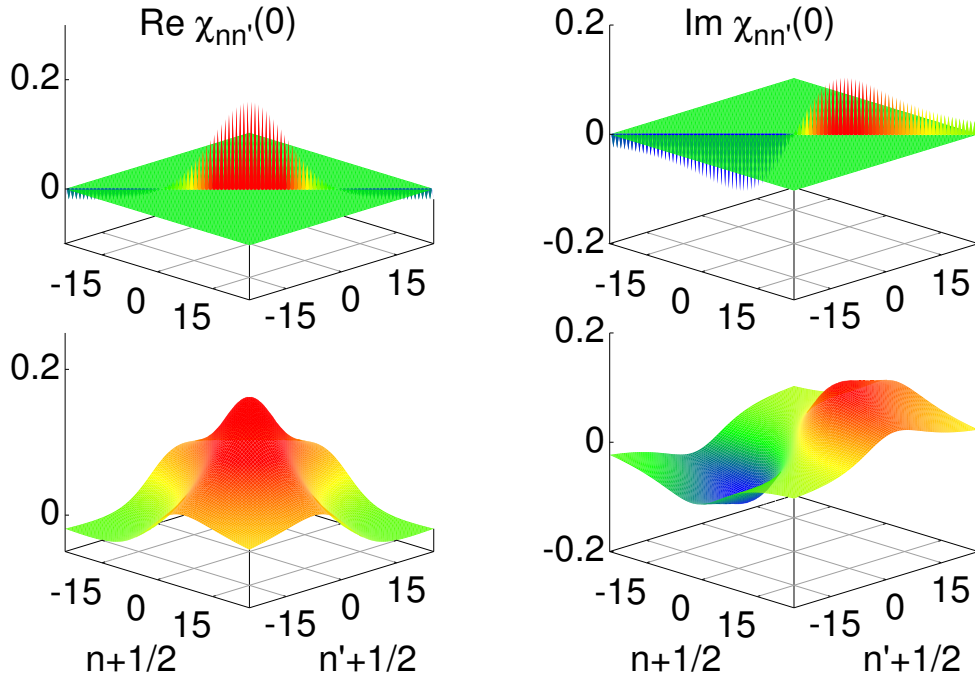
$$\left| \chi_{n+m,n'}^{\alpha\alpha'\alpha\alpha'}(i\omega_m) \right| = \left| \chi_{-n'-1,-n-m-1}^{\alpha\alpha'\alpha\alpha'}(i\omega_m) \right|.$$

### 2.7.3 Non-interacting case: Wick's theorem

For a non-interacting system Wick's theorem holds. It states that high-order Green functions can be factorized into products of lower-order Green function. For the two-particle Green function Wick's factorization yields

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = -\langle \mathcal{T} c_\alpha(\tau_1) c_{\gamma'}^\dagger(\tau_4) \rangle \langle \mathcal{T} c_\gamma(\tau_3) c_{\alpha'}^\dagger(\tau_2) \rangle = -G_{\alpha\gamma'}(\tau_{14}) G_{\gamma\alpha'}(-\tau_{23}). \quad (23)$$

If the two-particle Green function is written in this form, its periodicity properties can be directly derived from those of the one-particle Green function. For example, using as independent variables  $\tau_{12}$ ,  $\tau_{23}$ , and  $\tau_{34}$ , since  $\tau_{14} = \tau_{12} + \tau_{23} + \tau_{34}$ , one can verify that the susceptibility is periodic in the time associated with the bosonic frequency,  $\tau_{23}$ . As the single-particle Green function, the two-particle Green function has discontinuities associated with the jump coming from the time ordering operator. In Fig. 6 we see such jumps, e.g., along the line  $\tau_{12} = -\tau_{23}$  (for which  $\tau_{14} = 0^+$ ) and  $\tau_{12} = -\tau_{23} \pm \beta$  (for which  $\tau_{14} = \beta^+$  or  $\tau_{14} = \beta^-$ ).



**Fig. 7:** *Top: Real (left) and imaginary (right) part of  $\chi_{n,n'}^{\alpha\alpha\alpha\alpha}(0)$  for a non-interacting system, calculated for an energy level  $\varepsilon$  well above the Fermi level and  $\beta = 30 \text{ eV}^{-1}$ . Bottom: Real (left) and imaginary (right) part of the mean-field contribution. To better show the symmetries the center is shifted by  $(1/2, 1/2)$ . In all the plots the colors range from blue (minimum negative value) through green and yellow to red (maximum positive value).*

### 3 The dynamical susceptibility

#### 3.1 The magnetic susceptibility

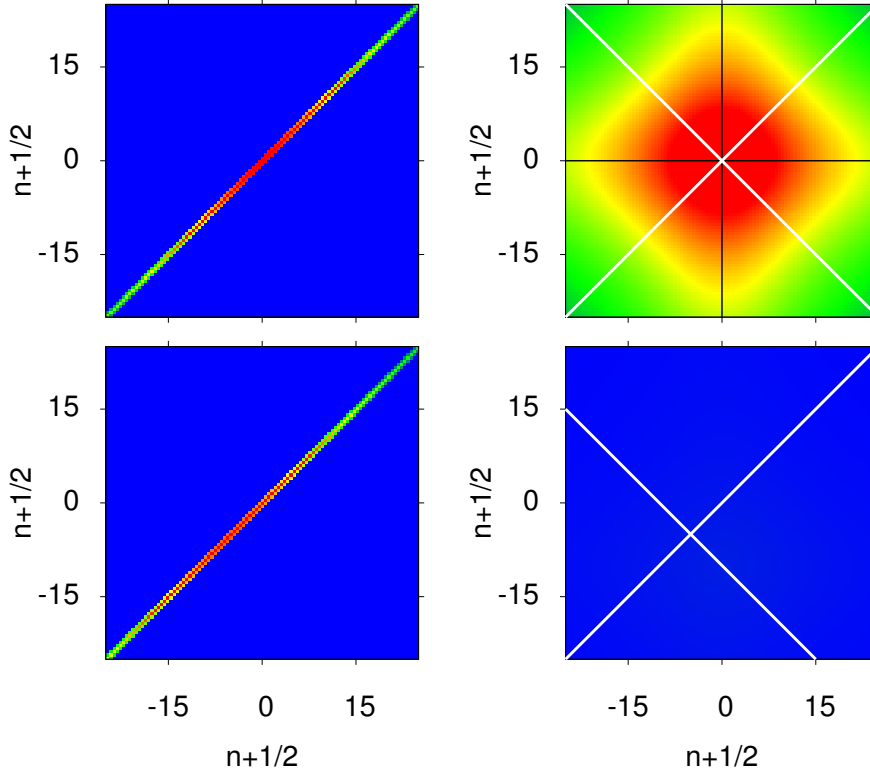
For a system made of well defined localized spins, as we have seen, the magnetic linear response function is proportional to the site susceptibility

$$\chi_{zz}^{i,i'}(\tau) = \chi_{zz}^{i,i'}(\tau) = \langle \mathcal{T} \hat{M}_z^i(\tau) \hat{M}_z^{i'}(0) \rangle_0 - \langle \hat{M}_z^i \rangle_0 \langle \hat{M}_z^{i'} \rangle_0,$$

where  $\hat{M}_z^i = -g\mu_B \hat{S}_z^i$  is the magnetization for lattice site  $i$ . Its Fourier transform is

$$\begin{aligned} \chi_{zz}(\mathbf{q}; i\omega_m) &= \sum_{ii'} e^{i\mathbf{q}\cdot(\mathbf{T}_i - \mathbf{T}_{i'})} \int d\tau e^{i\omega_m \tau} \chi_{zz}^{i,i'}(\tau) \\ &= \langle \hat{M}_z(\mathbf{q}; \omega_m) \hat{M}_z(-\mathbf{q}; 0) \rangle_0 - \langle \hat{M}_z(\mathbf{q}) \rangle_0 \langle \hat{M}_z(-\mathbf{q}) \rangle_0, \end{aligned} \quad (24)$$

where  $\omega_m$  is a bosonic Matsubara frequency. In actual calculations it is, however, often necessary to work with the full two-particle Green function tensor. Let us consider explicitly the case of the one-band Hubbard model; the tensor elements  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau)$  that are relevant for the magnetic susceptibility are those for which  $\alpha = \mathbf{k}_1\sigma$ ,  $\alpha' = \mathbf{k}_2\sigma$ ,  $\gamma = \mathbf{k}_3\sigma'$ , and  $\gamma' = \mathbf{k}_4\sigma'$ . Each



**Fig. 8:** *Left: Absolute value of  $\chi_{n,n'}^{\sigma\sigma}(0)$  (top) and  $\chi_{n,n'}^{\sigma\sigma}(i\omega_{10})$  (bottom) for a non-interacting system for an energy level  $\varepsilon$  well above the Fermi level and  $\beta = 30 \text{ eV}^{-1}$ . Right: Absolute value of the corresponding mean-field contribution. The white lines show symmetry axes. To better show the symmetries the center is shifted by  $(1/2, 1/2)$ . The colors range from blue (minimum value, here zero) through green and yellow to red (maximum positive value).*

flavor has a momentum  $\mathbf{k}_i$  associated, but, as we have seen for the frequencies, only three of the four  $\mathbf{k}_i$  vectors are independent (momentum conservation). Let us set  $\alpha = \mathbf{k}\sigma$ ,  $\alpha' = \mathbf{k} + \mathbf{q}\sigma$ ,  $\gamma = \mathbf{k}' + \mathbf{q}\sigma'$  and  $\gamma' = \mathbf{k}'\sigma'$  and write the tensor as a  $2N_{\mathbf{k}} \times 2N_{\mathbf{k}}$  matrix whose elements are defined as

$$[\chi(\mathbf{q}; \boldsymbol{\tau})]_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} = \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) = \langle \mathcal{T} c_{\mathbf{k}\sigma}(\tau_1) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger(\tau_2) c_{\mathbf{k}'+\mathbf{q}\sigma'}(\tau_3) c_{\mathbf{k}'\sigma'}^\dagger(\tau_4) \rangle_0 \quad (25)$$

$$- \langle \mathcal{T} c_{\mathbf{k}\sigma}(\tau_1) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger(\tau_2) \rangle_0 \langle \mathcal{T} c_{\mathbf{k}'+\mathbf{q}\sigma'}(\tau_3) c_{\mathbf{k}'\sigma'}^\dagger(\tau_4) \rangle_0.$$

The magnetic susceptibility is then given by

$$\chi_{zz}(\mathbf{q}; \boldsymbol{\tau}) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} \sigma\sigma' \chi^{\mathbf{q}\sigma\sigma'}(\boldsymbol{\tau}), \quad (26)$$

where  $\sigma = 1$  or  $-1$  for up and down, respectively, and

$$\chi^{\mathbf{q}\sigma\sigma'}(\boldsymbol{\tau}) = \frac{1}{\beta} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}\mathbf{k}'} [\chi(\mathbf{q}; \boldsymbol{\tau})]_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}. \quad (27)$$

After we Fourier transform with respect to imaginary time and sum over the fermionic Matsubara frequencies, we obtain the actual magnetic response function

$$\chi_{zz}(\mathbf{q}; i\omega_m) = (g\mu_B)^2 \frac{1}{4} \sum_{\sigma\sigma'} \sigma\sigma' \frac{1}{\beta^2} \sum_{nn'} \chi_{n,n'}^{\mathbf{q}\sigma\sigma'}(i\omega_m), \quad (28)$$

where

$$\chi_{n,n'}^{\mathbf{q}\sigma\sigma'}(i\omega_m) = \chi^{\mathbf{q}\sigma\sigma'}(\boldsymbol{\nu}) = \frac{\beta}{8} \iiint d\boldsymbol{\tau} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\tau}} \chi^{\mathbf{q}\sigma\sigma'}(\boldsymbol{\tau}).$$

### 3.1.1 One-band Hubbard model: Non interacting limit

In the non-interacting limit we can use Wick's theorem. It follows that the elements of the two-particle Green function tensor vanish if  $\mathbf{k} \neq \mathbf{k}'$ , and that, in the paramagnetic case, Eq. (26) becomes

$$\chi_{zz}(\mathbf{q}; \boldsymbol{\tau}) = -(g\mu_B)^2 \frac{1}{4} \frac{1}{\beta} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \sum_{\sigma} \mathcal{G}_{\mathbf{k}\sigma}(\tau_{14}) \mathcal{G}_{\mathbf{k}+\mathbf{q}\sigma}(-\tau_{23}).$$

For the frequency-dependent magnetic susceptibility Eq. (28) we have instead

$$\chi_{zz}(\mathbf{q}; i\omega_m) = (g\mu_B)^2 \frac{1}{4} \frac{1}{\beta^2} \sum_{nn'} \sum_{\sigma} \chi_{n,n'}^{\mathbf{q}\sigma\sigma}(i\omega_m),$$

where

$$\sum_{\sigma} \chi_{n,n'}^{\mathbf{q}\sigma\sigma}(i\omega_m) = -\beta \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \sum_{\sigma} \mathcal{G}_{\mathbf{k}\sigma}(i\nu_n) \mathcal{G}_{\mathbf{k}+\mathbf{q}\sigma}(i\nu_n + i\omega_m) \delta_{n,n'}. \quad (29)$$

The static susceptibility is given by

$$\chi_{zz}(\mathbf{q}; 0) = -(g\mu_B)^2 \frac{1}{4} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \sum_{\sigma} \frac{n_{\sigma}(\varepsilon_{\mathbf{k}+\mathbf{q}}) - n_{\sigma}(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}}.$$

Finally, in the  $\mathbf{q} \rightarrow 0$  and  $T \rightarrow 0$  limit we recover as expected the Pauli susceptibility

$$\begin{aligned} \chi_{zz}(\mathbf{0}; 0) &= \frac{1}{4} (g\mu_B)^2 \rho(\varepsilon_F), \\ \rho(\varepsilon_F) &= - \sum_{\sigma} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \left. \frac{dn_{\sigma}(\varepsilon_{\mathbf{k}})}{d\varepsilon_{\mathbf{k}}} \right|_{T=0}. \end{aligned}$$

If we consider the HTSCs dispersion relation Eq. (15) and assume  $t' = 0$ , at half filling the non-interacting static susceptibility exhibits a divergence at  $\mathbf{q} = \Gamma = (0, 0, 0)$ ; this is due to the van Hove singularity in the density of states at the Fermi level. It also diverges at, e.g.,  $X = (\pi/a, 0, 0)$  because of perfect nesting,  $\varepsilon_{\mathbf{k}+X} = -\varepsilon_{\mathbf{k}}$ . More details about the magnetic susceptibility of the non-interacting half-filled one-band Hubbard model with dispersion given by Eq. (15) can be found in Ref. [22].

### 3.1.2 One-band Hubbard model: Atomic limit

Let us now consider the opposite case, the atomic limit. First we use a simple approach, we directly calculate the right-hand side of Eq. (24) by summing up the contributions of the atomic states,  $|0\rangle$ ,  $c_{\uparrow}^{\dagger}|0\rangle$ ,  $c_{\downarrow}^{\dagger}|0\rangle$ ,  $c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}|0\rangle$ ; since the atoms are decoupled, only on-site terms  $i = i'$  contribute. The magnetic susceptibility, normalized to a single atom, is given by

$$\chi_{zz}(\mathbf{q}; 0) = (g\mu_B)^2 \frac{1}{4k_B T} \frac{e^{\beta U/2}}{1 + e^{\beta U/2}}. \quad (30)$$

The same expression can be obtained from the two-particle Green function tensor  $\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau})$ , defined in Eq. (25) for the Hubbard model. In the atomic limit it is better to work directly in real space; since only  $i = i'$  terms contribute, carrying out the  $\mathbf{k}$  sums in Eq. (27) we find

$$\chi^{q\sigma\sigma'}(\boldsymbol{\tau}) = \frac{1}{\beta} \sum_i \chi_{i\sigma' i\sigma}^{i\sigma i\sigma'}(\boldsymbol{\tau}).$$

As we have seen in Sec. 2.7.2, it is sufficient to calculate  $\chi_{i\sigma' i\sigma}^{i\sigma i\sigma'}(\boldsymbol{\tau})$  for positive times  $0 < \tau_{j4} < \beta$ . Because of the time ordering operator we have, however, to distinguish the various imaginary-time sectors. Let us consider first the case  $\tau_{j4} > \tau_{j+14}$  and label the corresponding  $\tau$ -vector as  $\boldsymbol{\tau}^+$ . Calculating the trace we obtain

$$\chi_{i\sigma' i\sigma}^{i\sigma i\sigma'}(\boldsymbol{\tau}^+) = \frac{1}{2(1 + e^{\beta U/2})} \left( e^{\tau_{12}U/2 + \tau_{34}U/2} + \delta_{\sigma\sigma'} e^{(\beta - \tau_{12})U/2 - \tau_{34}U/2} \right).$$

For a paramagnetic system the mean-field terms  $G_{\sigma}(\tau_{12})G_{\sigma'}(\tau_{34})$  cancel out in the actual susceptibility; thus we dropped them in the expression above. For a single atom, the imaginary-time magnetic susceptibility in the  $\boldsymbol{\tau}^+$  sector is then given by

$$\chi_{zz}(\boldsymbol{\tau}^+) = (g\mu_B)^2 \frac{1}{4} \frac{1}{\beta} \sum_{\sigma\sigma'} \sigma\sigma' \chi_{i\sigma' i\sigma}^{i\sigma i\sigma'}(\boldsymbol{\tau}) = \frac{(g\mu_B)^2}{4\beta} \frac{1}{(1 + e^{\beta U/2})} e^{(\beta - \tau_{12} - \tau_{34})U/2}.$$

The terms corresponding to the remaining imaginary-time sectors can be obtained in a similar way (see Appendix); summing up the various contribution to Eq. (28), i.e., to the Fourier transform  $\chi_{n,n'}^{\sigma\sigma'}(i\omega_n)$  we recover the initial expression Eq. (30).

In the atomic limit,  $\chi_{zz}(\mathbf{q}; 0)$  decreases for large temperatures as  $1/k_B T$ , i.e., it has a Curie behavior. This is very different from what we find in the  $U = 0$  limit. The non-interacting Pauli susceptibility  $\chi_{zz}(\mathbf{0}; 0)$  is weakly temperature-dependent; for the HTSCs dispersion relation, at half-filling the temperature dependence of  $\chi_{zz}(\mathbf{0}; 0)$  is enhanced for  $t' = 0$ , i.e., when the logarithmic van-Hove singularity is at the Fermi level [22].

## 3.2 The generalized susceptibility

In this section, we generalize what we have seen in the previous one to the case of the multi-band Hubbard model defined in (2); furthermore, we consider the linear response to a non-specified external field, not necessarily a magnetic field. Let us start from the site susceptibility in imaginary time

$$\chi_{\hat{P}_{\nu}^i \hat{O}_{\nu'}^{i'}}(\boldsymbol{\tau}) = \langle \mathcal{T} \Delta \hat{P}_{\nu}^i(\tau_1, \tau_2) \Delta \hat{O}_{\nu'}^{i'}(\tau_3, \tau_4) \rangle_0,$$

where the site operators  $\hat{P}_\nu^i$  and  $\hat{O}_{\nu'}^{i'}$  are defined as

$$\begin{aligned}\hat{P}_\nu^i(\tau_1, \tau_2) &= \sum_{\alpha} p_{\alpha}^{\nu} c_{i\alpha}^{\dagger}(\tau_2) c_{i\alpha}(\tau_1), \\ \hat{O}_{\nu'}^{i'}(\tau_3, \tau_4) &= \sum_{\gamma} o_{\gamma}^{\nu'} c_{i'\gamma}^{\dagger}(\tau_4) c_{i'\gamma}(\tau_3).\end{aligned}$$

The labels  $\alpha = (\alpha, \alpha')$ ,  $\gamma = (\gamma, \gamma')$  are, as usual, collective flavors, and for the multi-band Hubbard model include spin ( $\sigma$ ) and orbital ( $m$ ) quantum number, plus a fractional vector identifying a correlated basis atom in the unit cell ( $i_c$ ). The weight factors  $o_{\alpha}^{\nu}$  and  $p_{\gamma}^{\nu'}$ , in general complex numbers, identify the type of response we calculate. The imaginary-time site susceptibility is then given by

$$\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}(\boldsymbol{\tau}) = \sum_{\alpha\gamma} v_{\alpha\gamma} \chi_{\gamma_i'}^{\alpha_i}(\boldsymbol{\tau}),$$

where  $v_{\alpha\gamma} = p_{\alpha}^{\nu} o_{\gamma}^{\nu'}$ ,  $\alpha_i = (i\alpha, i\alpha')$ , and  $\gamma_{i'} = (i'\gamma, i'\gamma')$ . The function  $\chi_{\gamma_{i'}}^{\alpha_i}(\boldsymbol{\tau})$  is defined in Eq. (21) and its Fourier transform in time,  $\chi_{\gamma_{i'}}^{\alpha_i}(\boldsymbol{\nu})$ , in Eq. (22). If we perform the Fourier transform in both time and lattice vectors we find

$$\begin{aligned}\chi(\mathbf{q}; \boldsymbol{\nu}) &= \sum_{\alpha\gamma} v_{\alpha\gamma} \sum_{ii'} e^{i(\mathbf{T}_i - \mathbf{T}_{i'}) \cdot \mathbf{q}} \chi_{\gamma_{i'}}^{\alpha_i}(\boldsymbol{\nu}) = \sum_{\alpha\gamma} v_{\alpha\gamma} \frac{1}{N_{\mathbf{k}}^2} \sum_{\mathbf{k}\mathbf{k}'} \chi_{\gamma_{\mathbf{k}'}}^{\alpha_{\mathbf{k}}}(\boldsymbol{\nu}) \\ &= \sum_{\alpha\gamma} v_{\alpha\gamma} [\chi(\mathbf{q}; i\omega_m)]_{L_{\alpha}, L_{\gamma}},\end{aligned}$$

where  $\alpha_{\mathbf{k}} = (\alpha \mathbf{k}_1, \alpha' \mathbf{k}_2)$  and  $\gamma_{\mathbf{k}'} = (\gamma \mathbf{k}_3, \gamma' \mathbf{k}_4)$ ; as in the case of the magnetic susceptibility for the one-band Hubbard model,  $\mathbf{k}_1 = \mathbf{k}$ ,  $\mathbf{k}_2 = -\mathbf{k} - \mathbf{q}$ ,  $\mathbf{k}_3 = \mathbf{k}' + \mathbf{q}$  and  $\mathbf{k}_4 = -\mathbf{k}'$ . The terms  $\chi_{\gamma_{\mathbf{k}'}}^{\alpha_{\mathbf{k}}}(\boldsymbol{\nu})$  build a square matrix

$$\chi_{\gamma_{\mathbf{k}'}}^{\alpha_{\mathbf{k}}}(\boldsymbol{\nu}) \equiv [\chi(\mathbf{q}; i\omega_m)]_{\mathbf{k}L_{\alpha}, \mathbf{k}'L_{\gamma}}$$

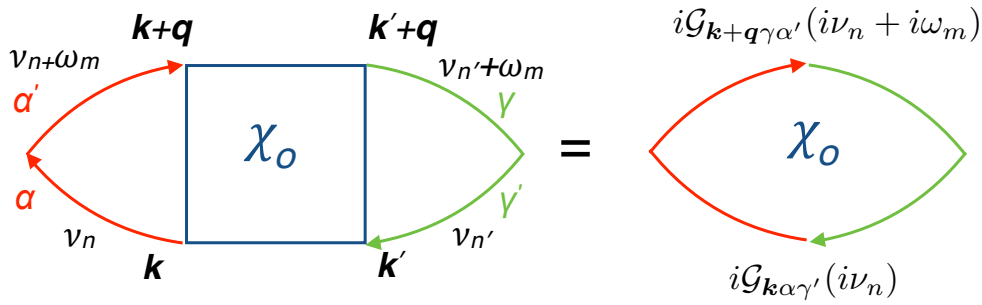
whose elements are labeled for convenience by the collective indices  $\mathbf{k}L_{\alpha} = (\alpha \mathbf{k}n, \alpha' \mathbf{k}n)$  and  $\mathbf{k}'L_{\gamma} = (\gamma \mathbf{k}'n', \gamma' \mathbf{k}'n')$ ; by summing over  $\mathbf{k}$  and  $\mathbf{k}'$  we obtain  $[\chi(\mathbf{q}; \omega_m)]_{L_{\alpha}, L_{\gamma}}$ . Finally, the actual linear response function is given by the sum over the fermionic Matsubara frequencies

$$\chi_{\hat{P}_\nu^i \hat{O}_{\nu'}^{i'}}(\mathbf{q}; i\omega_m) = \sum_{\alpha\gamma} v_{\alpha\gamma} \frac{1}{\beta^2} \sum_{nn'} [\chi(\mathbf{q}; \omega_m)]_{L_{\alpha}, L_{\gamma}}. \quad (31)$$

In the single-orbital case ( $\alpha = \alpha' = \sigma$  and  $\gamma = \gamma' = \sigma'$ ) when  $\hat{P}_\nu^i = \hat{M}_z^i = \hat{O}_\nu^i$  we have

$$o_{\alpha}^z = -g\mu_B \langle \sigma | \hat{\sigma}_z | \sigma \rangle, \quad p_{\alpha}^z = -g\mu_B \langle \sigma' | \hat{\sigma}_z | \sigma' \rangle,$$

and we recover the magnetic susceptibility for the one-band Hubbard model.



**Fig. 9:** Diagram contributing to the linear susceptibility for a non-interacting system. The red lines indicates that the creator/annihilator is originally from the operator  $\hat{P}_\nu$ , and the green lines indicate that the creator/annihilator is from the operator  $\hat{O}_\nu$ . The corresponding frequencies and momenta are explicitly assigned.

### 3.3 The generalized susceptibility in DMFT

The linear response function is nothing more than a generalized many-particle retarded Green function. Thus we can use, in principle, all standard many-body techniques for deriving a perturbation series for it. Let us consider a system described by the multi-band Hubbard model (2), which we write here as  $\hat{H}_e = \hat{H}_0 + \hat{H}_U$ , where  $\hat{H}_0$  is the non-interacting part. Let us now formally construct a perturbation series for  $\chi_{\hat{P}_\nu, \hat{O}_\nu}(\mathbf{q}; \omega_m)$  in the interaction  $\hat{H}_U$ . The first step is to calculate the zero-order contribution, i.e., the linear response function for the non-interacting term  $\hat{H}_0$ . Since for  $\hat{H}_0$  the Wick's theorem holds, we have

$$[\chi_0(\mathbf{q}; i\omega_m)]_{\mathbf{k}L_\alpha, \mathbf{k}'L_\gamma} = -\beta N_{\mathbf{k}} \mathcal{G}_{\mathbf{k}\alpha\gamma'}(i\nu_n) \mathcal{G}_{\mathbf{k}'+\mathbf{q}\alpha'\gamma}(i\nu_{n'} + i\omega_m) \delta_{n,n'} \delta_{\mathbf{k},\mathbf{k}'}. \quad (32)$$

The Feynman diagram corresponding to  $[\chi_0(\mathbf{q}; \omega_m)]_{L_\alpha, L_\gamma}$  is shown in Fig. 9. Once we switch on the interaction, many-body perturbation theory leads to the Bethe-Salpeter (BS) equation, pictorially shown in Fig. 10. Mathematically, it can be written in a matrix form as follows

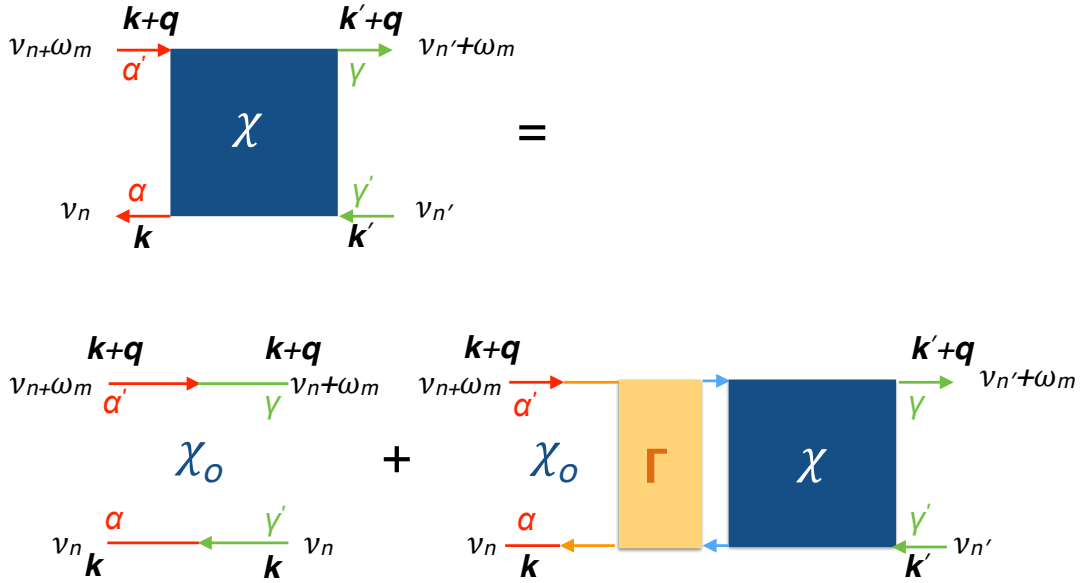
$$[\chi(\mathbf{q}; i\omega_m)]_{L_\alpha, L_\gamma} = \frac{1}{N_{\mathbf{k}}^2} \sum_{\mathbf{k}\mathbf{k}'} \left[ \chi_0(\mathbf{q}; i\omega_m) + \frac{1}{N_{\mathbf{k}}} \chi_0(\mathbf{q}; i\omega_m) \Gamma(\mathbf{q}; i\omega_m) \chi(\mathbf{q}; i\omega_m) \right]_{\mathbf{k}L_\alpha, \mathbf{k}'L_\gamma},$$

where the external sums on  $\mathbf{k}$  vectors are explicitly written. For systems for which dynamical mean-field is a good approximation, however, it is more convenient to construct a diagrammatic series starting from the DMFT linear response function rather than from the non-interacting term. If we do so,  $\chi_0(\mathbf{q}; \omega_m)$  in the Bethe-Salpeter equation is given by Eq. (32) with  $\mathcal{G}$  replaced by the DMFT Green function matrices

$$[\chi_0(\mathbf{q}; i\omega_m)]_{L_\alpha, L_\gamma} = -\beta \delta_{nn'} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} G_{\alpha\gamma'}^{\text{DMFT}}(\mathbf{k}; i\nu_n) G_{\alpha'\gamma}^{\text{DMFT}}(\mathbf{k} + \mathbf{q}; i\nu_n + i\omega_m).$$

There is a catch, however. How do we calculate the vertex matrix  $[\Gamma(\mathbf{q}; \omega_m)]_{\mathbf{k}L_\alpha, \mathbf{k}'L_\gamma}$ ? In the infinite dimension limit it has been shown that, in the BS equation, the vertex can be replaced





**Fig. 10:** Diagrammatic representation of the Bethe-Salpeter equation for the linear susceptibility. The red lines indicates a creator/annihilator stemming from the operator  $\hat{P}_\nu$  and the green lines from the operator  $\hat{O}_{\nu'}$ . The box labeled with  $\Gamma$  is the vertex function, the one labeled with  $\chi$  the full susceptibility, and  $\chi_0$  is the pair-bubble term.

by a local quantity [15, 23, 24]; assuming that, in the spirit of the dynamical mean-field approximation, for a real 3-dimensional system we can still do the same, the BS equation becomes

$$[\chi(\mathbf{q}; i\omega_m)]_{L_\alpha, L_\gamma} = [\chi_0(\mathbf{q}; \omega_m) + \chi_0(\mathbf{q}; i\omega_m)\Gamma(i\omega_m)\chi(\mathbf{q}; i\omega_m)]_{L_\alpha, L_\gamma}.$$

By solving it formally we find

$$[\chi^{-1}(\mathbf{q}; i\omega_m)]_{L_\alpha, L_\gamma} = [\chi_0^{-1}(\mathbf{q}; i\omega_m) - \Gamma(i\omega_m)]_{L_\alpha, L_\gamma}. \quad (33)$$

To actually obtain  $\chi(\mathbf{q}; i\omega_m)$  from this equation we still need the local vertex. The latter can be calculated by means of a further approximation, i.e., assuming that (33) is also satisfied if we replace the  $\mathbf{q}$ -dependent susceptibilities with their local counterparts, defined as

$$\begin{aligned} [\chi_0(i\omega_m)]_{L_\alpha^{i_c}, L_\gamma^{i_c}} &= \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q}} [\chi_0(\mathbf{q}; i\omega_m)]_{L_\alpha^{i_c}, L_\gamma^{i_c}}, \\ [\chi(i\omega_m)]_{L_\alpha^{i_c}, L_\gamma^{i_c}} &= \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q}} [\chi(\mathbf{q}; i\omega_m)]_{L_\alpha^{i_c}, L_\gamma^{i_c}}. \end{aligned}$$

Since the local response function is the same for all equivalent correlated basis sites  $i_c$  we work with the matrix block of a given site; to make this explicit we renamed the corresponding elements  $L_\alpha$  as  $L_\alpha^{i_c}$ . The local term  $\chi(i\omega_m)$  is obtained via the quantum impurity solver in the final iteration of the DMFT self-consistency loop. By inverting the local BS equation we have the vertex

$$[\Gamma(i\omega_m)]_{L_\alpha, L_\gamma} = [\chi_0^{-1}(i\omega_m)]_{L_\alpha, L_\gamma} - [\chi^{-1}(i\omega_m)]_{L_\alpha, L_\gamma}. \quad (34)$$

Replacing  $\Gamma(i\omega_m)$  obtained via Eq. (34) into Eq. (33) yields the  $\mathbf{q}$ -dependent susceptibility. It has to be noticed that, although the two equations (33) and (34) look innocent, solving them numerically is a delicate task because the local susceptibility is in general not diagonal in  $n, n'$  and does not decay very fast with the frequencies. There are, however, various ways around based on extrapolations [25] or using auxiliary polynomials [26] or other methods.

### 3.4 The $\chi_0(\mathbf{q}; \omega)$ diagram

It is tempting to stop at the first term in the expansion,  $\chi_0(\mathbf{q}; \omega)$ . In the non-interacting case,  $\chi_0(\mathbf{q}; \omega)$  is the exact solution by construction; for small  $U$  we can expect that  $\chi_0(\mathbf{q}; \omega)$  is a reasonable approximation. Can we use it as an approximated linear response function more in general, i.e., also for intermediate or even large  $U$ ? Unfortunately the answer is no. In the large  $U$  limit  $\chi_0(\mathbf{q}; \omega)$  is very different from the exact susceptibility. To understand this point let us calculate the static large  $U$  magnetic susceptibility for the half-filled one-band Hubbard model. We consider two cases, the atomic limit and the insulating regime (small  $t/U$  limit); for the latter we use an approximate expression for the self-energy.

#### 3.4.1 One-band Hubbard model: Atomic limit

In the atomic limit, using the atomic Green function instead of  $\mathcal{G}$  in Eq. (32), we obtain

$$\chi_{n,n'}^{\sigma\sigma'}(0) = -\beta\delta_{nn'}\delta_{\sigma\sigma'}\frac{1}{4}\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right]\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right].$$

By performing the Matsubara sums

$$\chi_{zz}^0(0) = \frac{1}{4}(g\mu_B)^2 \sum_{\sigma} \frac{1}{\beta^2} \sum_n \chi_{n,n}^{\sigma\sigma}(0) = \frac{1}{4}(g\mu_B)^2 \frac{\beta e^{\beta U/2}}{1 + e^{\beta U/2}} \left[ \frac{1}{1 + e^{\beta U/2}} + \frac{1}{U\beta} \left( \frac{1 - e^{-\beta U}}{1 + e^{-\beta U/2}} \right) \right]$$

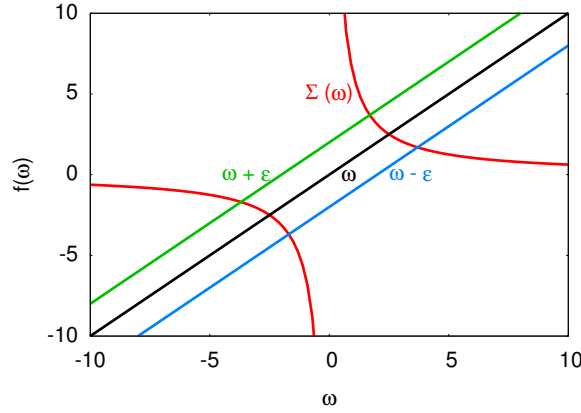
If we assume that  $U$  is finite, for very large temperatures ( $\beta U \rightarrow 0$ ) we find  $\chi_{zz}^0(0) \sim \beta(g\mu_B)^2/8$ . In realistic cases, however, the temperature is in the range 0-1000 K and  $U$  is of the order of few eV; under these conditions the atomic spin  $S = 1/2$  is well defined. In such a large  $\beta U$  limit  $\chi_{zz}^0(0) \sim (g\mu_B)^2/4U$ , i.e., the term  $\chi_{zz}^0(0)$  does not exhibit the Curie behavior. The approximated susceptibility  $\chi_{zz}^0(0)$  should be compared with the actual magnetic susceptibility of our idealized atom which, as we have seen in Sec. 3.1, is given by

$$\chi_{zz}(0) = (g\mu_B)^2 \frac{1}{4} \left[ \frac{\beta e^{\beta U/2}}{1 + e^{\beta U/2}} \right] \stackrel{\beta U \rightarrow \infty}{\sim} \frac{(g\mu_B S)^2}{k_B T}.$$

#### 3.4.2 One-band Hubbard model: Mott-insulating regime

Let us now consider the half-filled Hubbard model with HTCSs dispersion; the latter is defined in Eq. (15). For simplicity, we assume that all hopping integrals except  $t$  are zero. In the atomic limit ( $t = 0$ ) we can rewrite the atomic Green function as

$$G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)},$$



**Fig. 11:** Graphical solution of the equation  $\omega + \varepsilon + \Sigma(\omega) = 0$  yielding the poles  $E^+$  and  $E^-$  of the Green function defined in Eq. (36).

where  $\mu = U/2$  and the self-energy is given by

$$\Sigma(i\nu_n) = \mu + \frac{U^2}{4} \frac{1}{i\nu_n}. \quad (35)$$

In the Mott insulating regime, i.e., for small but finite  $t/U$ , we can assume that the self-energy can be still written in the form given in Eq. (35), with  $\mu$  replaced by the actual chemical potential and  $U^2/4$  by a quantity which plays the role of a dimensionless *order parameter* [24] for the insulating phase  $r_U U^2/4$ , defined as

$$\frac{1}{r_U} \frac{4}{U^2} = \int_{-\infty}^{+\infty} d\varepsilon \frac{\rho(\varepsilon)}{\varepsilon^2},$$

where  $\rho(\varepsilon)$  is the density of states per spin; the integral  $4/r_U U^2$  diverges in the metallic phase. The Green function can then be rewritten as

$$G_{\mathbf{k}}(i\nu_n) = \frac{1}{i\nu_n - \Sigma(i\nu_n) - \varepsilon_{\mathbf{k}}} = \frac{1}{E_{\mathbf{k}}^+ - E_{\mathbf{k}}^-} \left[ \frac{E_{\mathbf{k}}^+}{i\nu_n - E_{\mathbf{k}}^+} - \frac{E_{\mathbf{k}}^-}{i\nu_n - E_{\mathbf{k}}^-} \right] \quad (36)$$

where  $E_{\mathbf{k}}^+$  and  $E_{\mathbf{k}}^-$  are the two roots of the equation  $\omega - \Sigma(\omega) - \varepsilon_{\mathbf{k}} = 0$ ,

$$E_{\mathbf{k}}^{\pm} = \frac{1}{2} \varepsilon_{\mathbf{k}} \pm \frac{1}{2} \sqrt{\varepsilon_{\mathbf{k}}^2 + r_U U^2}.$$

By performing the Matsubara sums, one finds

$$\begin{aligned} \chi_{zz}^0(\mathbf{q}; 0) &= (g\mu_B)^2 \frac{1}{4} \sum_{\sigma} \frac{1}{\beta^2} \sum_n \chi_{n,n}^{\sigma\sigma}(0) \\ &= (g\mu_B)^2 \frac{1}{2} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \left[ \underbrace{-I_{\mathbf{k},\mathbf{q}}^{++} - I_{\mathbf{k},\mathbf{q}}^{--}}_{A_{\mathbf{k},\mathbf{q}}} + \underbrace{I_{\mathbf{k},\mathbf{q}}^{+-} + I_{\mathbf{k},\mathbf{q}}^{-+}}_{B_{\mathbf{k},\mathbf{q}}} \right] \end{aligned}$$

where, setting  $\alpha = \pm$  and  $\gamma = \pm$ ,

$$I_{\mathbf{k},\mathbf{q}}^{\alpha\gamma} = \frac{E_{\mathbf{k}}^{\alpha} E_{\mathbf{k}+\mathbf{q}}^{\gamma}}{(E_{\mathbf{k}}^+ - E_{\mathbf{k}}^-)(E_{\mathbf{k}+\mathbf{q}}^+ - E_{\mathbf{k}+\mathbf{q}}^-)} \frac{n(E_{\mathbf{k}}^{\alpha}) - n(E_{\mathbf{k}+\mathbf{q}}^{\gamma})}{E_{\mathbf{k}}^{\alpha} - E_{\mathbf{k}+\mathbf{q}}^{\gamma}}.$$

In the  $\mathbf{q} \rightarrow \mathbf{0}$  limit we find

$$A_{\mathbf{k},\mathbf{0}} = \beta \left[ \frac{(E_{\mathbf{k}}^+)^2}{\varepsilon_{\mathbf{k}}^2 + r_U U^2} n(E_{\mathbf{k}}^+) [1 - n(E_{\mathbf{k}}^+)] + \frac{(E_{\mathbf{k}}^-)^2}{\varepsilon_{\mathbf{k}}^2 + r_U U^2} n(E_{\mathbf{k}}^-) [1 - n(E_{\mathbf{k}}^-)] \right]$$

$$B_{\mathbf{k},\mathbf{0}} = \frac{r_U U^2}{2(\varepsilon_{\mathbf{k}}^2 + r_U U^2)^{3/2}} [n(E_{\mathbf{k}}^-) - n(E_{\mathbf{k}}^+)].$$

In the large  $\beta U$  limit, the  $A_{\mathbf{k},\mathbf{0}}$  term, proportional to the density of states at the Fermi level, vanishes exponentially; the  $B_{\mathbf{k},\mathbf{0}}$  term yields the dominant contribution

$$\chi_{zz}^0(\mathbf{0}; 0) \sim (g\mu_B)^2 \frac{1}{4} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \frac{r_U U^2}{[\varepsilon_{\mathbf{k}}^2 + r_U U^2]^{3/2}} \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U} U} \left[ 1 - \frac{3}{2} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}^2}{r_U U^2} + \dots \right].$$

The right-hand side is equal to the atomic  $\chi_{zz}^0(0)$  minus a correction; hence the term  $\chi_{zz}^0(\mathbf{0}; 0)$  for a Mott insulator has basically the same defects as  $\chi_{zz}^0(0)$  for an idealized one-level atom. What about the  $\mathbf{q}$ -dependence of  $\chi_{zz}^0(\mathbf{q}; 0)$ ? The one-band Hubbard model has an antiferromagnetic instability in the Mott-insulating regime due to superexchange [22, 27]. Let us therefore calculate  $\chi_{zz}^0(\mathbf{q})$  at the  $\mathbf{q}$  vector associated with antiferromagnetic order,  $\mathbf{q}_C = (\pi/a, \pi/a, 0)$ . Since at  $\mathbf{q}_C$  the band dispersion satisfies the perfect nesting condition ( $\varepsilon_{\mathbf{k}+\mathbf{q}_C} = -\varepsilon_{\mathbf{k}}$ ) we find

$$A_{\mathbf{k},\mathbf{q}_C} = \frac{1}{2} \frac{r_U U^2}{\varepsilon_{\mathbf{k}}^2 + r_U U^2} \frac{n(E_{\mathbf{k}}^+ - \varepsilon_{\mathbf{k}}) - n(E_{\mathbf{k}}^+)}{\varepsilon_{\mathbf{k}}}$$

$$B_{\mathbf{k},\mathbf{q}_C} = \frac{1}{2} \frac{\varepsilon_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}^2 + r_U U^2} \frac{n(E_{\mathbf{k}}^+ - \varepsilon_{\mathbf{k}}) - n(E_{\mathbf{k}}^+)}{\varepsilon_{\mathbf{k}}} - \frac{1}{2} \frac{1}{\sqrt{\varepsilon_{\mathbf{k}}^2 + r_U U^2}} [n(E_{\mathbf{k}}^+) - n(E_{\mathbf{k}}^-)],$$

and therefore

$$\chi_0(\mathbf{q}_C; 0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U} U} \left[ 1 - \frac{1}{2} \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}^2}{r_U U^2} \right].$$

Thus  $\chi_0(\mathbf{q}; 0)$  is larger at  $\mathbf{q} = \mathbf{q}_C$  than at  $\mathbf{q} = \mathbf{0}$ ; it does not exhibit, however, Curie-Weiss instabilities. The latter appear as soon as we take the vertex into consideration. In line with the results above, we express  $\chi_0(\mathbf{q}; 0)$  as

$$\chi_0(\mathbf{q}; 0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U} U} \left[ 1 - \frac{1}{2} \frac{J_0}{\sqrt{r_U} U} - \frac{1}{4} \frac{J_{\mathbf{q}}}{\sqrt{r_U} U} \right],$$

where  $J_{\mathbf{q}} = 2J[\cos q_x + \cos q_y]$  with  $J \propto t^2/U$ . Next we take the exact atomic susceptibility in the large  $\beta U$  limit as local term and calculate the vertex as

$$\Gamma \sim \left[ \frac{1}{\chi_{zz}^0(0)} - \frac{1}{\chi_{zz}(\mathbf{q}; 0)} \right] \sim \frac{1}{(g\mu_B)^2} \left[ 4\sqrt{r_U} U \left( 1 + \frac{1}{2} \frac{J_0}{\sqrt{r_U} U} \right) - 4k_B T \right].$$

Therefore,

$$\chi_{zz}(\mathbf{q}; 0) = \frac{1}{[\chi_{zz}^0(\mathbf{q}; 0)]^{-1} - \Gamma} \sim (g\mu_B)^2 \frac{1}{4} \frac{1}{k_B T + J_{\mathbf{q}}/4} = \frac{(g\mu_B)^2}{k_B} \frac{1}{4} \frac{1}{T - T_{\mathbf{q}}}.$$

Thus, including the vertex correction we recover the Curie-Weiss behavior expected for a system with coupled localized spins; we also correctly find the antiferromagnetic instability, since  $\mathbf{q}_C$  is the vector for which  $T_{\mathbf{q}}$  is largest. In conclusion, we have seen that  $\Gamma$  is essential to properly describe the magnetic response function of strongly-correlated systems.

### 3.5 The local susceptibility $\chi(\omega)$

The local susceptibility can be obtained in various ways. Here we briefly recollect the essential steps for calculating it via a quantum Monte Carlo approach. A more detailed description of quantum Monte Carlo approaches can be found in the lecture of Fakher Assaad.

#### 3.5.1 Hirsch-Fye QMC quantum impurity solver

For the one-band Hubbard model, the typical quantum-impurity problem used in DMFT calculations is the Anderson Hamiltonian

$$\hat{H} = \underbrace{\sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}}_{\hat{H}_{\text{loc}}} + \underbrace{\sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}}_{\hat{H}_{\text{bth}}} + \underbrace{\sum_{\sigma} \sum_{\mathbf{k}} [V_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{d\sigma} + \text{h.c.}]}_{\hat{H}_{\text{hyb}}}.$$

This Hamiltonian describes a correlated site, e.g., site  $i = 0$  in the original lattice Hubbard model, whose states are labeled with  $d$ , coupled to a non-correlated bath, whose states have for quantum numbers the momentum  $\mathbf{k}$  and the spin  $\sigma$ , via the hybridization  $V_{\mathbf{k}}$ . The Anderson model was originally introduced in the context of the single-impurity Kondo problem [28].

The Hirsch-Fye quantum Monte Carlo approach [29] is based on *imaginary-time discretization*. To calculate a physical observable a crucial ingredient is the partition function

$$Z = \text{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}.$$

If all eigenvalues and eigenvectors were known, the partition function would be of course also known. How do we calculate a physical observable without this information? If we split the interval  $\tau = [0, \beta]$  in time steps  $\Delta\tau = \beta/L$  we can rewrite the partition function as follows

$$Z = \text{Tr} \prod_{l=1}^L e^{-\Delta\tau(\hat{H} - \mu\hat{N})}. \quad (37)$$

In the Anderson model, the interaction term is  $\hat{H}_{\text{loc}}$ ; we therefore rewrite the Hamiltonian  $\hat{H}$  as  $\hat{H} = \hat{H}_0 + \hat{H}_U$ , where  $\hat{H}_0 = \hat{H}_{\text{bth}} + \hat{H}_{\text{hyb}}$  and  $\hat{H}_U = \hat{H}_{\text{loc}}$ . If  $\Delta\tau$  is small, we can approximate the partition function via the Trotter decomposition

$$Z = \text{Tr} \prod_{l=1}^L e^{-\Delta\tau(\hat{H}_0 - (\mu\hat{N} - \mu_d\hat{N}_d))} e^{-\Delta\tau(\hat{H}_U - \mu_d\hat{N}_d)} + O(\Delta\tau^2), \quad (38)$$

where  $\hat{N}_d = n_{d\uparrow} + n_{d\downarrow}$  is the impurity electron number operator, and  $\mu_d\hat{N}_d$  yields a shift. The equivalence between Eq. (37) and Eq. (38) up to first order can be verified, e.g., by performing a first-order Taylor expansion of both expressions and comparing the results. Remarkably, Eq. (38) can be rewritten in a simpler form using the Hubbard-Stratonovich transformation. Taking  $\mu_d = \varepsilon_d + U/2$  we obtain, for a given  $\Delta\tau$

$$e^{-\Delta\tau[\hat{H}_{\text{loc}} - \mu_d\hat{N}_d]} = e^{-\Delta\tau U[n_{d\uparrow}n_{d\downarrow} - \frac{1}{2}(n_{d\uparrow} + n_{d\downarrow})]} = \frac{1}{2} \sum_{s=\pm 1} e^{s\lambda(n_{d\uparrow} - n_{d\downarrow})}$$

where  $s$  is an auxiliary Ising variable and can take two values,  $s = -1$  or  $s = +1$ , and  $\cosh \lambda = e^{\Delta\tau U/2}$ . One can verify this relation by applying the left and right operator to the basis states. The result is summarized in the table below

	$e^{-\Delta\tau U[n_{d\uparrow}n_{d\downarrow} - \frac{1}{2}(n_{d\uparrow} + n_{d\downarrow})]}$	$\frac{1}{2} \sum_{s=\pm 1} e^{s\lambda(n_{d\uparrow} - n_{d\downarrow})}$
$ 0\rangle$	1	1
$c_{\sigma}^{\dagger} 0\rangle$	$e^{\Delta\tau U/2}$	$\cosh \lambda$
$c_{d\uparrow}^{\dagger}c_{d\downarrow}^{\dagger} 0\rangle$	1	1

Thus, via the auxiliary-field decoupling we replaced the two-particle term  $Un_{d\uparrow}n_{d\downarrow}$  with two single-particle terms, much easier to handle. If we introduce one Ising spin per  $\Delta\tau$  interval, i.e.,  $L$  in total,  $\{s_i\} = s_1, \dots, s_L$ , the partition function becomes

$$Z = \frac{1}{2^L} \sum_{\{s_i\}} \text{Tr} \prod_{l=1}^L e^{-\Delta\tau(\hat{H}_0 - \mu\hat{N} + \mu_d\hat{N}_d) + \lambda s_l(n_{d\uparrow} - n_{d\downarrow})} + O(\Delta\tau^2).$$

For a specific configuration of Ising spins, i.e., for a given set of values for the variables  $\{s_i\}$ , the contribution to the partition function of the auxiliary model has the form

$$Z_{\{s_i\}} = \text{Det}[O_{\{s_i\}}^{\uparrow}] \text{Det}[O_{\{s_i\}}^{\downarrow}],$$

Taking the inverse of  $O_{\{s_i\}}^{\sigma}$  yields the Green function matrix  $G_{\{s_i\}}^{\sigma}$ . The latter has dimension  $NL \times NL$  where  $N$  is the total number of sites (bath plus impurity) and satisfies the Dyson equation

$$G_{\{s_j\}}^{\sigma} = [A^{\sigma}]^{-1} G_{\{s_i\}}^{\sigma}, \quad A^{\sigma} = 1 + [1 - G_{\{s_i\}}^{\sigma}] \left[ e^{V_{\{s_i\}} - V_{\{s_j\}}} - 1 \right],$$

where  $\{s_j\}$  and  $\{s_i\}$  are two different configurations and the matrix  $V_{\{s_i\}} = \lambda\sigma s_i(l)|d\rangle\langle d|$  is a potential acting only on the impurity site. Since the potential is local, the impurity Green function  $G_d$  satisfies the Dyson equation

$$[G_d^{\sigma}]_{\{s_j\}} = [A_d^{\sigma}]^{-1} [G_d^{\sigma}]_{\{s_i\}}, \quad A_d^{\sigma} = 1 + [1 - [G_d^{\sigma}]_{\{s_i\}}] \left[ e^{V_{\{s_i\}} - V_{\{s_j\}}} - 1 \right].$$

By summing over all possible configurations, we have

$$Z = \sum_{\{s_i\}} Z_{\{s_i\}}, \quad G_d^{\sigma} = \sum_{\{s_i\}} w_{\{s_i\}} [G_d^{\sigma}]_{\{s_i\}}$$

where

$$w_{\{s_i\}} = \frac{Z_{\{s_i\}}}{\sum_{\{s_i\}} Z_{\{s_i\}}}.$$

Thus, if  $w_{\{s_i\}}$  were positive definite, it could be used as Boltzmann weight for importance sampling. Unfortunately the ratio of determinants can be negative for some configurations, giving rise to the minus-sign problem. Still, we can define  $|w_{\{s_i\}}|$  as Boltzmann weight and keep track of the sign of the product of determinants.

Remarkably, the ratio of the ‘Boltzmann weights’ of two different configurations

$$\frac{w_{\{s_j\}}}{w_{\{s_i\}}} = \frac{\text{Det}O_{\{s_j\}}^\uparrow \text{Det}O_{\{s_j\}}^\downarrow}{\text{Det}O_{\{s_i\}}^\uparrow \text{Det}O_{\{s_i\}}^\downarrow} = R_\uparrow R_\downarrow.$$

can be obtained via the Dyson equation; in particular, if we flip a spin at time slice  $l$

$$R_\sigma = 1 + \left[ 1 - [[G_d^\sigma]_{\{s_i\}}]_{l,l} \right] [e^{-2\lambda s_i(l)} - 1].$$

Thus, we do not need to calculate the determinants. If a new configuration is accepted we have, however, to recalculate the Green function. In conclusion, the Green function can be obtained as

$$G_d^\sigma \sim \frac{\sum_{\{c\}} \langle G_d^\sigma \rangle_c \text{sign}(w_c)}{\sum_{\{c\}} \text{sign}(w_c)},$$

where  $\{c\}$  are the visited configurations. The linear response function  $\chi_\alpha$  is obtained similarly

$$\chi_\alpha \sim \frac{\sum_{\{c\}} \langle \chi_\alpha \rangle_c \text{sign}(w_c)}{\sum_{\{c\}} \text{sign}(w_c)}.$$

Since the Wick theorem holds for a given configuration, we have  $\langle \chi_\alpha \rangle_c = \langle G_{\alpha,\gamma'} \rangle_c \langle G_{\gamma,\alpha'} \rangle_c$ .

The Hirsch-Fye algorithm can be generalized to more complex local interactions, such as the density-density Coulomb interaction in the multi-orbital Hubbard model, by introducing additional Ising fields  $s$  and correspondingly additional parameters  $\lambda$ .

### 3.5.2 CT-HYB QMC quantum impurity solver

In continuous-time QMC [30] the partition function is expanded in either the hybridization (CT-HYB) or the interaction (CT-INT). Here we discuss shortly the first algorithm, in which the expansion series is in powers of  $\hat{H}_{\text{hyb}}$ . We follow the notation of Ref. [31]. Since for this algorithm we do not need to specify the form of the local interaction, let us consider the most general quantum-impurity Hamiltonian  $\hat{H} = \hat{H}_{\text{loc}} + \hat{H}_{\text{bth}} + \hat{H}_{\text{hyb}}$ , where

$$\begin{aligned} \hat{H}_{\text{loc}} &= \sum_{\alpha\bar{\alpha}} \tilde{\epsilon}_{\alpha\bar{\alpha}} c_\alpha^\dagger c_{\bar{\alpha}} + \frac{1}{2} \sum_{\alpha\alpha'} \sum_{\bar{\alpha}\bar{\alpha}'} U_{\alpha\alpha'\bar{\alpha}\bar{\alpha}'} c_\alpha^\dagger c_{\alpha'}^\dagger c_{\bar{\alpha}'} c_{\bar{\alpha}}, \\ \hat{H}_{\text{bth}} &= \sum_{\gamma} \epsilon_\gamma b_\gamma^\dagger b_\gamma, \\ \hat{H}_{\text{hyb}} &= \sum_{\gamma} \sum_{\alpha} [V_{\gamma,\alpha} c_\alpha^\dagger b_\gamma + h.c.]. \end{aligned}$$

This is a generalized Anderson model that describes a multi-orbital correlated impurity, e.g., site  $i = 0$  in the original multi-band Hubbard model (2), coupled to a bath; it is the typical local impurity model which we have to solve in a realistic DMFT calculation. The combined index  $\alpha = m\sigma$  labels spin and orbital degrees of freedom. For the bath we can use, without loss of generality, the basis that diagonalizes  $\hat{H}_{\text{bth}}$ , with quantum numbers  $\gamma$ . Finally, we define

$\tilde{\varepsilon}_{\alpha\bar{\alpha}} = \varepsilon_{\alpha\bar{\alpha}} - \Delta\varepsilon_{\alpha\bar{\alpha}}^{\text{DC}}$ , where  $\varepsilon_{\alpha\bar{\alpha}}$  is the crystal-field matrix and  $\Delta\varepsilon_{\alpha\bar{\alpha}}^{\text{DC}}$  is the double-counting correction. We work in the interaction picture, and therefore

$$\hat{H}_{\text{hyb}}(\tau) = e^{\tau(\hat{H}_{\text{bth}} + \hat{H}_{\text{loc}})} \hat{H}_{\text{hyb}} e^{-\tau(\hat{H}_{\text{bth}} + \hat{H}_{\text{loc}})}.$$

By expanding the partition function in powers of  $\hat{H}_{\text{hyb}}$  we obtain the series

$$Z = \text{Tr} \left[ e^{-\beta(\hat{H}_{\text{bth}} + \hat{H}_{\text{loc}})} \mathcal{T} e^{-\int_0^\beta d\tau \hat{H}_{\text{hyb}}(\tau)} \right] = \sum_{m=0}^{\infty} (-1)^m \int d\boldsymbol{\tau}^{(m)} \text{Tr} \mathcal{T} \left[ e^{-\beta(\hat{H}_{\text{bth}} + \hat{H}_{\text{loc}})} \prod_{i=m}^1 \hat{H}_{\text{hyb}}(\tau_i) \right],$$

where  $\mathcal{T}$  is again the time-ordering operator,  $\boldsymbol{\tau} = (\tau_1, \tau_2, \dots, \tau_m)$  with  $\tau_{i+1} \geq \tau_i$  and

$$\int d\boldsymbol{\tau}^{(m)} \equiv \int_0^\beta d\tau_1 \dots \int_{\tau_{m-1}}^\beta d\tau_m.$$

In the trace, only terms containing an equal number of creation and annihilation operators in both the bath and impurity sector, i.e., only even expansion orders  $m = 2n$ , yield a finite contribution. Introducing the bath partition function  $Z_{\text{bth}} = \text{Tr} e^{-\beta\hat{H}_{\text{bth}}}$ , the partition function can be factorized as

$$\frac{Z}{Z_{\text{bth}}} = \sum_{n=0}^{\infty} \int d\boldsymbol{\tau}^{(n)} \int d\bar{\boldsymbol{\tau}}^{(n)} \sum_{\alpha\bar{\alpha}} z_{\alpha\bar{\alpha}}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}}), \quad (39)$$

with  $z_{\alpha\bar{\alpha}}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}}) = t_{\alpha\bar{\alpha}}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}}) d_{\bar{\alpha}\alpha}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}})$ . The first factor is the trace over the impurity states

$$t_{\alpha\bar{\alpha}}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}}) = \text{Tr} \mathcal{T} \left[ e^{-\beta(\hat{H}_{\text{loc}} - \mu\hat{N})} \prod_{i=n}^1 c_{\alpha_i}(\tau_i) c_{\bar{\alpha}_i}^\dagger(\bar{\tau}_i) \right],$$

where  $c_{\alpha}^{(\dagger)}(\tau) = e^{\tau(\hat{H}_{\text{loc}} - \mu\hat{N})} c_{\alpha}^{(\dagger)} e^{-\tau(\hat{H}_{\text{loc}} - \mu\hat{N})}$  and  $N$  is the total number of electrons on the impurity. For expansion order  $m = 2n$ , the vector  $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_n)$  gives the flavors  $\alpha_i$  associated with the  $n$  annihilation operators on the impurity at imaginary times  $\tau_i$ , while the  $\bar{\boldsymbol{\alpha}} = (\bar{\alpha}_1, \bar{\alpha}_2, \dots, \bar{\alpha}_n)$  are associated with the  $n$  creation operators at  $\bar{\tau}_i$ . The second factor is the trace over the non-interacting bath, which is given by the determinant

$$d_{\bar{\alpha}\alpha}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}}) = \det[F_{\bar{\alpha}\alpha}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}})]$$

of the  $n \times n$  square hybridization-function matrix with matrix elements  $[F_{\bar{\alpha}\alpha}^{(n)}(\boldsymbol{\tau}, \bar{\boldsymbol{\tau}})]_{i',i} = F_{\bar{\alpha}_{i'}\alpha_i}(\bar{\tau}_{i'} - \tau_i)$  given by

$$F_{\bar{\alpha}\alpha}(\tau) = \sum_{\gamma} \frac{V_{\gamma,\bar{\alpha}} \bar{V}_{\gamma,\alpha}}{1 + e^{-\beta\epsilon_{\gamma}}} \times \begin{cases} -e^{-\epsilon_{\gamma}\tau} & \tau > 0 \\ e^{-\epsilon_{\gamma}(\beta+\tau)} & \tau < 0. \end{cases}$$

On the fermionic Matsubara frequencies,  $\omega_n$ , its Fourier transform

$$F_{\bar{\alpha}\alpha}(\omega_n) = \sum_{\gamma} \frac{V_{\gamma,\bar{\alpha}} \bar{V}_{\gamma,\alpha}}{i\omega_n - \epsilon_{\gamma}}$$



is related to the bath Green-function matrix  $\mathcal{G}$  by

$$F_{\bar{\alpha}\alpha}(\omega_n) = i\omega_n \delta_{\bar{\alpha}\alpha} - \tilde{\epsilon}_{\bar{\alpha}\alpha} - (\mathcal{G})_{\bar{\alpha}\alpha}^{-1}(\omega_n),$$

as can be shown by downfolding the original multiband Hubbard model, Eq. (2), to the impurity block (say, the  $i = i_0$  site)

$$(\mathcal{G})^{-1}(\omega_n) = \left( \begin{array}{c|ccc} i\omega_n I_{i_0} - H_{i_0} & V_{1,i_0} & V_{2,i_0} & \dots \\ \hline \bar{V}_{1,i_0} & i\omega_n - \epsilon_1 & 0 & \dots \\ \bar{V}_{2,i_0} & 0 & i\omega_n - \epsilon_2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{array} \right).$$

Here the matrix elements of  $H_{i_0}$  and  $I_{i_0}$  are given by  $(H_{i_0})_{\alpha\bar{\alpha}} = \tilde{\epsilon}_{\alpha\bar{\alpha}}$  and  $(I_{i_0})_{\alpha\bar{\alpha}} = \delta_{\alpha,\bar{\alpha}}$ , while  $(V_{i_0,i})_{\bar{\alpha}i} = V_{\bar{\alpha},i}$ , and  $(\bar{V}_{i,i_0})_{i\alpha} = \bar{V}_{i,\alpha}$ . The partition function defined in Eq. (39) can be seen as the sum over all configurations  $c = \{\alpha_i \tau_i, \bar{\alpha}_i \bar{\tau}_i, n\}$  in imaginary time and flavors. In a compact form, similar to the case of the Hirsch-Fye algorithm, we have

$$Z = \sum_c \langle Z \rangle_c = \sum_c w_c \sim \sum_{\{c\}} \text{sign}(w_{\{c\}}),$$

where in the last term the sum is over a sequence of configurations  $\{c\}$  sampled by Monte Carlo using  $|w_c|$  as the probability of configuration  $c$ .

Finally, a generic observable  $O$  can then be obtained as the Monte Carlo average

$$O \sim \frac{\sum_{\{c\}} \langle O \rangle_c \text{sign}(w_c)}{\sum_{\{c\}} \text{sign}(w_c)}$$

where  $\langle O \rangle_c$  is the value of the observable for configuration  $c$ . The average expansion order increases linearly with the inverse temperature.

The Green function matrix can, e.g., be obtained as the Monte Carlo average with

$$\langle O \rangle_c = \langle G_{\alpha\bar{\alpha}} \rangle_c = \sum_{ij=1}^n \Delta(\tau, \tau_j - \bar{\tau}_i) [M^{(n)}]_{ji} \delta_{\alpha_j \alpha} \delta_{\bar{\alpha}_i \bar{\alpha}}.$$

Here  $M^{(n)} = [F^{(n)}]^{-1}$  is the inverse of the hybridization-function matrix, updated at each accepted move, and  $\Delta$  is given by

$$\Delta(\tau, \tau') = -\frac{1}{\beta} \begin{cases} \delta(\tau - \tau') & \tau' > 0 \\ -\delta(\tau - (\tau' + \beta)) & \tau' < 0, \end{cases}$$

where the  $\delta$ -function is discretized. Alternatively, we can calculate the Green function matrix from its Legendre coefficients [26], i.e., use the Fourier-Legendre series. The Legendre polynomials  $\{P_l(x)\}$  form a complete orthogonal system over the interval  $[-1, 1]$  and therefore the Green function may be expanded in terms of them as

$$G_{\alpha\bar{\alpha}}(\tau) = \sum_{l=0}^{\infty} \frac{\sqrt{2l+1}}{\beta} P_l(x(\tau)) G_{\alpha\bar{\alpha}}^l, \quad (40)$$

with  $x(\tau) = 2\tau/\beta - 1$ . The first four Legendre polynomials are

$$P_l(x) \begin{array}{c|cccc} & l=0 & l=1 & l=2 & l=3 \\ \hline & 1 & x & \frac{1}{2}(3x^2 - 1) & \frac{1}{2}(5x^3 - 3x) \end{array}$$

The coefficients of the expansion are given by

$$G_{\alpha\bar{\alpha}}^l = \sqrt{2l+1} \int_0^\beta d\tau p_l(x(\tau)) G_{\alpha\bar{\alpha}}(\tau). \quad (41)$$

This can be verified by replacing (40) into (41) and then using the orthogonality property of the Legendre polynomials

$$\int_{-1}^1 dx P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{l,l'}.$$

We can then sample directly the Legendre coefficients; for a given configuration

$$\begin{aligned} \langle G_{\alpha\bar{\alpha}}^l \rangle_c &= \sum_{i,j=1}^n \tilde{P}_l(\tau_j - \bar{\tau}_i) [M^{(n)}]_{j,i} \delta_{\alpha_j \alpha} \delta_{\bar{\alpha}_i \bar{\alpha}} \\ \tilde{P}_l(\tau) &= -\frac{\sqrt{2l+1}}{\beta} \times \begin{cases} P_l(x(\tau)), & \tau > 0 \\ -P_l(x(\tau + \beta)), & \tau < 0 \end{cases} \end{aligned}$$

Since the coefficients  $G_l$  decay fast for large  $l$ , it is often convenient to work with the Legendre rather than with the Matsubara representation, or with a mixed representation. In particular, the Bethe-Salpeter equation can be rewritten in terms of Legendre coefficients for the susceptibility. Let us first start from the Green function matrix

$$\begin{aligned} G_{\alpha\gamma}(\nu_n) &= \int_0^\beta d\tau_{12} e^{i\nu_n \tau_{12}} G_{\alpha\gamma}(\tau_{12}) = \sum_l T_{n,l} G_{\alpha\gamma}^l \\ T_{n,l} &= \frac{\sqrt{2l+1}}{\beta} \int_0^\beta d\tau_{12} e^{i\nu_n \tau_{12}} p_l(x(\tau_{12})). \end{aligned}$$

We can now express the non-interacting susceptibility in terms of the transformation matrices  $T_{n,l}$  and the Legendre coefficients  $\chi_0^{l,l'}(\omega_m)$

$$\begin{aligned} [\chi_0(\omega_m)]_{n,n'} &= \frac{1}{16} \iiint d\boldsymbol{\tau} e^{i[\nu_n \tau_{12} + \nu_{n'} \tau_{34}]} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau}) e^{-i\omega_m \tau_{23}} \\ &= -\frac{1}{16} \iiint d\boldsymbol{\tau} e^{i[\nu_n \tau_{12} + \nu_{n'} \tau_{34}]} G_{\alpha\gamma'}(\tau_{14}) G_{\gamma\alpha'}(-\tau_{23}) e^{-i\omega_m \tau_{23}} \\ &= \sum_{l'} T_{n,l} \chi_0^{l,l'}(\omega_m) T_{n',l}^*. \end{aligned}$$

A similar relation holds for the full susceptibility  $[\chi(\omega_m)]_{n,n'} = \sum_{l,l'} T_{n,l} \chi^{l,l'}(\omega_m) T_{n',l}^*$ .

## 4 Conclusion

In this lecture, I have introduced some of the fundamental aspects of linear-response theory, with focus on strongly correlated materials. Along the way, we have seen an important theorem connecting the linear susceptibility and the correlation function, the fluctuation-dissipation theorem; we have discussed the analytic and symmetry properties of the linear susceptibility tensor; we have introduced the thermodynamic- and the f-sum rule. In the second part of the lecture, we have seen how to calculate the susceptibility using dynamical mean-field theory, the state-of-the art approach for strongly correlated materials. Within this method, the local susceptibility is obtained via the quantum-impurity solver; the  $\mathbf{q}$ -dependent susceptibility can, instead, be calculated solving the Bethe-Salpeter equation in the local-vertex approximation. We have seen that the vertex in the Bethe-Salpeter equation plays a crucial role. As representative examples we have used the one-band Hubbard model and when possible the generalized multi-band Hubbard model. Finally, we have presented two impurity solvers, the Hirsch-Fye QMC and the hybridization-expansion continuous-time QMC method.

Linear response functions are of fundamental importance when we want to compare our theory of a given phenomenon to experiments. In addition, the linear susceptibility tensor is a key ingredient of extensions of DMFT such as, e.g., the dual-fermion and the dual-boson approach.

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## Appendix

### Atomic units

In this lecture, formulas are expressed in atomic units unless specified otherwise. The unit of mass  $m_0$  is the electron mass ( $m_0 = m_e$ ), the unit of charge is the electron charge ( $e_0 = e$ ), the unit of length is the Bohr radius ( $a_0 = a_B \sim 0.52918 \text{ \AA}$ ), and the unit of time  $t_0 = 4\pi\epsilon_0\hbar a_0/e^2$ . In these units, the numerical value of the Bohr radius  $a_B$ , of the electron charge  $e$ , of the electron mass  $m_e$ , of  $1/4\pi\epsilon_0$ , and of  $\hbar$  is 1. Furthermore, the speed of light is  $c = 1/\alpha \sim 137$ , the Bohr magneton  $\mu_B = 1/2$ , and the unit of energy is the Hartree (1 Ha  $\sim 27.211 \text{ eV}$ ).

### Fourier transforms

We use the following conventions for the Fourier transforms. For the direct and inverse Fourier transform in frequency and time

$$f(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}$$

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) e^{-i\omega t}.$$

For the direct and inverse transform in spatial/momentum coordinates

$$g(\mathbf{q}) = \int d\mathbf{r} g(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$g(\mathbf{r}) = \int \frac{d\mathbf{q}}{(2\pi)^3} g(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{r}}.$$

For ideal lattices and  $\mathbf{k}$  vectors in the first Brillouin Zone

$$\frac{1}{N_s} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{T}} = \delta_{\mathbf{T},\mathbf{0}},$$

$$\frac{1}{N_s} \sum_{\mathbf{T}} e^{i\mathbf{k}\cdot\mathbf{T}} = \sum_{\mathbf{G}} \delta_{\mathbf{k},\mathbf{G}},$$

where  $N_s$  is the number of lattice sites.

### Dirac delta function

The Dirac delta function is defined as

$$\delta(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega x}.$$

Some of the properties of the delta function:

$$\begin{aligned}\int f(x)\delta(x-b)dx &= f(b), \\ \delta(x) &= \delta(-x), \\ \delta(ax) &= \frac{1}{|a|}\delta(x), \\ \delta(\mathbf{r}) &= \delta(x)\delta(y)\delta(z).\end{aligned}$$

## Heisenberg representation

Real time:

$$\hat{A}(t) = e^{i(\hat{H}-\mu\hat{N})t} \hat{A} e^{-i(\hat{H}-\mu\hat{N})t}.$$

Imaginary time:

$$\hat{A}(\tau) = e^{(\hat{H}-\mu\hat{N})\tau} \hat{A} e^{-(\hat{H}-\mu\hat{N})\tau},$$

$$[\hat{A}(\tau)]^\dagger = e^{-(\hat{H}-\mu\hat{N})\tau} \hat{A}^\dagger e^{(\hat{H}-\mu\hat{N})\tau} = \hat{A}^\dagger(-\tau)$$

## Fermi-Dirac distribution function

The Fermi-Dirac distribution function is defined as

$$n(\varepsilon) = \frac{1}{1 + e^{\beta\varepsilon}}.$$

In the lecture we used the following relations

$$\begin{aligned}1 - n(\varepsilon) &= \frac{e^{\beta\varepsilon}}{1 + e^{\beta\varepsilon}} = n(-\varepsilon), \\ n(\varepsilon)[1 - n(\varepsilon)] &= \frac{e^{\beta\varepsilon}}{(1 + e^{\beta\varepsilon})^2} = -\frac{1}{\beta} \frac{dn(\varepsilon)}{d\varepsilon}, \\ \frac{dn(\varepsilon)}{d\varepsilon} &= -\frac{dn(-\varepsilon)}{d\varepsilon}.\end{aligned}$$

Furthermore

$$\begin{aligned}\lim_{T \rightarrow 0} \beta n(\varepsilon)[1 - n(\varepsilon)] &= \delta(\varepsilon), \\ \lim_{\Delta \rightarrow 0} \frac{1}{\Delta} [n(\varepsilon) - n(\varepsilon + \Delta)] &= \delta(\varepsilon).\end{aligned}$$

## Analytic functions

Here, we shortly summarize the properties of complex functions which have been used in the lecture. A complex function is said to be *analytic* on a domain  $D$  in the complex plane if it is differentiable at every point inside  $D$ . If  $f(z)$  is analytic at all points within and on a closed path  $\mathcal{C}$  (traversed in anti-clockwise direction) the Cauchy integral theorem holds

$$\oint_{\mathcal{C}} f(z)dz = 0. \quad (42)$$

The points on which a function  $f(z)$  is not analytic are called *singularities*. There are two types of singularities, *isolated* (i.e., at some specific  $z = z_0$ ) and *extended* singularities. If a function  $f(z)$  has an isolated singularity in  $z = z_0$  and there is an integer  $n$  such that for  $m \geq n$  the function  $(z - z_0)^m f(z)$  is analytic in  $z_0$ , then  $z_0$  is said to be a *pole of order  $n$*  of the function  $f(z)$ . Apart from poles, other types of isolated singularities are *essential singularities*, *logarithmic singularities* and *removable singularities*. Let us consider some examples of complex functions that we have used in this lecture. The function

$$f(z) = \frac{1}{z - z_0}$$

has a single pole in  $z_0$ ; this pole is of first order. The Fermi-Dirac distribution function

$$f(z) = \frac{1}{1 + e^{\beta z}}$$

has instead infinite poles, all the fermionic Matsubara frequencies  $z = i\nu_n = i(2n + 1) \pi/\beta$ . In a similar way the Bose distribution function

$$f(z) = \frac{1}{e^{\beta z} - 1}$$

has infinite poles at the bosonic Matsubara frequencies  $z = i\omega_m = i2m \pi/\beta$ .

If within the contour  $\mathcal{C}$  a function  $f(z)$  is analytic except for a set of poles  $\{z_n\}$  of order one, the residue theorem holds

$$\begin{aligned} \oint_{\mathcal{C}} f(z)dz &= 2\pi i \sum_{\{z_n\}} \text{Res}[f(z_n)], \\ \text{Res}[f(z_n)] &= \lim_{z \rightarrow z_n} f(z)(z - z_n), \end{aligned}$$

where the term  $\text{Res}[f(z_n)]$  is called residue of the function  $f(z)$  at the point  $z_n$ .

Extended singularities are of two types, *natural boundaries* and *branch cuts*. The latter are curves (e.g., lines or segments) in the complex plane across which a multi-valued function is discontinuous. Let us consider as example the function  $f(z) = \sqrt{z}$ ; this function is double-valued, for example, in  $z = 1$  it can take both the values  $\pm 1$ . Let us define the principal value of the function  $\sqrt{z}$  as the positive square root (+1), and let us rewrite  $z = |z|e^{i\phi}$ ; the function  $\sqrt{z}$  has then a branch cut at  $\phi = 2\pi$ , i.e., along the line  $y \geq 0$ .

## Spin and magnetization operators

The spin operators  $\hat{S}_\nu$  are defined as

$$\hat{S}_\nu = \frac{1}{2} \sum_{\sigma\sigma'} c_\sigma^\dagger \sigma_\nu c_{\sigma'},$$

where  $\nu = x, y, z$  and  $\hat{\sigma}_\nu$  are the Pauli matrices

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The magnetization operators  $\hat{M}_\nu$  are defined as  $\hat{M}_\nu = -g\mu_B \hat{S}_\nu$ .

## Useful formulas

- Sokhotski-Plemelj formula

$$\frac{1}{\omega + i\delta} = \mathcal{P} \frac{1}{\omega} - i\pi\delta(\omega)$$

- Cauchy principal value

$$\int_{-\infty}^{\infty} \mathcal{P} \frac{1}{\omega} d\omega = \int_{-\infty}^{-\varepsilon} \frac{1}{\omega} d\omega + \int_{\varepsilon}^{\infty} \frac{1}{\omega} d\omega,$$

- Fourier representation of  $\Theta(t)$  function

$$\Theta(t) = i \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} e^{-i\omega''t} \frac{1}{\omega'' + i\delta},$$

- Integral of imaginary exponential

$$I(x) = \int_0^{\infty} e^{ixt} dt = \frac{i}{x + i\delta}, \quad \delta = 0^+.$$

## Atomic magnetic susceptibility

Let us consider an idealized single-level atom described by the Hamiltonian  $\hat{H}_U = U n_\uparrow n_\downarrow$ . The eigenstates of this system,  $|\Psi_i^N\rangle$ , as well as the expectation values  $E_i = \langle \Psi_i^N | \hat{H}_U - \mu \hat{N} | \Psi_i^N \rangle$  at half-filling, are given in the table below

$ \Psi_i^N\rangle$	$N$	$E_i = \langle \Psi_i^N   \hat{H}_U - \mu \hat{N}   \Psi_i^N \rangle$
$ 0\rangle$	0	0
$c_\sigma^\dagger  0\rangle$	1	$-U/2$
$c_\uparrow^\dagger c_\downarrow^\dagger  0\rangle$	2	0

The magnetic susceptibility in Matsubara space is given by

$$[\chi_{zz}]_{nn'}(i\omega_m) = \beta \frac{1}{4} (g\mu_B)^2 \sum_P \text{sign}(P) f_P$$

$$f_P(i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34} e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} f_P(\tau_{14}, \tau_{24}, \tau_{34})$$

where  $P = A, B, \dots$  are the six possible permutations of the indices (123) and

$$f_P(\tau_{14}, \tau_{24}, \tau_{34}) = \frac{1}{Z} \sum_{\sigma\sigma'} \sigma\sigma' \text{Tr} e^{-\beta(\hat{H} - \mu\hat{N})} \left[ \hat{o}_{P_1}(\tau_{14}) \hat{o}_{P_2}(\tau_{24}) \hat{o}_{P_3}(\tau_{34}) c_{\sigma'}^\dagger \right]$$

$$= \frac{1}{Z} \sum_{\sigma\sigma'} \sigma\sigma' \sum_{ijkl} e^{-\beta E_i} \langle i | \hat{o}_{P_1} | j \rangle \langle j | \hat{o}_{P_2} | k \rangle \langle k | \hat{o}_{P_3} | l \rangle \langle l | c_{\sigma'}^\dagger | i \rangle$$

$$\times \left[ e^{\Delta E_{ij}\tau_{14} + \Delta E_{jk}\tau_{24} + \Delta E_{kl}\tau_{34}} \right],$$

where  $\Delta E_{ij} = E_i - E_j$ . For the identity permutation the operators are  $\hat{o}_{P_1} = c_\sigma$ ,  $\hat{o}_{P_2} = c_\sigma^\dagger$ , and  $\hat{o}_{P_3} = c_{\sigma'}$  and the frequencies are  $\omega_1 = \nu_n$ ,  $\omega_2 = -\omega_m - \nu_n$ ,  $\omega_3 = \omega_m + \nu_{n'}$ . This expression can be used to calculate the magnetic susceptibility of any one-band system whose eigenvalues and eigenvectors are known, e.g., via exact diagonalization. In the case of our idealized atom

$$f_E(\tau_{14}, \tau_{24}, \tau_{34}) = \frac{1}{(1 + e^{\beta U/2})} e^{\beta U/2} e^{-(\tau_{12} + \tau_{34})U/2} = \frac{1}{(1 + e^{\beta U/2})} g_E(\tau_{14}, \tau_{24}, \tau_{34}).$$

The frequencies and functions  $f_P(\tau_{14}, \tau_{24}, \tau_{34})$  for all permutations are given in the table below

	$\omega_{P_1}$	$\omega_{P_2}$	$\omega_{P_3}$	$g_P(\tau_{14}, \tau_{24}, \tau_{34})$	$\text{sign}(P)$
$E(123)$	$\nu_n$	$-\omega_m - \nu_n$	$\omega_m + \nu_{n'}$	$e^{\beta U/2} e^{-(\tau_{12} + \tau_{34})U/2}$	+
$A(231)$	$-\omega_m - \nu_n$	$\omega_m + \nu_{n'}$	$\nu_n$	$-e^{\beta U/2} e^{-(\tau_{12} + \tau_{34})U/2}$	+
$B(312)$	$\omega_m + \nu_{n'}$	$\nu_n$	$-\omega_m - \nu_n$	$-e^{+(\tau_{12} + \tau_{34})U/2}$	+
$C(213)$	$-\omega_m - \nu_n$	$\nu_n$	$\omega_m + \nu_{n'}$	$-e^{\beta U/2} e^{-(\tau_{12} + \tau_{34})U/2}$	-
$D(132)$	$\nu_n$	$\omega_m + \nu_{n'}$	$-\omega_m - \nu_n$	$-e^{+(\tau_{12} + \tau_{34})U/2}$	-
$F(321)$	$\omega_m + \nu_{n'}$	$-\omega_m - \nu_n$	$\nu_n$	$e^{+(\tau_{12} + \tau_{34})U/2}$	-

The missing ingredient is the integral

$$I_P(x, -x, x; i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34} e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} e^{x(\tau_{14} - \tau_{24} + \tau_{34})}$$

$$= + \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau \int_0^{\tau_{14} - \tau} d\tau' e^{(i\omega_{P_1} + i\omega_{P_2} + i\omega_{P_3} + x)\tau_{14} - i(\omega_{P_2} + \omega_{P_3})\tau} e^{-(i\omega_{P_3} + x)\tau'}$$

$$= + \frac{1}{i\omega_{P_3} + x - i\omega_{P_2} + x} \left[ \frac{1}{i\omega_{P_1} + x} \frac{1}{n(x)} + \beta \delta_{\omega_{P_1} + \omega_{P_2}} \right]$$

$$+ \frac{1}{i\omega_{P_3} + x} \frac{1 - \delta_{\omega_{P_2} + \omega_{P_3}}}{i(\omega_{P_2} + \omega_{P_3})} \left[ \frac{1}{i\omega_{P_1} + x} - \frac{1}{i(\omega_{P_1} + \omega_{P_2} + \omega_{P_3}) + x} \right] \frac{1}{n(x)}$$

$$+ \delta_{\omega_{P_2} + \omega_{P_3}} \frac{1}{i\omega_{P_3} + x} \left\{ \left[ \frac{1}{(i\omega_{P_1} + x)} \right]^2 \frac{1}{n(x)} - \beta \left[ \frac{1}{(i\omega_{P_1} + x)} \right] \frac{1 - n(x)}{n(x)} \right\}.$$

where  $x = \pm U/2$ , depending on the permutation. The general expression of the integral  $I_P(\Delta E_{ij}, \Delta E_{jk}, \Delta E_{kl}; i\omega_1, i\omega_2, i\omega_3)$  can be found in Refs. [32, 33].



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