

Impurities and other defects in correlated lattice electrons: Friedel oscillations and interference patterns

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We study interference patterns and Friedel oscillations (FO) due to scattering from two or more localized impurities and scattering from extended inhomogeneities in the two-dimensional lattice systems of interacting fermions. Correlations between particles are accounted for by using an approximate method based on the real-space dynamical mean-field theory and a homogeneous self-energy approximation (HSEA), where the site-dependent part of the self-energy is neglected. We find that the interference maxima and minima change systematically as we vary the relative distance between the two impurities. At the same time, the increase of the interaction does not shift the position of interference fringes but only reduces their intensities. A comparison with the single impurity cases clearly shows complex patterns in FO fringes induced by additional multiple scattering processes. In the case of an extended steplike potential the system becomes more homogeneous when the interaction increases. FO and interference patterns are not present in the Mott insulating phase in both single and many impurity models.

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I. INTRODUCTION

The presence of an external inhomogeneous potential or localized defects in metallic systems modulates the electronic charge density around these lattice imperfections due to scatterings of the electrons near the Fermi surface. These charge density oscillations are known as the Friedel oscillations (FO) and are mostly visible at low temperatures [1–3]. FO occur in real materials due to the presence of adatoms, interstitial defects, or surface irregularities after cleavage. The studies of FO can be significant for a wide range of systems as we discussed in [4–6]. To mention a few, FO have been observed experimentally in quantum corals, metal surfaces like Cu(111), semiconductor surfaces like GaAs(111) around point defects using scanning tunneling microscopy (STM) at around 4–5 K [7–10]. FO have been seen to produce an asymmetry in the quantum transport at the interface of monolayer and bilayer graphene, which can be used as an application in novel quantum switching devices [11]. It has been demonstrated that the FO, due to the topological defects in the carbon nanotubes, are important for understanding properties like selective dot growth, magnetic interaction through carbon nanotubes and optical spectroscopy of interface states using the tight-binding model [12]. Kolesnychenko *et al.* observed, using a scanning tunneling microscopy (STM), anisotropic FO while studying the surface electronic structure of transition metal Cr(001) produced by the cleavage of a single crystal having surface areas where impurity concentrations slightly

exceeded the bulk concentration due to the existence of a high dopant zone in the crystal [13].

In order to understand theoretically the FO in Cr or other transition metals, which belongs to the class of correlated electronic systems, it is important to consider the Coulomb interaction between the electrons. FO have been studied in one-dimensional (1d) interacting fermions using several theories, e.g., the bosonization method or the density-matrix renormalization group [14,15], and the Bethe-Ansatz local-density approximation [16]. The Fermi liquid theory for two-dimensional (2d) and three-dimensional (3d) systems [17] was applied to investigate FO. The FO induced by nonmagnetic impurities in 2d Hubbard model in the presence of interactions have been studied using the slave-boson technique, which involves the static renormalization of the impurity potential [18]. FO seen around the Kondo screening cloud in the presence of magnetic impurities using the *t*-matrix formalism have been reported in [19].

The dynamical mean-field theory (DMFT) is considered an advanced and suitable technique to capture the effects of correlations, particularly around the Mott metal to insulator transition, which is significant for describing the compounds with partially filled *d* and *f* shells, e.g., transition metals and their oxides [20–25]. A real space extension of DMFT (R-DMFT) is needed to treat strongly correlated inhomogeneous systems [26–29].

In our previous work we investigated the behavior of FO in models of correlated lattice systems in the metallic and Mott insulating phases in the presence of a single impurity potential using the R-DMFT [4,6]. We reported that the oscillations get

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damped with increasing the interaction, and disappear at the Mott transition and beyond it in the Mott insulating phase.

In reality, a single-site impurity potential could be a too idealized model when we deal with inhomogeneities on surfaces of true materials. There are usually more than one defect or contamination. One even encounters extended inhomogeneities and interface effects in multilayered nanostructures, for example as discussed in Ref. [30]. Grosu *et al.* studied the problem of FO in a 1d noninteracting electron gas in the presence of two impurities, modeled by a double delta function separated by a finite distance, using a linear response theory [31]. They showed that the presence of the second impurity significantly changes the density oscillations (changing the positions of the maxima and minima) depending on the distance between the impurities. The studies of two-impurity scattering have been further extended to a 1d interacting fermionic system using the bosonization method in [32]. The scattering and quasiparticle interference from two and multiple magnetic impurities adsorbed on 2d and 3d interacting hosts have been probed using the *t*-matrix formalism and the numerical renormalization group [33,34]. However, in these studies the interference effects are discussed in the local density of states in the presence of interactions and not in the particle density oscillations.

We thus see that the studies of FO in the presence of two or multiple impurities have been conducted mostly for 1d interacting systems, while an attempt to understand real materials requires models in two and higher dimensions. Moreover, the behavior of FO in the Mott insulating regime for models with many imperfections has not been addressed. Also the current state of knowledge lacks any quantitative treatment of the screening and interference effects in systems with interparticle interactions.

A proper description of FO in real materials with strong electronic correlations demands a realistic modeling combining the density functional theory within the local density approximation and DMFT (LDA+DMFT) [35,36] and its extension in real space. Such techniques are computationally nontrivial in the presence of inhomogeneities, particularly if it is not just an adatom but an impurity atom embedded in the host, e.g., Cr atom in a Pb surface [37]. The translational invariance of the lattice is broken in such a case.

Motivated by this state of art we extend our earlier study [6] by adding to the simple one-band Hubbard model various types of impurity potentials and inhomogeneities. The correlations are treated by using an approximate self-energy based on DMFT where the site-dependent part of the self-energy is neglected. We name this approximation the homogeneous self-energy approximation (HSEA) and discuss it in Sec. II. We investigate both noninteracting and interacting two-dimensional finite lattice systems.

In this paper we address the following questions: (a) How do the FO change due to the interference effects when we introduce the second impurity? (b) How does the interference change when we vary the distance between the impurities and switch on the interaction? (c) How does the whole picture change if we generalize the two impurities to multiple impurities scattered over the lattice or the extended inhomogeneity? (d) Do we see any interference effect or FO for any of these models of impurity potential in the Mott insulating phase?

Our investigation shows that the interaction reduces the interference pattern in FO and the impurity screening. However, the interaction does not alter the position of the interference maxima and minima for the particle-hole symmetric case.

The paper is organized as follows. In Sec. II we discuss lattice models and methods used to solve them. We introduce there physical quantities describing physical properties of these systems. Afterwards in Sec. III we present our numerical results for (a) two impurities, (b) multiple impurities, (c) a chain of impurities or a domain wall, and (d) extended inhomogeneity. Finally, in Sec. IV we conclude our results and provide an outlook.

II. MODELS AND FORMALISM

A. Models

We consider the one-band Hubbard model [38–40] with an external inhomogeneous potential

$$H = \sum_{ij,\sigma} t_{ij} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \sum_{i\sigma} V_{i\sigma} \hat{a}_{i\sigma}^\dagger \hat{a}_{i\sigma} + U \sum_i \hat{n}_{i\downarrow} \hat{n}_{i\uparrow}, \quad (1)$$

where $\hat{a}_{i\sigma}$ ($\hat{a}_{i\sigma}^\dagger$) is the annihilation (creation) fermionic operator with spin σ on the *i*th lattice site, and t_{ij} is the hopping matrix element between the *i*th and *j*th sites with $t_{ii} = 0$. The second term describes the external (inhomogeneous) potential given by $V_{i\sigma}$, which is assumed to be real. The third term models the local part of the electronic interaction between two fermions with opposite spins located on the same lattice site.

We consider a two-dimensional square lattice with the number of lattice sites $N_L = 31^2$ (the size of the lattice is 31×31) and the following models of the external (inhomogeneous) spin independent potential:

(i) Two single-site impurities placed either along the diagonal direction of the lattice or along a vertical direction of the lattice for different relative distances. Mathematically, $V_i = V_{01} \delta_{ii_{01}} + V_{02} \delta_{ii_{02}}$.

(ii) A more general case where several impurities are irregularly distributed over various lattice sites. This aims to model a contaminated surface with various dopant zones or interstitial defects. Mathematically, $V_i = V_{01} \delta_{ii_{01}} + V_{02} \delta_{ii_{02}} + V_{03} \delta_{ii_{03}} + \dots$.

(iii) A chain of impurities placed along the diagonal and vertical directions of the lattice aimed to model a domain wall or an interface. In freshly cleaved samples such domain walls can be found connecting large lattice inhomogeneities and can be observed experimentally using STM.

(iv) A steplike potential or extended inhomogeneity across the lattice aimed to describe inhomogeneous surface irregularities after a cleavage. Mathematically, $V_{i\sigma} = V_0 \Theta(X_i - X_0)$, where X_0 is the horizontal lattice coordinate where the steplike potential begins [i.e., the Heaviside function $\Theta(x)$ is nonzero].

B. Method

All single-particle properties of the system are obtained from the retarded Green's function obtained by inverting the matrix Dyson equation [41] in the lattice position space:

$$\mathbf{G}(z) = [(z + \mu)\mathbf{I} - \mathbf{t} - \mathbf{V} - \Sigma(z)\mathbf{I}]^{-1}, \quad (2)$$

where $z = \omega + i0^+$ is the energy approaching the real axis from above and μ is the chemical potential ($\hbar = 1$). $\Sigma(z)$

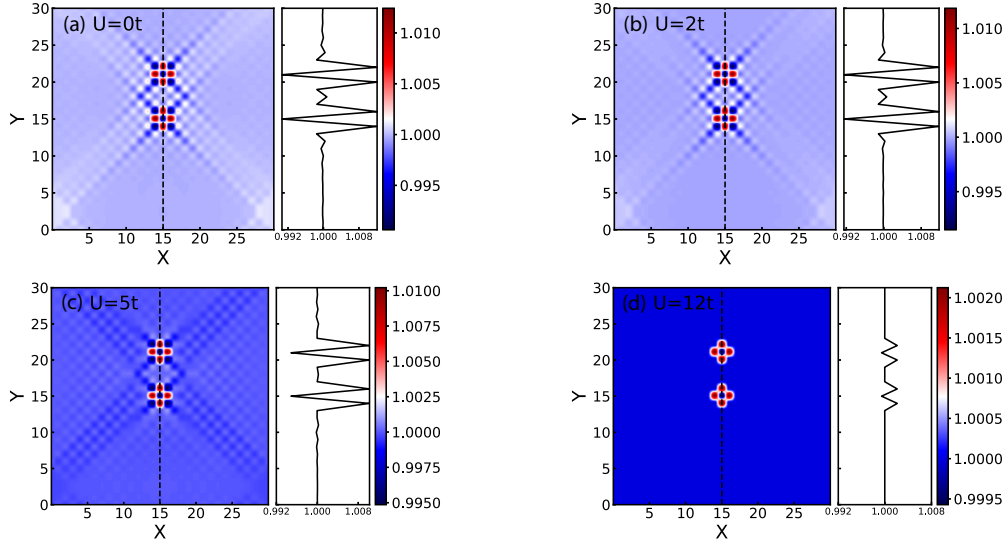


FIG. 1. Friedel oscillations (FO) in particle densities (\bar{n}_i) due to two impurities of equal magnitude, i.e., $V_{01} = V_{02} = 24t$, placed at $\vec{R}_{01} = (15a, 15a)$ and $\vec{R}_{02} = (15a, 22a)$, respectively, along the vertical axis of the (31×31) square lattice. We show the change in interference pattern of FO due to scattering from the two impurities for (a) $U = 0t$, (b) $U = 2t$, (c) $U = 5t$, and (d) $U = 12t$. The insets (on the right) show oscillations along the vertical line passing through the impurities. The color scale is spanned in between the highest and the lowest values of the density in the system. The color scale changes for different U since the minimal value of the density increases with it. We do not show the actual densities on the impurity sites, which are substituted by the second lowest values in the plots. Otherwise the impurity contribution would overshadow any contributions in \bar{n}_i .

is the site independent homogeneous part of the self-energy which approximates the effect of correlations and is calculated using the DMFT for the same parameters of the corresponding homogeneous Hubbard Hamiltonian. Hereafter, all matrices are expressed in bold faced notation. The nondiagonal matrix \mathbf{t} corresponds to the hopping amplitudes t_{ij} and the diagonal matrix \mathbf{V} reflects the on-site inhomogeneous potential V_i . The unity matrix is written as $\mathbf{1}$.

In the DMFT the self-energy is diagonal in lattice site indices and accounts for all local dynamic correlation effects. In case of homogeneous lattice systems, all lattice sites are equivalent. In this case, the self-energy is computed by mapping a lattice site into an effective single impurity Anderson model (SIAM) and solving it by using standard techniques like continuous time quantum Monte Carlo, an exact diagonalization, a numerical renormalization group method (NRG), etc. However, in the presence of external impurities, translational invariance of the lattice is broken and the lattice sites are nonequivalent. Hence, it is essential now to solve the SIAM separately at each lattice site and the local self-energy becomes explicitly site dependent. In other words, in an inhomogeneous system the self-energy has a homogeneous part due to the electron-electron interactions and an inhomogeneous part due to the contribution from the interaction and the external impurities. Owing to the site dependent part of the self-energy, the result of the impurity potential in the system is not static but effectively dynamic [5]. Ideally, in order to get the full picture of a correlated inhomogeneous system we should consider both the homogeneous and inhomogeneous parts of the self-energy solving the full real-space DMFT (R-DMFT) equations self-consistently [5].

Unfortunately, deciphering the full R-DMFT equations is computationally exhaustive, especially for higher-

dimensional systems with a large number of lattice sites. Hence, as a first approximation we omit the inclusion of the inhomogeneous, site-dependent part of the self-energy in our present studies to obtain some initial insights on the behavior of the system with correlations. We call this approximation

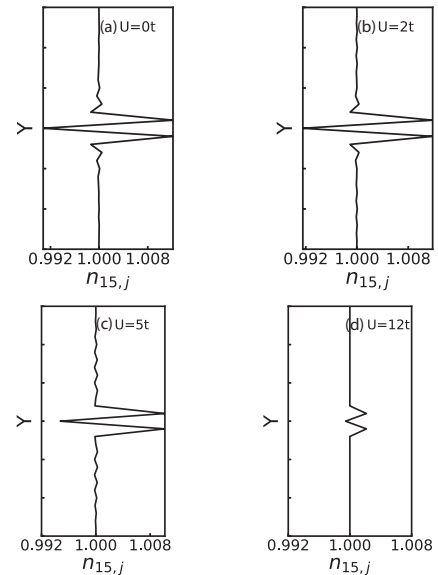


FIG. 2. FO in particle densities (\bar{n}_i) in the square lattice in the presence of a single impurity $V_0 = 24t$ in the center [$\vec{R}_0 = (15a, 15a)$]. All other model parameters and plotting style is the same as in Fig. 1. We show (a) $U = 0t$, (b) $U = 2t$, (c) $U = 5t$, and (d) $U = 12t$. We only show the vertical line passing through sites containing the impurity for a comparison with Fig. 1. A complete density profile for the single impurity case is available in [6].

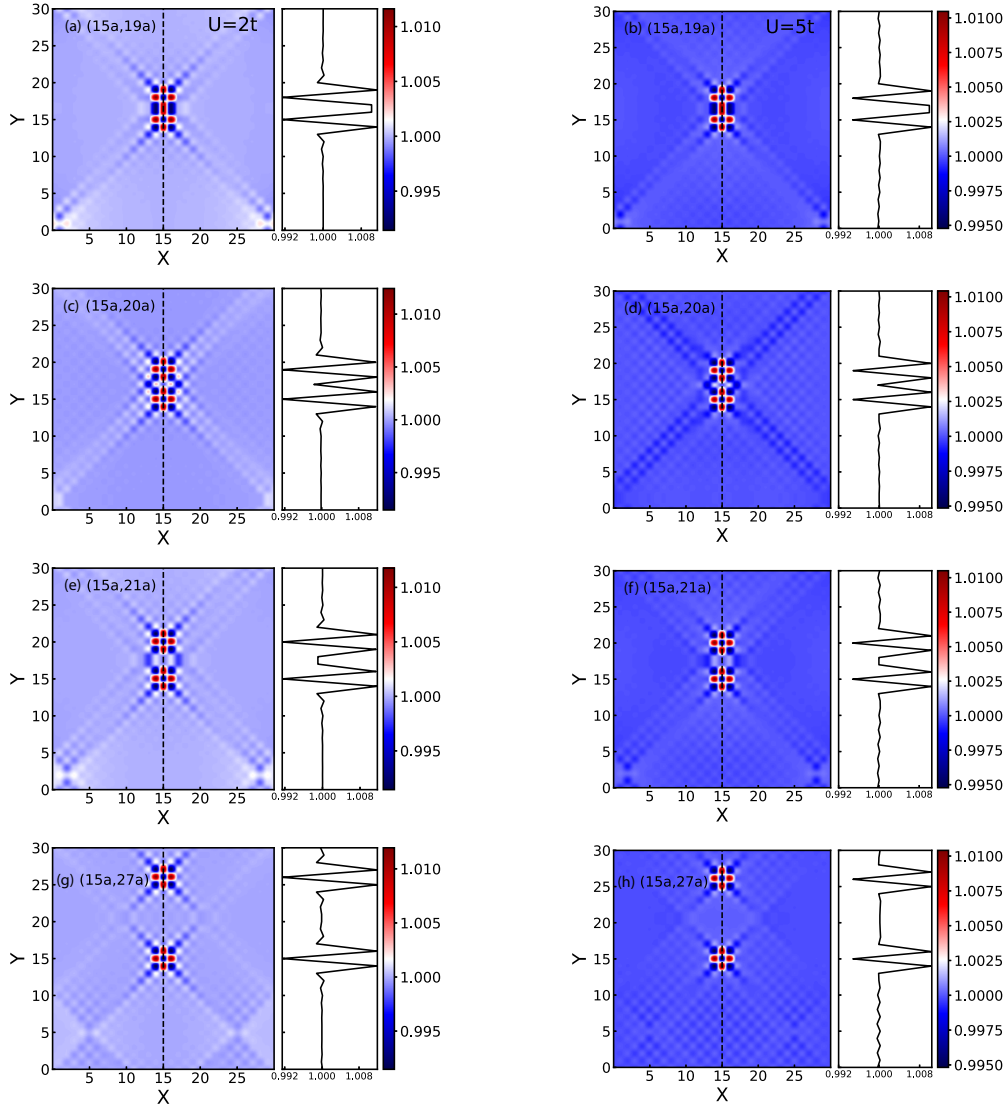


FIG. 3. The variation in the interference patterns in the FO of particle densities (\bar{n}_i) for different relative distances between the two impurities of equal magnitude $V_{01} = V_{02} = 24t$. The first impurity V_{01} is kept fixed at $\vec{R}_{01} = (15a, 15a)$ and the position of the second impurity is shifted along the vertical line and placed at $\vec{R}_{02} = (15a, 19a)$, $\vec{R}_{02} = (15a, 20a)$, $\vec{R}_{02} = (15a, 21a)$, $\vec{R}_{02} = (15a, 27a)$ (from top to bottom, respectively). We show the interactions $U = 2t$ (a,c,e,g) and $U = 5t$ (b,d,f,h). All other model parameters and the plotting style are the same as in Fig. 1.

the homogeneous self-energy approximation [6]. The homogeneous part of the self-energy is computed by solving the DMFT self-consistency equations for infinite homogeneous system at zero temperature and half filling (particle-hole symmetric case) by using the NRG method [42]. This essentially implies setting the parameter $V_{i\sigma} = 0$ in Eq. (1). The open-source code “NRG Ljubljana” [43,44] is used for this purpose. The computed self-energy (the HSEA) is then transferred to the real space Dyson equation (2) containing the impurity potential $V_{i\sigma} \neq 0$ and used to obtain the one-particle Green’s function. We note here that although the self-energies are computed for a homogeneous system, the Green’s function is still obtained by inverting the Dyson equation containing the impurity potential in the real space and thus inhomogeneity of the system is taken into account.

A detailed discussion of the R-DMFT and HSEA is presented in [6], wherein we also show that the results obtained

from these two methods qualitatively agree for a single impurity potential. It might be an interesting future project to compare the results obtained from the full R-DMFT and from the HSEA for our models of the multiple impurity potentials. However, we do not expect significant changes because even in the metallic regime the FO decay quickly in space with a power law. We also observe that a possible change in the density of particles due to a change of the self-energy by inhomogeneous potential is a higher order effect beyond the linear response regime.

C. Physical quantities

Once we know the Green’s function of the system from Eqs. (1) and (2) we obtain the local spectral function as

$$A_{i\sigma}(\omega) = -\frac{1}{\pi} \text{Im} G_{i\sigma}(\omega). \quad (3)$$

Having (3) we compute the spin resolved local density of particles at zero temperature as

$$\bar{n}_{i\sigma} = \int_{-\infty}^{E_F} A_{i\sigma}(\omega) f(\omega) d\omega. \quad (4)$$

We consider spin rotational invariant systems, i.e., $\bar{n}_{i\uparrow} = \bar{n}_{i\downarrow}$, and the total number of particles per site is given by

$$\bar{n} = \frac{1}{N_L} \sum_{i=1}^{N_L} \bar{n}_i, \quad (5)$$

where $\bar{n}_i = n_{i\uparrow} + n_{i\downarrow}$. Equation (4) is the most relevant for our studies of FO.

We further quantify the screening and interference effects in the system by the screening charge defined by

$$Z = \sum_{i\sigma} \left(\bar{n}_{i\sigma} - \frac{\bar{n}_{\text{hom}}}{2} \right), \quad (6)$$

where the summation runs over all the lattice sites and \bar{n}_{hom} corresponds to the density of particles of the reference homogeneous system (i.e., with $V_i = 0$).

III. NUMERICAL RESULTS

We choose the chemical potential $\mu = U/2$ such that the homogeneous system is at half filling, i.e., $\bar{n} = 1$. In all cases the hopping amplitude $t_{ij} = t$ is only between nearest neighbors. We set $t = 1$ to define the energy units and set the lattice constant $a = 1$ to define the length units in our numerical calculations. The band-width W of the system is given by $W = 2zt$, where z is the coordination number. The system is subjected to the periodic boundary conditions with a finite number of the lattice sites N_L . We perform our simulations at zero temperature ($T = 0$).

The strength of electronic correlation is controlled by tuning the parameter U . We study the 2d homogeneous system for different U values and see that the Mott transition occurs at $U_c \approx 11.5t$. Hence, we choose $U = 0t, 2t, 5t$, and $12t$ values to represent a noninteracting lattice gas, a weakly interacting metallic phase, an intermediate interacting metallic phase, and a Mott insulating phase of the inhomogeneous system, respectively.

A. Two impurities

We start with the case where two impurities are present in the system. In Fig. 1 we show the interference patterns in FO due to two impurities of equal magnitude $V_{01} = V_{02} = 24t$ placed in the lattice sites $(15a, 15a)$ and $(15a, 22a)$ along the vertical direction of the square lattice for the noninteracting system and the interacting system with $U = 2t, 5t$, and $12t$. We further compare with the case where only a single impurity is present in the system in Fig. 2. On comparing Figs. 1 and 2, the interference effect induced by the second impurity is visible. We see that within the HSEA the interaction does not change the position of the interference maxima and minima but reduces their heights and intensities as seen in $U = 2t$ and $5t$ cases. This is analogous to the damping of FO with the interactions in the single impurity case. Such behavior is attributed to the particle-hole symmetry in the system. The na-

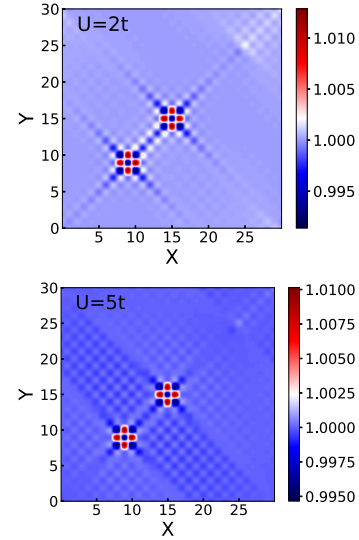


FIG. 4. Friedel oscillations (FO) in particle densities (\bar{n}_i) in the presence of two impurities of equal magnitude, i.e., $V_{01} = V_{02} = 24t$, placed at $\vec{R}_{01} = (9a, 9a)$ and $\vec{R}_{02} = (15a, 15a)$, respectively, along the diagonal direction of the square lattice. The interactions $U = 2t$ (upper panel) and $U = 5t$ (lower panel). The model, all other parameters, and the plotting style are the same as in Fig. 1.

tures of the noninteracting system and the weakly interacting one with $U = 2t$ are very similar. No interference effects and FO are visible in the Mott insulating phase at $U = 12t$. The disappearance of the FO in the Mott insulating phase is due to a gap opening around the Fermi level, and the Fermi edge cutoff, responsible for oscillatory behavior, is absent.

In order to investigate how the interference maximum and minimum changes as we vary the relative distance between the impurities, in Fig. 3 we fix the position of the first impurity at $(15a, 15a)$ and vary the position of the second impurity to $(15a, 19a)$, $(15a, 20a)$, $(15a, 21a)$, and $(15a, 27a)$. We show only the cases for $U = 2t$ and $5t$ since the behavior of the noninteracting system is very similar to the $U = 2t$ one and no interference effects were seen in the system with $U = 12t$. We see the occurrence of a minimum for $(15a, 19a)$ and a maximum for $(15a, 20a)$. Beyond a certain crossover distance, e.g., for $(15a, 27a)$, the interference effects are negligible and the inhomogeneities behave independently as in the diluted impurity regime. Again, on comparing the cases $U = 2t$ and $U = 5t$ we see that the interaction does not change the positions of the maximum and minimum but reduces their height. In other words, we conclude that the interaction reduces the interference effects.

We now place two impurities of equal magnitude $V_{01} = V_{02} = 24t$ along the diagonal direction of the lattice at sites $(10a, 10a)$ and $(15a, 15a)$ and show the cases for $U = 2t$ and $U = 5t$ in Fig. 4. Comparing Figs. 4 and 3, we already see that the interference patterns are qualitatively different when the impurities are placed along the diagonal. Particularly, for $U = 5t$ alternate regions of high and low density along the diagonal of the lattice are clearly visible. The interference pattern in the interstitial region between the two impurities is the most dominant. No FO or scattering interference effects are visible for $U = 12t$.

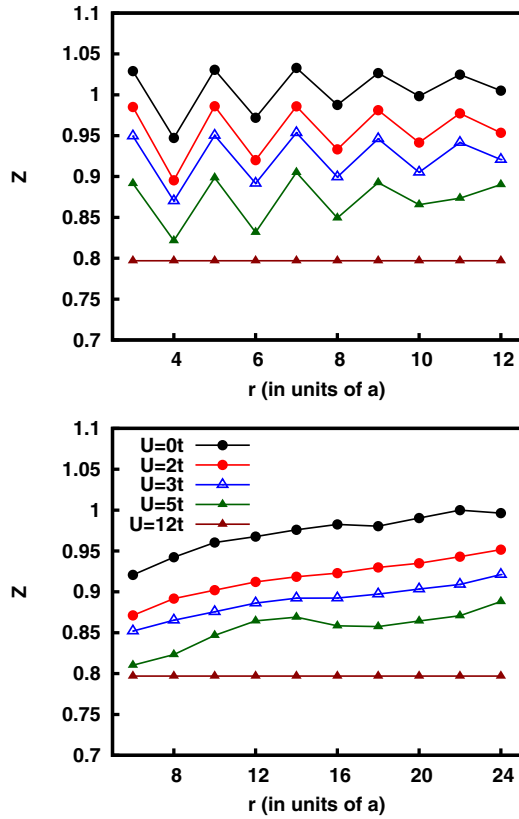


FIG. 5. Variation of the screening charge defined by Eq. (6) with relative (Manhattan) distance between the impurities ($V_{01} = V_{02} = 24t$). The impurities are placed in the vertical (diagonal) directions in the upper (lower) panel. Different values of the parameter U correspond to different interactions. We show $U = 0t, 2t, 5t$, and $12t$. The legend for the plot in the upper panel (not shown) is same as that of the lower panel.

In order to get a quantitative description of the interference effects with the relative distance between the impurities we study the dependence of the screening charge as defined by Eq. (6) for different positions of the second impurity, i.e., when placed along the vertical or along diagonal directions as shown in Fig. 5 (top and bottom panels) respectively. When the two impurities are placed along the vertical line, an oscillatory behavior is seen in the screening charge, i.e., maxima (minima) appear when the impurities are separated by an odd (even) number of lattice sites both for the noninteracting and interacting systems. The screening charge does not change with distance and reaches its constant residual value in the Mott phase ($U = 12t$), again confirming the absence of any FO or interference effects in this regime.

The oscillatory behavior in screening charge with the distance is absent when the impurities are placed along the diagonal direction as seen in Fig. 5 (bottom panel). Along the diagonal direction the Manhattan distance between the two sites is always even and, hence, there are always interference minima in the FO. If one compares the evolution of Z for even lattice spacings in the upper panel with the same ones in the lower panel, they almost match perfectly. The screening charge reaches the same constant residual value for $U = 12t$ as in the case when the impurities are placed along the vertical

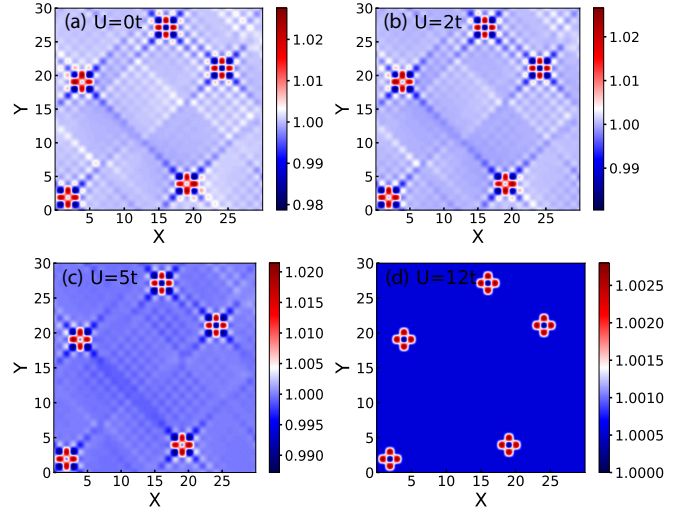


FIG. 6. FO in particle densities (\bar{n}_i) in the presence of five impurities each of magnitude $V_1 = V_2 = V_3 = V_4 = V_5 = 10t$ distributed on the lattice sites located at $\vec{R} = (3a, 3a), (20a, 5a), (5a, 20a), (25a, 22a),$ and $(17a, 28a)$ of the square lattice. We show the interference in FO due to the impurities for (a) a noninteracting system ($U = 0t$) and the systems with the interactions (b) $U = 2t$, (c) $U = 5t$, and (d) $U = 12t$. All other model parameters and the plotting style are the same as in Fig. 1.

direction. In both cases, at any given distance the screening charge is reduced with increasing interactions, which is in agreement with the case when only a single impurity is present in the system [6].

B. Multiple impurities

We now move to a more complex case where we extend our studies to several impurities randomly distributed over the surface. This aims to model a contaminated surface of a transition metal in the presence of dopant/defects, e.g., the Cr 001 surface in [13]. We use the square lattice also to predict the behavior on the surfaces of 3d systems, exploiting the fact that lower dimensions can also mimic the higher dimensions in the DMFT approximation due to the momentum independence in the self-energy. This feature has also been exploited in [6].

In Fig. 6, we consider five impurities each of magnitude $V_0 = 10t$, distributed on the lattice at sites: $(3a, 3a), (20a, 5a), (5a, 20a), (25a, 22a), (17a, 28a)$ for the noninteracting system and systems with $U = 2t, U = 5t$, and $U = 12t$. We see oscillations around the impurities together with a complex interference pattern (like a checkerboard) in the interstitial spaces between the impurities for the noninteracting system and systems with $U = 2t, 5t$. Interference effects get localized around the impurities with increasing interactions (cf. $U = 5t$). No FO are observed in the Mott insulator for ($U = 12t$). This is in agreement to our previous studies where a single impurity or two impurities are present in the system. Thus we conclude that, at least within HSEA, the absence of FO and any interference effects due to scattering in the Mott insulating phase is rather universal irrespective of the model of the inhomogeneous potential.

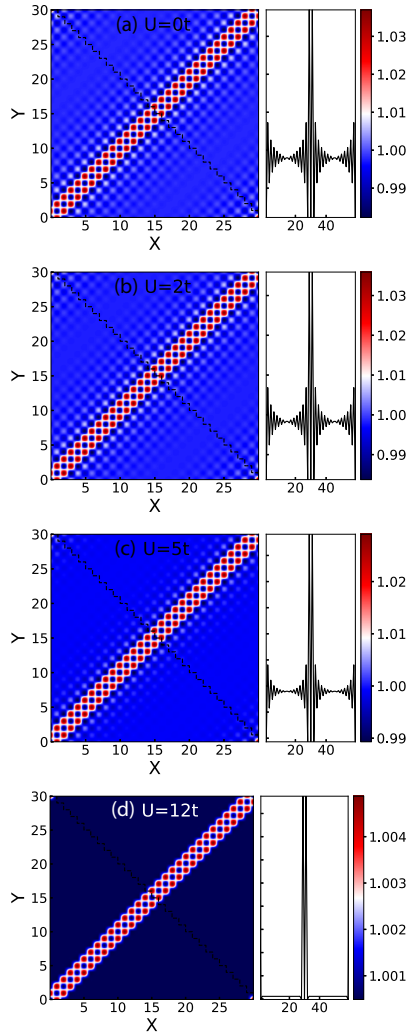


FIG. 7. FO in particle densities (\bar{n}_i) due to the scattering from a chain of impurity atoms of equal magnitude $V_0 = 24t$ along the diagonal direction of the square lattice. Interference effects on FO are shown for (a) noninteracting system ($U = 0t$), (b) $U = 2t$, (c) $U = 5t$, and (d) $U = 12t$. The model, all other parameters, and the plotting style are the same as in Fig. 1.

C. A chain of impurities

Next, we study the case where a chain of impurities each of magnitude ($V_0 = 24t$) is placed along the diagonal direction and a vertical direction of the square (31×31) lattice. This aims to model a domain wall or an interface. We investigate the behavior of FO for these two orientations of the chain with the different interactions. First, in Fig. 7 we present the case for a diagonally oriented chain for the noninteracting system and systems with $U = 2t$, $5t$, and $12t$. The insets show a projection of the densities along a zigzag line oriented perpendicularly to the diagonal direction. FO are visible around the chain and the behavior is similar for the noninteracting system and $U = 2t$, as in the other previously presented cases. FO get localized around the chain with increasing interaction (cf. $U = 5t$). On the ends of the cut (corners of the lattice) we observe an increase of oscillations, which is due to the imposed periodic boundary conditions in a finite (small) system. In the case of a Mott insulator with $U = 12t$ no FO are

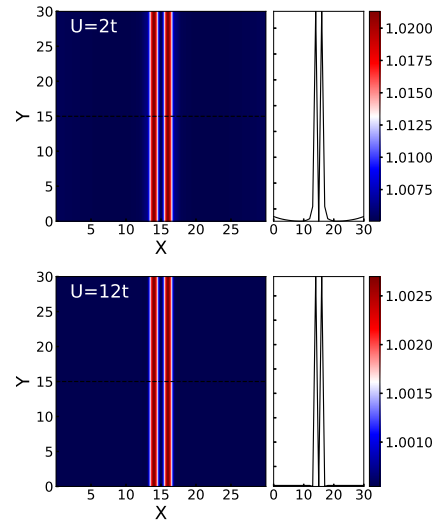


FIG. 8. FO in particle densities (\bar{n}_i) due to the scattering from a chain of impurity atoms of equal magnitude $V_0 = 24t$ along the vertical line of the square lattice. Interference effects on FO are shown for (a) $U = 2t$ and (b) $U = 12t$. The model, all other parameters, and the plotting style are the same as in Fig. 1.

visible. The chain creates an interface and effectively forms two subsystems separated in space.

In Fig. 8 we show the behavior for the system with interactions if the chain of impurities is oriented along the vertical direction. The inset shows a horizontal cut perpendicular to the chain. In contrast to the previous case we do not see any FO but just a density minimum corresponding to the repulsive potential for both the noninteracting and interacting systems. We only show the cases for $U = 2t$ and $U = 12t$ since the behavior of the system does not change much with the interactions. This different behavior as compared to the diagonally oriented chain lies in the geometrical orientation of the impurities with respect to each other. If the chain is vertically oriented, each impurity site has two neighboring sites occupied by impurities. On the other hand, if the chain is diagonally oriented, each impurity site is completely surrounded by nearest neighboring sites without impurities. Hence, in the latter case the distance between the impurity sites and the sites on a perpendicular cut, measured in Manhattan metric, is always even, in contrast to the former case, where it is always odd. This difference makes the interference pattern between FO created by each impurity from the chain always constructive in the diagonal case, while it is destructive in the vertical case.

In Fig. 9 we compare the FO from the diagonally oriented chain (blue line) and from the vertically oriented chain (green line) of impurities, presented above, with the FO of a one-dimensional lattice having a single impurity potential (red line), with $N_L = 32$ sites and a single impurity $V_0 = 12t$ placed in the center. We also show the FO from a single impurity potential in the square lattice (black line). We consider the noninteracting systems for all these cases. The comparison shows that none of the 2d systems could be simplified to an assembly of 1d chains with a single impurity potential. While the vertically oriented chain shows no oscillations, the decay of FO due to the diagonally oriented chain is not

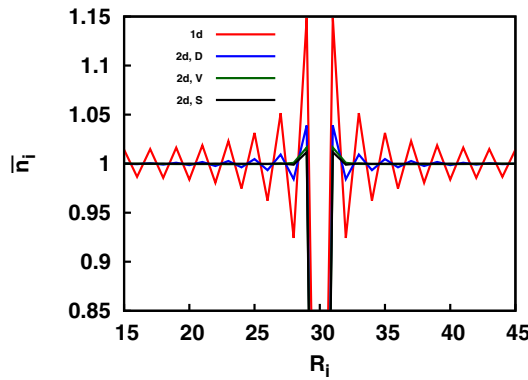


FIG. 9. Comparison of FO along a 1d lattice chain with $N_L = 32$ sites and a single impurity potential $V_0 = 12t$ placed at the center (1d), across the perpendicular cut for a chain of impurities $V_0 = 24t$ along the diagonal chain (D), vertical chain (V), and a single impurity potential $V_0 = 24t$ placed at the center of the square lattice (S). We show the noninteracting case $U = 0t$.

exactly similar to the 1d chain. Eventually, the FO from both the vertically and diagonally oriented chains are also quite different compared to a chain from a 2d lattice with a single impurity potential at the center. Hence, the substantial role of the geometrical orientation of the chain of impurities on the interference effect prevents one from simplifying this system to equivalent 1d chains with single impurity potentials assembled together.

D. Extended inhomogeneity

Next, we apply a steplike potential across the square lattice (32×32), i.e., for all the lattice sites with x coordinates $X_i \leq 15a$ the potential is $V_0 = 3t$ and in the rest of the system it is $V_0 = 0$. This potential models an extended inhomogeneity which could correspond to the surface irregularities in materials developed during the process of cleavage. In Fig. 10 we show local densities in the noninteracting system (upper panel) and in the interacting system with $U = 12t$ (middle panel). The steplike potential divides the lattice into two half planes with a different average occupation (\bar{n}_i). FO is visible for $U = 0$, but the period of oscillations differs in the two half planes as illustrated in the inset, where we show the FO in the cut perpendicular to the potential edge. Different oscillation periods originate from different uniform densities of particles in each half of the systems. Any signature of FO is absent for the Mott phase ($U = 12t$); cf. the bottom panel of Fig. 10. In Fig. 10 (bottom panel) the influence of interactions in this system is studied, taking cuts perpendicular to the step of the potential. We see that the system becomes more homogeneous and the screening charge decreases with the increasing interaction.

1. Going beyond a simple HSEA scheme

The extended steplike potential discussed here preserves partially mirror point symmetries of the lattice. Therefore, it is natural to extend our earlier HSEA scheme and determine homogeneous self-energies, which correspond to the left side of the system and to the right side independently. In the right side the external potential is zero and the corresponding infi-

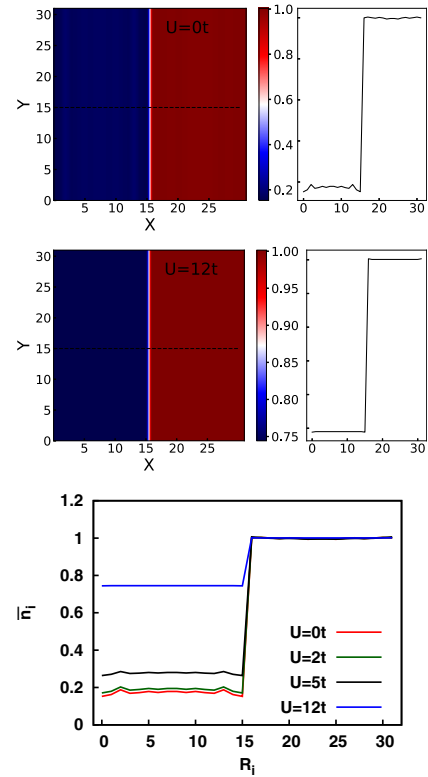


FIG. 10. Interference effect on FO due to the scattering from an extended inhomogeneity: A steplike potential is applied in half of the square lattice (32×32), such that on the left side of the vertical symmetry line the potential is $V_0 = 3t$ and on the right side of it $V_0 = 0$. We show the noninteracting case (upper panel) and Mott phase ($U = 12t$) (middle panel). The right insets show oscillations on a cut (dotted line in the main panels) perpendicular to the step of the potential. In the bottom panel we compare a similar cut for the different interactions $U = 0t, 2t, 5t$, and $12t$.

nite system is at half filling. On the left side a finite potential $V_i = 3t$ corresponds to a change of the chemical potential in the corresponding infinite system. Therefore, the reference system is away from half filling.

We used two different homogeneous self-energies, obtained by solving DMFT equations using the NRG method, for the infinite homogeneous systems and the chemical potentials $\mu = 0$ and $\mu = -V_i$, for the left and the right sides respectively. Then from solving the Dyson equation (2) we obtain actual densities of particles.

In the results, shown in Fig. 11, we see that the main difference is in changing the average density on left side of the system. However, shapes and characters of oscillations seem to be very similar to those seen in Fig. 10. Hence we conclude that the HSEA does not take into account very precisely the Hartree (static) term in the self-energy, which on the impurity sites is quite different from the homogeneous case. However, regarding how the particle density oscillates around the average density, it seems to be independent of this Hartree term.

To make sure that our reasoning is correct we determined the particles densities in the case of few impurities randomly distributed on the lattice, as in Fig. 6 in Sec. III B, but with a modified HSEA scheme. That is, on the impurity sites either

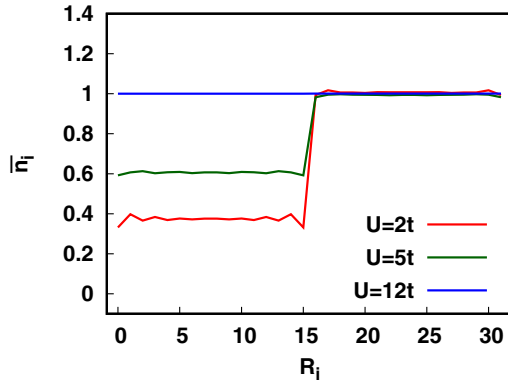


FIG. 11. The same cut as in Fig. 10 using the self-energy from a doped Hubbard model.

the self-energy is taken to be zero, cf. upper panels in Fig. 12, or the self-energy is equal to the interaction, cf. lower panels in Fig. 12. Comparing Figs. 12 and 6 we conclude that the FO oscillations are still the same.

IV. CONCLUSIONS

We have studied the interference effects in FO due to the scattering from two impurities, multiple impurities, and extended inhomogeneities in noninteracting and interacting fermion systems. On comparing the FO in the presence of a single impurity we see that in two-impurity systems the additional impurity induces interference effects on FO. The interference maxima and minima change with the relative position of the impurities up to a certain crossover distance, beyond which the impurities behave independently. At half filling, the interaction does not change the positions of maxima and minima but reduces their intensity and consequently the interference effects. The screening charge shows an oscillatory behavior with the even and odd lattice spacing between the impurities along a vertical column. A more complex pattern is seen in the presence of multiple impurities but the FO still localize around the impurities with the increase in interaction. In case of extended inhomogeneities the system also becomes more homogeneous with increasing interaction. In case of a chain of impurities in the square lattice, FO is present for a diagonal chain while it is absent for a vertical chain due to constructive and destructive of FO in these two geometries respectively. In all the models of the impurity potential no FO or interference effects are seen in the Mott insulating phase.

We have used a homogeneous self-energy approximation based on DMFT for most of our studies, where the inhomogeneous part of the self-energy due to the contribution from the impurities is neglected. However, in the case of extended inhomogeneity we show that the inclusion of the inhomogeneous

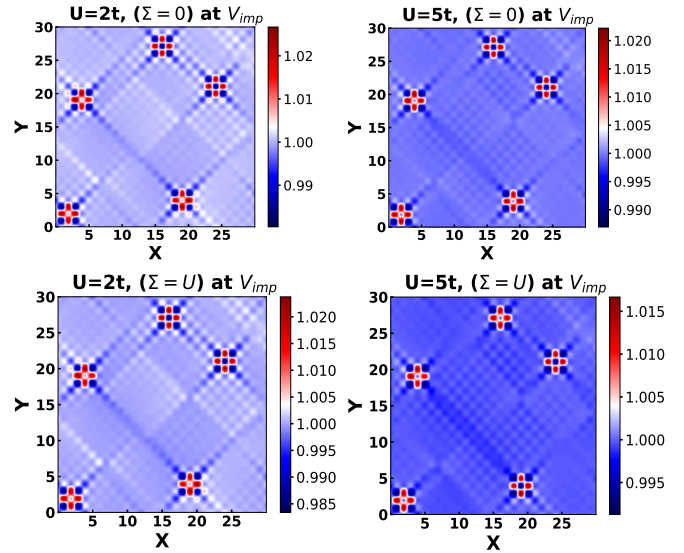


FIG. 12. FO in particle densities (\bar{n}_i) in the presence of five impurities each of magnitude $V_1 = V_2 = V_3 = V_4 = V_5 = 10t$ randomly distributed over the same lattice sites as in Fig. 6. We put the self-energy to zero (top panel) and the self-energy to be equal to U (bottom panel) at the impurity sites. We do not see any changes from the HSEA.

part of the self-energy does not qualitatively alter the pattern of FO. It is a promising future work to compare the results of HSEA and full R-DMFT accounting for the inhomogeneous part of the self-energy for the models of multiple discrete impurity potential. We do not expect significant changes with the single-site R-DMFT since a possible change in the density of particles due to a change of the self-energy by the inhomogeneous potential is a higher order effect beyond the linear response regime. Hence, one can further probe beyond the single-site DMFT, taking into account the spatial correlations and nonlocal part of the self-energy, and see if the positions of interference maxima/minima are altered by the interactions. Our model studies should further motivate a realistic modeling of FO in real materials like transition metal oxides and transition metal dichalcogenides using LDA+DMFT in real space and its validation through STM experiments.

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