Dynamical vertex approximation in its parquet implementation: application to Hubbard nano-rings

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We have implemented the dynamical vertex approximation (DΓA) in its full parquet-based version to include spatial correlations on all length scales and in all scattering channels. The algorithm is applied to study the electronic self-energies and the spectral properties of finite-size one-dimensional Hubbard models with periodic boundary conditions (nanoscopic Hubbard rings). From a methodological point of view, our calculations and their comparison to the results obtained within dynamical mean-field theory, plain parquet approximation, and the exact numerical solution, allow us to evaluate the performance of the DΓA algorithm in the most challenging situation of low dimensions. From a physical perspective, our results unveil how non-local correlations affect the spectral properties of nanoscopic systems of various sizes in different regimes of interaction strength.

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I. INTRODUCTION

Models and materials with reduced dimensionality typically show enhanced correlation effects beyond the limit of standard density-functional or perturbation theory-based schemes, calling for corresponding developments of theoretical tools. From a general point of view, the challenge for a theoretical description is much bigger than in bulk systems: In three dimensions (3D), even in the presence of strong electronic correlations, very accurate material calculations can be performed by means of the dynamical mean-field theory (DMFT) \cite{georges1996} combined with \textit{ab-initio} methods \cite{ceperley1980, kohn1965}. This is possible, because DMFT captures, non-perturbatively, the purely local part of electronic correlations, which drives most important phenomena of correlated electrons in the bulk, such as, e.g., the Mott-Hubbard metal-insulator transition (MIT) \cite{mott1947}. Formally, DMFT becomes exact in the limit of infinite dimensions \cite{georges1996} where all non-local correlations in space are averaged out. Corrections to DMFT in finite-dimensional systems originate from non-local correlations. While, in 3D, deviations from the DMFT description become predominant only in specific parameter regimes \cite{zwanziger2007}, e.g., in the proximity of a second order phase transition \cite{zwanziger2007}, the situation is completely different in case of lower dimensions. In fact, reducing the dimensionality magnifies effects of non-local correlations, undermining the main assumption of DMFT. Already for extended 2D systems, the physics deviates qualitatively from the DMFT predictions, e.g., the Mott-Hubbard MIT is found to disappear in a weak-coupling crossover in the phase-diagram of the 2D Hubbard model \cite{zhang1988, zuhland2011}. Evidently, even stronger non-local effects can be expected if the dimensionality is further reduced towards 1D or 0D.

As for the theoretical description of electronic correlations at the nanoscale, several algorithmic implementations based on DMFT have recently been implemented under the name of nano or real-space DMFT \cite{varma1986, wang1990, mittal1994, mittal1995, sengupta1997, schafer1996, rohringer2004}. Despite some technical differences, all these algorithms essentially extend the DMFT scheme to finite-size and possibly non-translational invariant systems. The common idea consists in solving simultaneously several single impurity problems for calculating, separately, the local self-energies of the different sites composing the system of interest, while the DMFT self-consistency is then enforced at the level of the whole nanostructure. This way, a number of interesting results have been obtained both for model \cite{valli2011, valli2014, valli2015} and realistic studies \cite{valli2013, valli2014a, valli2014b}. However, the applicability of these DMFT-based methods is restricted to the weakly correlated and/or the high-temperature regime, where the effects of non-local correlations are weaker \cite{valli2013, valli2014a, valli2014b} and can be, to a certain extent, neglected. Such limitations were also openly discussed in the previous literature \cite{valli2014, valli2015} where numerical comparisons between DMFT-based calculations and exact solutions (where available) have shown large deviations already in the intermediate coupling regime.

A promising theoretical answer to this challenging situation has already been proposed, but not implemented, in Ref. \cite{valli2015}. The application of diagrammatic extensions \cite{bulla2004, bulla2006, bulla2007, bulla2008, bulla2012} of DMFT such as the dynamical vertex approximation (DΓA) \cite{valli2015} for nanoscopic systems (nano-DΓA). The basic idea of DΓA is the following: Instead of assuming the locality of the one-particle self-energy \( \Sigma(k, \omega) = \Sigma(\omega) \), as in DMFT, one raises the assumption of the locality to a higher level of the diagrammatics, i.e., from the one- to the two-particle irreducible vertex \( \Gamma_{\text{irr}}(k, \omega) \). Once local vertex functions are computed, e.g., with the same impurity solvers used for the standard DMFT \cite{georges1996, schafer1996, rohringer2004, sengupta1997}, non-local correlation ef-
fects can be directly included through diagrammatic relations e.g., in the most general case, through the parquet equations.\textsuperscript{41}

In the specific case of the DΓA implementation for nanoscopic systems\textsuperscript{17} the nano-DΓA algorithm requires a separate calculation of the local irreducible vertex function for each inequivalent site of the nanostructure. The inclusion of the non-local effects should be performed at the level of the whole nanostructure via a self-consistent solution of the parquet equations. This procedure is less demanding than the exact treatment of the corresponding quantum Hamiltonian: the exponential scaling with the number of sites required for a diagonalization of the Hamiltonian, is replaced by a polynomial effort to solve the parquet equations. Moreover, the necessity of calculating the vertex functions only locally, mitigates secondary (but important) numerical problems such as the sign-problem in quantum Monte Carlo (QMC) solvers. Nonetheless, the overall numerical efforts for treating the parquet equations has limited, so far, a wide application of DΓA-based methods in their more complete (parquet-based) form: Hitherto, all successful applications of DΓA to 2D and 3D systems have been performed in cases where fluctuations in a given scattering channel predominate.\textsuperscript{9,13,42} In this case the solution of the parquet equation can be replaced by a much simpler ladder resummation performed in the most relevant channel only.\textsuperscript{42} We note, in passing, that such considerations apply, with very few exceptions,\textsuperscript{42} also to almost all other diagrammatic extensions of DMFT. For similar reasons, no application of the nano-DΓA algorithm, as illustrated in Refs.\textsuperscript{17} and \textsuperscript{22} has been realized hitherto. Exploiting the constant improvements of the numerical performance both in the DMFT calculations of vertex functions\textsuperscript{26,37,40} as well as in the numerical solution of the parquet equations,\textsuperscript{26,37,40} we will present here our first results of the full (i.e., parquet-based) nano-DΓA, applied to a set of correlated nanoscopic rings of increasing size.

The importance of the results presented in the following is twofold, and goes beyond the demonstration of a full applicability of the algorithm proposed in Ref.\textsuperscript{17}. Physically, our calculations allow to understand the interplay of local and non-local correlations in spectral and transport properties of finite systems of different sizes; from a methodological perspective, the application of a full (parquet-based) DΓA scheme to these nanoscopic systems represent one of the most severe benchmarks conceivable for this theoretical approach. In fact, the accuracy of a DΓA calculation depends on the correctness of the locality assumption for the two-particle irreducible vertex functions. Heuristically, this assumption looks plausible for 3D and 2D systems with local interactions, where strong spin, charge, and pair fluctuations are already generated by the corresponding collective modes built on local irreducible vertexes. Numerically, a direct verification of the DΓA assumption is difficult in 2D or 3D: While the irreducible vertex surely displays a strong frequency dependence,\textsuperscript{36,37} taken into account by the DΓA, its independence on momentum has been shown explicitly only in few calculations\textsuperscript{23} beyond DMFT, where the momentum-dependence was found to be weak. In this work, we focus instead on systems where an exact numerical solution is available, so that both, the DΓA performances and assumptions, can be tested. Let us emphasize that the low connectivity and the peculiarities of 1D physics represent the most challenging situation for DΓA. In this perspective, our numerical analysis will also allow to draw conclusions, on a more quantitative ground, on the physical content of parquet-based approximations. The paper is organized as follows: In Sec. II, we introduce the general properties of the nanoscopic systems under consideration, namely Hubbard-rings of different sizes. In Sec. III, we discuss the parquet implementation of DΓA. In Sec. IV, we present the numerical results. Finally, Sec. V provides a summary and our conclusions.

II. MODELLING THE NANO-RINGS

The correlated nanoscopic rings considered in the following consist of $N$ isolated correlated atoms, arranged in a chain with periodic boundary conditions, and described by the Hubbard Hamiltonian

$$ H = -t \sum_{\sigma} \sum_{i=1}^{N} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} \quad (1) $$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) denote the creation (annihilation) operators of an electron on site $i$ with spin $\sigma$, fulfilling the periodic boundary conditions $c_{i+N\sigma} = c_{i\sigma}$, while $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ denotes the number operator; the parameters $t$ and $U$ denote the nearest-neighbor (NN) hopping amplitude and the on-site Hubbard interaction, respectively. Due to the translational invariance of the system, granted by the periodic boundary conditions of the ring, it is convenient to formulate the hopping term in the reciprocal space, yielding a tight-binding dispersion $\epsilon(k) = -2t \cos(ka) - \mu$, where $\mu$ is the chemical potential.

![FIG. 1. (Color online) Energy-momentum dispersion relation $\epsilon(k)$ with respect to the Fermi level $\mu$ (dashed line) for nano-rings with $N = 4, 6, 8$ sites. The symbols denote the discrete eigenstates corresponding to the allowed values of the momentum: $k = 2\pi n / N$, with $n \in \mathbb{N}$.](image-url)
In the following, we set the lattice spacing $a = 1$ and consider rings with $N = 4, 6, 8$ sites. We restrict ourselves to the half-filled case, i.e., $\mu = U/2$, where electronic correlations stemming from the local Hubbard interaction are expected to be most effective. Under these conditions, the rings display a particle-hole symmetric density of states, and in particular, in the non-interacting case ($U = 0$) the systems display either a "band" gap (as in the case of the $N = 6$ sites ring) or a 2-fold degenerate state at the Fermi level (as in the case of $N = 4, 8$ sites rings). The rings considered in this work and the corresponding dispersions $\epsilon(k)$ are shown in the upper and lower panel of Fig. 1, respectively.

III. PARQUET-BASED IMPLEMENTATION OF THE NANO-DΓA

We recall that the idea of DΓA is to apply the locality assumption of DMFT at an higher level of the diagrammatics: While in DMFT all one-particle irreducible (1PI) one-particle diagrams (i.e., the self-energy $\Sigma$) are assumed to be purely local, DΓA confines the locality to the two-particle irreducible (2PI) two-particle diagrams, i.e., the fully irreducible vertex $\Gamma_{irr}$ is approximated by all local Feynman diagrams. Hence, in the DΓA framework, the purely local, but frequency-dependent 2PI vertex $\Gamma_{irr} = \Lambda_{\nu\nu'}^{\omega}$ is calculated for a site $i$ and then used as the input for the parquet equations. In practice, this vertex is obtained by solving the Anderson impurity model (AIM) numerically. Hence, non-local correlations on top of the DMFT solution are generated in all scattering channels by the (numerical) solution of the parquet equations without any restriction to specific (ladder) subsets of diagrams. For the sake of clarity, we should emphasize here that this is different from the so-called parquet approximation (PA). In fact, the PA corresponds to approximating the 2PI vertex with the bare interaction of the theory (e.g., $\Gamma_{irr} = U$) in a merely perturbative fashion. On the contrary, in DΓA all non-perturbative DMFT correlations, which control, e.g., the physics of the Mott-Hubbard transition, are actually included through the frequency dependent $\Gamma_{irr} = \Lambda_{\nu\nu'}^{\omega}$, and non-local correlations beyond DMFT are generated via the solution of the parquet equations.

The specific implementation of the parquet-based DΓA scheme for the case of nanoscopic systems, such as the Hubbard nano-rings, is briefly sketched in the flowchart of Fig. 2 and incorporates all main aspects of the original proposal of Ref. 17. Let us start by recalling the DMFT scheme for a nanoscopic system with $N$ constituents (e.g., atoms), which is self-consistent at the one-particle level only. The first step consists in mapping the full problem onto a set of auxiliary AIMs, one for each of the $N$ sites of the nanostructure. Each auxiliary problem is characterized by a dynamical Weiss field (i.e., the non-interacting Green’s function of the AIM) $G_0^{\nu}(\nu)$. The numerical solution of the AIM yields the local Green’s function $G_{ii}(\nu)$ and the local DMFT self-energy $\Sigma_{ii}(\nu) = G_{0,ii}^{-1}(\nu) - G_{ii}^{-1}(\nu)$. Through the Dyson equation the local (yet site-dependent) DMFT self-energies determine the new non-local Green’s function $G_{ij}$, and the self-consistency is realized at the level of the whole nanostructure.

In the case of the DΓA this procedure is raised to the two-particle level. For each inequivalent AIM, the local 2PI vertex function is computed as following (for the sake of clarity, we omit the temporal and spatial indexes in this derivation, and yet recall that those steps are performed at the local level of each AIM). Typically, one first calculates the full vertex $F$ from the generalized local susceptibility $\chi$ as

$$\chi = \chi_0 - \frac{1}{\beta}\chi_0 F \chi_0,$$

where $\chi_0$ is the bubble part of $\chi$, while $F$ includes all possible vertex corrections, computed with the impurity solver of the AIM. In order to obtain the fully irreducible vertex $\Lambda$, it is necessary to separate the two-particle reducible ($\Phi_r$) and irreducible ($\Gamma_r$) contributions to the full vertex $F$ in each scattering channel $r$, by solving the corresponding Bethe-Salpeter equation

$$F = \Gamma_r + \Phi_r = \Gamma_r + \int \Gamma_r G F.$$

Hence, the fully irreducible vertex $\Lambda$ is obtained from $F$ by inverting the parquet equation of the AIM

$$F = \Lambda + \sum_r \Phi_r.$$
For further details, Ref. 36 provides a comprehensive discussion of the local two-particle vertex functions and of the parquet equations in a unified formalism. Once all inequivalent local 2PI vertexes $\Lambda_{iii}$ are obtained for each site $i$, they are used as an input for the (self-consistent) solution of the parquet equations of the whole nanoscopic system. This yields the non-local full two-particle vertex function $F_{ijkl}$ and, through the Dyson-Schwinger equation, the non-local self-energy $\Sigma_{ij}$, as shown in the flowchart of Fig. 2. Finally, after having determined $\Sigma_{ij}$ one can either skip the outermost loop, i.e., updating the AIM and simply start from $G_{ii}$ of DMFT, as we did in the present paper, or one can perform fully self-consistent calculations; In the latter case the $G_{ii}$ of the corresponding inequivalent AIMS has to be adjusted to yield the given DΓA $G_{ii}$ from the previous iteration before recalculating the vertex (defined diagrammatically in terms of $U$ and $G_{ii}$). One then needs to iterate this scheme until convergence. We refer to Refs. 44 and 45 for a more detailed discussion of the local two-particle vertex functions and all the equations. From the flowchart of the algorithm, one can clearly see how in the DΓA non-local correlations beyond DMFT are systematically generated in all scattering channels in a two-particle self-consistent framework.

Previous applications of the DΓA to bulk systems were carried out within the ladder approximation of the DΓA scheme, which is obtained by replacing the solution of the parquet equations in the flowchart of the algorithm with the simpler calculations at the level of Bethe-Salpeter equations. In practice, this means that only a vertex irreducible in a specific channel, e.g., for the spin channel ($\Gamma_s$), is assumed to be local and needs to be extracted from the solution of the AIM. The application of the ladder approximation is justified in case the system displays predominating fluctuations in a given scattering channel, which is known a priori, e.g., in the case of the antiferromagnetic instability in the 3D Hubbard model at half-filling. The significant numerical simplification of avoiding the solution of the direct and inverse parquet equations has the price of violating the Ward identities, which is mitigated by performing the so-called Moriya correction.  

In practice, the correction is done at the level of the propagator of the (e.g., spin) fluctuations, obtained from the generalized susceptibility by performing the sum over the fermionic Matsubara frequencies and corresponding momenta. The correction is performed by adding a mass term $\lambda$ to the propagator, so that in the selected (spin) channel it reads

$$\chi^{-1}_s(q) \rightarrow \chi^{-1}_s(q) + \lambda.$$  

We note that, as the mass is determined by imposing a condition over the local physics, the procedure mimics to some extent the effect of a full self-consistency of the algorithm, where also the local 2PI vertex would be renormalized by non-local spatial correlations.

### IV. RESULTS

In the following we present the numerical results for all Hubbard nano-rings discussed in Sec. III characterized by the dispersions $\epsilon(k)$ shown in Fig. 1 (lower panels). For each system we compare different approximations, i.e., DMFT, PA, and parquet DΓA, to the ladder DΓA and to the exact QMC solution. Each method is associated to a specific diagrammatic content, as discussed in Sec. III which allows us to understand the relevance of specific subsets of Feynman diagrams for the description of the system. We will discuss the results obtained for the electronic self-energy $\Sigma_{ii}(k, \omega_n)$, the local Green’s function $G_{ii}(\tau)$, and the two-particle irreducible vertex function $\Lambda_{i\alpha\mu\nu}^{\omega\nu\prime\omega'}$. The analysis of the self-energy allows to resolve a $k$-selective behavior in the (discrete) reciprocal space. In particular, we analyze two low-energy parameters, i.e., the scattering rate $\gamma(k) = -2\text{Im}\Sigma(k, \omega_n \rightarrow 0)$, which corresponds to a damping or to the inverse lifetime of quasi-particle excitations in the Fermi liquid regime, and the (static) renormalization of the bare dispersion $\Delta(k) \equiv \text{Re}\Sigma(k, \omega_n \rightarrow 0)$. We will discuss the effect of the local and non-local self-energy on the low-energy spectral properties of the system which can be deduced by the local Green’s function, and is related to the $k$-resolved spectral function $A(k, \nu)$ by

$$G_{ii}(\tau) = \sum_k \int_{-\infty}^{\infty} d\nu \frac{e^{-\tau\nu}}{1 + e^{\beta\nu}} A(k, \nu).$$

The value of the Green’s function at $\tau = \beta/2$ represents an estimate of the value of the local spectral function at the Fermi level (averaged over an energy window proportional to the temperature $T$), i.e.,

$$-\beta G_{ii}(\beta/2) \approx \pi \sum_k A(k, 0).$$

In order to understand the non-local self-energy corrections beyond mean-field, we will also relate our results to the frequency structure of the local 2PI vertex ($\Lambda_{iii}$), which is the input for the parquet equations of the DΓA. To this end, the generalised susceptibility of the AIM is computed with an exact diagonalization impurity solver (with $N_b = 4$ bath sites and a frequency grid large enough to obtain a smooth asymptotics for the irreducible vertexes) and the 2PI vertex is obtained following the steps discussed in Sec. III. For the analysis of the 2PI vertex we will adopt the notation of Refs. 36 and 34, and in particular we will consider the 2PI vertex in the (particle-hole) density and magnetic channels, with respect to their static asymptotics, i.e., $\Lambda_{i\alpha\mu\nu}^{\omega\nu\prime\omega'} \mp U$. Moreover, the comparison to numerically exact two-particle vertex functions, and in particular the fully irreducible one, will also allow us to directly test the assumption behind the DΓA, i.e., the locality of $\Lambda$.

In the following, we will start presenting in Sec. IV A the numerical results for the $N = 6$ sites nano-ring before turning, in Sec. IV B to nano-rings with $N = 4, 8$
sites. The reason for this choice is that the low-energy physics of the $N=6$ sites ring is controlled by an energy scale $\Delta_0 = 2t$, associated to the gap in the non-interacting density of states, which makes the system behave more similarly to a correlated band insulator. On the other hand, the $N=4,8$ sites rings are both characterized by the presence of a 2-fold degenerate state at the Fermi energy, which induces a physical behavior similar to the one of a correlated metal.

A. $N=6$: "insulating" ring

In previous works, we analyzed by means of nano-DMFT the electronic and transport properties in a $N=6$ Hubbard nano-ring in the presence of hybridization with a substrate. In particular, it was shown that in the weak-hybridization regime, and in particular in the case of an isolated nanostructure considered here, non-local correlations beyond DMFT are not negligible and have an important effect on the electronic and transport properties of the system. In fact, local electronic correlations within DMFT shrink the gap with respect to the value predicted, e.g., within a Hückel picture, akin to what happens in bulk correlated band insulators. Instead, the numerically exact solution (obtained by means of Hirsch-Fye QMC simulations) shows that non-local correlations yield a wider spectral gap due to the effective renormalization of the hopping parameter by a non-negligible NN self-energy in real space. With increasing hybridization between the correlated sites and the substrate, non-local spatial correlations are gradually suppressed, while local correlations remain sizeable. We now extend the analysis done in previous works including non-local correlations via the parquet DΓA, which yields a qualitative and quantitative agreement with exact QMC simulations. We note that the DΓA results for the $N=6$ sites ring presented in this section, are expected to hold also for generic semiconducting nano structures in the weak- and intermediate-coupling regime, i.e., where the bare interaction $U$ is comparable with the size of the gap. We have tested this claim to hold for another gapped Hubbard ring with $N=10$ sites (not shown). In Fig. 3 we compare the local DMFT self-energy with the $k$-resolved self-energy for representative $k$ points in the discrete Brillouin zone (DBZ), namely $k=0$ and $k=\pi/3$, obtained by means of PA, DΓA and exact QMC solution. Concerning the imaginary part of the self-energy $\mathrm{Im}\Sigma(k,\nu_n)$, one can note that all the approximations employed provide a qualitative and quantitative agreement with the exact solution. The system displays a low scattering rate $\gamma(k)$, which is consistent with the picture of an insulating ground state reminiscent of the band gap of the non-interacting spectral function (renormalized by electronic correlations), rather than driven by a Mott MIT. More specifically, the exact QMC self-energy displays a weak $k$-dependence at low frequencies, resulting in a slightly different scattering rate $\gamma(k)$ for different $k$ points in the DBZ. While this feature cannot

![FIG. 3. (Color online) Comparison between the local DMFT self-energy in Matsubara representation and the $k$-resolved self-energy obtained within PA, parquet DΓA, and exact QMC solution, for representative $k$-points in the DBZ. Parameters: $N=6$, $U=2t$ and $T=0.1t$.](image)

![FIG. 4. (Color online) $k$-resolved ladder DΓA self-energy in Matsubara representation, obtained after performing the Moriyasque correction to the spin propagator, for representative $k$-points in the DBZ. Parameters: $N=6$, $U=2t$ and $T=0.1t$.](image)
be reproduced within DMFT by definition, it is well captured including non-local correlations beyond mean-field.

Concerning the real part of the self-energy, we observe that within DMFT \( \text{Re}\Sigma(\nu_n) = 0 \), i.e., all contributions averaging out in the local picture, except for the Hartree term, which is included in the redefinition of the chemical potential, i.e., \( \mu \to \mu - U/2 \) at half-filling. On the contrary, including non-local correlations beyond mean-field we find a sizeable \( k \)-dependent self-energy \( \text{Re}\Sigma(k,\nu_n) \).

In all cases the exact self-energy is quantitatively well reproduced. While the results are quite convincing, one may also note that the ladder DΓA self-energy, shown for comparison in Fig. 4 obtained by a resummation of the ladder diagrams in the magnetic (spin) channel, displays a slightly larger deviation from the exact solution with respect to the parquet-based DΓA. This observation suggests that, although at half-filling the physics is dominated by spin fluctuations, considering all the scattering channels on the same footing (and their interplay) leads to quantitative corrections, in this parameter regime.

Fig. 5 shows the effect of non-local correlations on the local Green’s function \( G_{ii}(\tau) \). In the case of the \( N = 6 \) sites ring, the interpretation of the results is straightforward. In fact, all methods predict an insulating solution, and this is reflected by \( G_{ii}(\beta/2) \approx 0 \) (which is a measure for the spectral weight in an energy interval \( \sim T \) around the chemical potential; it is exactly zero only in the limit \( T \to 0 \)). However, at a closer look one can notice that the DMFT predicts more spectral weight \( A(0) \) than the other methods, and even of the non-interacting case. This is clearly shown in the inset of Fig. 5 where we plot the difference \( \Delta G_{ii}(\tau) \) of the local Green’s function obtained in the non-interacting case, DMFT, and DΓA with respect to the one of the exact solution. This suggests different size of the spectral gap for the approximations considered. Hence, we can “disentangle” the roles played by local and non-local correlations on an insulator considering that: i) the inclusion of local correlations alone, within DMFT, reduces the non-interacting spectral gap \( \Delta_{\text{exact}} \), and ii) non-local correlations in the exact solution display the opposite trend, as correctly described by the DΓA. Indeed, the analytic continuation of the Green’s function by means of the maximum entropy method confirms the expectations, yielding a spectral gap \( \Delta \approx 1.9t \) within DMFT and \( \Delta \approx 2.2t \) within PA, DΓA and the exact solution, to be compared to the non-interacting value \( \Delta_0 = 2t \) (not shown).

We can understand the results obtained for both the self-energy and the local Green’s function within the different approximations, by taking a closer look at the local fully irreducible vertex calculated from the DMFT Green’s function. The isolines and the density plot in the left and right panels of Fig. 6, respectively, highlight the sign and the logarithmic intensity of the frequency structure of \( \Lambda_{d,m} \). The vertex displays the typical butterfly structure previously reported with positive and negative lobes and no features at high frequency. We see that the 2PI vertex corrections beyond the static asymptotics are quite small with respect to the bare interaction \( U \). This is due to the presence of a gap in the spectral function of the non-interacting system, resulting in an insulating Green’s functions already within DMFT. The inversion of sign at low frequencies in the first and third quarter of the \( (\nu,\nu') \) plane originates, instead, from the precursor lines of the Mott transition recently found in

\[ \beta \]

\[ \beta \]

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the DMFT phase diagram. The negligible frequency structure of the local 2PI vertex explains why the DΓA self-energy does not deviate from the plain PA result in this case. On the other hand, the quantitative agreement with the exact QMC solution, suggests that the local DΓA assumption of the 2PI is justified in this system. The direct numerical analysis of the exact 2PI vertex confirms that, besides a structure in momentum space, its overall values yield moderate corrections to the bare interaction $U = 2t$ (not shown).

B. $N=4$ and $N=8$: “correlated metallic” rings

In contrast to the previous system, both the $N=4$ and $N=8$ sites rings are characterized by the presence of a (doubly degenerate) eigenstate at the Fermi level of the non-interacting density of states. This suggests that they will display a similar behavior, and a different low-energy physics with respect to the $N=6$ sites ring. As we will show, this expectation is only partially true.

Let us start discussing the $k$-resolved self-energy of the $N=4$ ring, shown in Fig. 7 for representative $k$ points in the DBZ, namely $k = 0$ and $k = \pi/2$ (the latter at the Fermi surface). In this case the DMFT self-energy displays a non-Fermi liquid behavior, characterized by a large yet finite scattering rate $\gamma(k)$ (obviously independent on $k$). As we will see below, the system is not gapped in DMFT. The DMFT picture, however, is substantially changed by non-local correlations, as reflected in a strong $k$-dependent behavior of the self-energy, found within all approximations considered. In particular, away from the Fermi surface (e.g., at $k = 0$) all approximations yield a low scattering rate $\gamma(k = 0)$ due to the bending towards zero of $\Im \Sigma(k, \nu_n)$. The situation is drastically different at the Fermi surface (e.g., at $k = \pi/2$), where in the exact solution, the divergent tendency of the self-energy marks the opening of a gap in the spectral function. Taking into account all scattering channels within the parquet DΓA formalism leads to an improvement with respect to the DMFT results. While the PA yields a sizeable scattering rate $\gamma(k = \pi/2) \approx 0.4$, including the frequency dependence of the fully irreducible vertex within DΓA further enhances $\gamma(k = \pi/2)$ and reproduce correctly the qualitative trend of the exact self-energy, as well as an overall better description of the $\Re \Sigma(k, \nu_n)$ with respect to PA and DMFT. The quantitative difference between the parquet DΓA and the exact solution may originate either from the momentum dependence of the 2PI vertex, neglected in DΓA, or by the lack of self-consistency. Further insights can be obtained by considering the spin propagator $\chi^s(q)$, in particular at $\omega = 0$. Within DMFT, we find that $\chi^s(q = \pi) < 0$. The unphysical value of the susceptibility indicates that the system is below the Néel temperature of DMFT, i.e., $T < T_N^{DMFT}$, while no ordering is expected at finite temperature. Including non-local spatial correlations within the parquet DΓA scheme reduces $T_N$. However, it is plausible that the local physics described by DMFT, and hence the information encoded into the 2PI vertex of DMFT, can be very different from the local physics of the exact solution. A different result is found within the ladder DΓA. In particular, the large $\gamma(k = \pi/2)$ at the Fermi surface is well captured by the ladder DΓA self-energy, shown in Fig. 8, where the ladder resummation is performed in the spin

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FIG. 7. (Color online) As in Fig. 4 but for the $N=4$ ring.

FIG. 8. (Color online) As in Fig. 4 but for the $N=4$ ring.
channel, associated to the predominant fluctuations at half-filling. In this case, the Moriyasque correction can mimic the self-consistency of the local vertex.\textsuperscript{34,42,43}

It is interesting to discuss the effect of local and non-local correlations on the Green’s function (as we did for the $N=6$ sites ring). In general, the small, not vanishing values of $G_{ii}(\beta/2)$ suggest a metallic spectral function for DMFT, PA, and DΓA, in contrast to the exact solution. However, the corresponding self-energy on the Fermi surface in Fig. 7 displays a non-Fermi liquid behavior, with a large scattering rate $\gamma(k)$. This should indeed correspond to a local minimum in the spectral function at the Fermi level (pseudo gap). Hence, we have shown that the DΓA, in its full implementation, yields a qualitative improvement of the self-energy results with respect to the other approximations considered. This is reflected in a higher reduction of the low-energy spectral weight within DΓA with respect to the other schemes. The agreement of the DΓA with the numerically exact solution is, however, not perfect: The non-local correlations stemming from the 2PI local vertex of DMFT are not yet strong enough to completely open a well-defined gap in the spectral function, which is instead present in the exact solution.

A deeper understanding of the above results can be obtained by the analysis of the frequency and momentum structure of the 2PI vertex. Let us first discuss the local 2PI vertex, shown in Fig. 10. The most striking feature of the vertex of the $N=4$ sites ring is the strongly enhanced low-frequency structure which now exhibits strong deviations from the bare interaction $U=2t$. In fact, the vertex corrections are orders of magnitude larger than for the $N=6$ insulating ring, and the low-frequency structure is also more complex. In particular, one can observe additional negative "spots" (of highest intensity) which are generated by the change of sign of several eigenvalues of the generalized local susceptibility.\textsuperscript{30,31,37} This low-frequency structure of the local 2PI vertex is responsible for a $k$-selective enhancement of the DFA self-energy over the one obtained within the PA. The direct numerical evaluation of the exact 2PI vertex indicates that it also displays a strong momentum dependence. According to our numerical data for the $N=4$ sites ring, the exact 2PI vertex $\Lambda_{2PI}$ is strongly enhanced, for $\omega=0$ and $q=0$, close to the Fermi surface, i.e., at low-frequencies and at the Fermi momenta ($k=k'=\pm\pi/2$), while it becomes much smoother away from the Fermi surface (not shown). Such a large frequency and momentum dependence of the exact 2PI vertex can be possibly interpreted in terms of a proximity to a non-perturbative instability of the Bethe-Salpeter equations, such as those already reported for the Hubbard and Falikov-Kimball models.\textsuperscript{30,31,37} A momentum dependence of the 2PI is certainly to be expected in low-dimensional systems. However, it is important to notice that the exact results for the $N=4$ sites ring are already well approximated by the ladder DΓA with Moriya correction. This suggests that it is not the momentum structure of the 2PI to control the (large) self-energy, but rather the enhanced scattering induced by a strongly renormalized local vertex. Hence, it is likely that similar results can also be obtained within a fully self-consistent parquet DΓA scheme, where the local vertex will be further enhanced with respect to DMFT by non-local correlations.

We finally discuss the results for the $N=8$ sites ring, where the presence of additional structure in the non-interacting density of states, besides the (doubly degenerate) eigenstate at the Fermi level and the one at the band edge lead to a somewhat different physical situation. Let us start discussing the $k$-resolved self-energy shown in Fig. 11. As $N$ increases, the number of inequivalent $k$ points in the DBZ increases with respect to the previous cases. By symmetry it is sufficient to consider $k=0$, $k=\pi/4$, and $k=\pi/2$ (the latter at the Fermi surface). In this case, in contrast to the $N=4$ sites ring, the DMFT self-energy shows a metallic bending, with a scattering rate $\gamma(k)\approx0.1$, independent on $k$. The comparison

FIG. 10. (Color online) As in Fig. 6 but for the $N=4$ ring.

FIG. 9. (Color online) As in Fig. 5 but for the $N=4$ sites ring.
with the exact solution shows that the largest corrections with respect to DMFT are the enhanced scattering rate at the Fermi surface, $\gamma(k = \pi/2)$, and the renormalization of the dispersion $\Delta(k = 0, \pi/4) = \text{Re}\Sigma(k, \nu_n \rightarrow 0)$. The PA and the DΓA give rise to similar non-local correlations, displaying a strong $k$-dependent scattering rate, $\gamma(k = \pi/2) \approx 0.3$, respectively. The large scattering rate reflects physically in the Green’s function through a suppression of $G_{ii}(\tau)$, and hence of the low-energy spectral weight, with respect to DMFT, as shown in Fig. 13. Although DΓA provides an overall better description of the low-energy physics of the system with respect to DMFT, also in this case the parquet-based approximations fail to reproduce the divergent behavior of $\text{Im}\Sigma(k = \pi/2, \nu_n)$. On the other hand, the Moriya corrected ladder approximation, shown in Fig. 12, seems able to better capture the low-energy physics and in particular the non-Fermi liquid trend of the exact self-energy. This could again indicate a significant renormalization of the local 2PI vertex with respect to the one of DMFT.

As for the interpretation of the results, from the similarity of the PA and DΓA results for the $N=8$ sites ring one would not expect a strong frequency dependence of the local 2PI vertex, as confirmed from the numerical data shown in Fig. 14. The 2PI vertex qualitatively resembles the one of the $N=6$ sites ring, with the difference that there is no suppression of the low-frequency structure. On the other hand, the difference between DΓA and
the exact solution might suggest an important momentum structure of the 2PI vertex. Unfortunately in this case a direct analysis is not feasible, due to the extremely high computational effort required to calculate the exact momentum-dependent two-particle vertex functions for the $N = 8$ site ring. While a strong momentum dependence of the exact 2PI vertex is possible, also in this case the deviation observed between the parquet DΓA and the exact solution might be induced by the poor approximation of the local physics of the system provided by the 2PI vertex of DMFT. This scenario, supported by the qualitatively correct behavior found within the Moriya corrected ladder approximation, suggests that the parquet DΓA results might be further performing a fully self-consistent calculation.

V. SUMMARY AND CONCLUSIONS

In this paper we have presented a numerical study of correlated Hubbard nano-rings, employing the DΓA algorithm, which we implemented in its parquet-based version. This algorithm corresponds to the actual realization of the original DΓA idea, in which the local (DMFT) assumption is made only at the level of the 2PI local vertex of the theory, while non-local correlations beyond DMFT are computed simultaneously in all channels by solving the corresponding parquet equations, as opposed to the ladder DΓA algorithms used hitherto, where additional approximations (e.g., restriction to a given subset of ladder diagrams) were performed. The direct solution of the parquet equations makes it possible to determine the dominant instability in the presence of competing orders, and to address the interplay between different channels. The overall numerical effort of a full DΓA calculation is clearly larger than in the case of ladder-approximations, but the numerical workload is still manageable in 1D and 2D. Specifically, we have shown results of the DΓA in its full implementation for correlated Hubbard rings of different sizes $N = 4, 6, 8$, and compared them with the corresponding ones of DMFT, ladder DΓA, plain PA, and numerically exact QMC solutions of the problem. This way we could achieve a twofold goal: On the methodological side, we could test the accuracy of the DΓA approximation for 1D systems, the arguably most challenging regime for the locality assumption of the 2PI vertex. On the physical side, we could understand the different roles played by local and non-local correlations in determining the spectral properties of systems.

Our calculations show how, in the case of $N = 6$ nanorings, the DΓA reproduces essentially the exact results, improving over the corresponding local description of DMFT. This is ascribed to the presence of a spectral gap already in the non-interacting density of states resulting in strongly damped correlation effects at the level of the 2PI vertex, which essentially reduces to the local bare interaction $U$. Hence, the DΓA, and even the parquet approximation, yield “de facto” the exact many-body solution for these systems, as one can actually see by comparing the self-energy and the Green’s function. Minor deviations from the exact solution are obtained within the ladder DΓA, which has to be expected when the physics is not dominated by fluctuation in a specific scattering channel. This scenario should be also applicable to generic semiconducting nanostructures, if the Hubbard interaction is not much larger than the spectral gap.

The situation changes when considering Hubbard rings with $N = 4$ and $N = 8$ correlated sites, where the non-interacting energy spectrum displays a doubly degenerate state at the Fermi level. Correspondingly the 2PI vertex strongly deviates from $U$ already at the local level of DMFT, inducing deviations between a plain PA and a parquet DΓA calculation. The comparison of our numerical data shows that in these cases the agreement of the parquet DΓA with the exact solution is not perfect, though it yields always an improvement over DMFT and plain PA. Deviations of DΓA from the exact results are certainly not surprising for these 1D systems, and the analysis of their origin allows us to understand more profoundly how correlations of different type determine the physics. The deviations between the DΓA and the exact solution has two possible origins: (i) a significant momentum dependence of the 2PI vertex, and (ii) a poor description of the local physics encoded in the 2PI vertex of DMFT. In the latter case, one could expect the results to improve by performing a fully self-consistent DΓA calculation, which is, however, beyond the scope of this work.

In conclusion, we have shown how the parquet DΓA algorithm can be implemented and applied with success to analyze the physics of correlated Hubbard nano-rings. Exploiting the recent improvements in the calculation of the local vertex of DMFT and in the numerical solution of the parquet equations, we obtain results, which are obtained in one of the most difficult regimes for the DΓA, pave the path for a more accurate theoretical treatment of strongly correlated electron systems.

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Due to the particle-hole symmetry and to the degeneracy of the non-interacting eigenstates, the other components of the $k$-resolved self-energy can display, at most, a sign change with respect to the ones shown here.

We recall that a $n$-particle Feynman diagram is defined fully (or "$n$-particle") irreducible if it cannot be split in two by cutting $n$ fermionic (Green’s function) lines. At the one-particle level, this corresponds to $\Sigma$, at the two-particle level to the fully 2PI vertex function. For more details and explicit diagrammatic expression see Refs. 36 and 44, whose notation is adopted in the following.

According to the notation of Ref. 36, we recall that in the SU(2) symmetric case the particle-hole density and magnetic channels are given by the symmetric and antisymmetric combination of the vertexes of the up-up and up-down spin sectors, respectively, i.e., $\Lambda^{\nu\nu'\nu'\nu}_{\omega m} = \Lambda^{\nu\nu'\nu'\nu}_{\omega m} \pm \Lambda^{\nu\nu'\nu'\nu}_{\omega m}$.

As for the frequency dependence of the 2PI vertex, we recall that in the case of a time-independent interaction all two-particle vertex functions depend on two fermionic Matsubara ($\nu, \nu'$) frequencies of the incoming particles and on the bosonic transfer frequency ($\omega$) of the scattering process. For further details see Ref. 36.

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