I. INTRODUCTION

The Hubbard model has been initially introduced, inter alia, to describe metallic magnetism [1,2]. This is frequently forgotten in recent research which focuses on other instabilities which are hidden and not so easy to investigate, as the instabilities of the Fermi surface or the superconductivity [3]. The ferromagnetic (FM) state is easily derived from the Stoner criterion and occurs at sufficiently large local Coulomb interaction $U$. The Stoner instability of a nonmagnetic state is determined using the Hartree-Fock approximation and is thus predicted for any lattice and filling of a nondegenerate band. However, it was soon realized that it does not imply ferromagnetism as electron correlations strongly renormalize the Stoner parameter which follows from the Hartree-Fock approach and remove the FM instability in most cases. The metallic state of strongly correlated electrons in the nondegenerate Hubbard model is a correlated Fermi liquid which is characterized by the Fermi liquid parameters. In the frequently considered model of a rectangular density of states, the FM instability is absent at commensurate fillings. This conclusion follows also by considering the Fermi-liquid antisymmetric parameter $F_0$, which was found to be close to $-3/4$ [4]. Indeed, experimentally there exist only very few systems in nature which could be classified as itinerant ferromagnets with a single band, such as a weak itinerant ferromagnet ZrZn$_2$ [5].

After several decades of research on the Hubbard model, it became clear that the mechanism of itinerant ferromagnetism is subtle and other effects are needed to stabilize it. One of them is high degeneracy of the ground state [3] realized when the band is flat [7,8]. Ferromagnetism in realistic flat-band systems has been proposed for a triangular lattice of Na$_2$CoO$_2$ [10] and for the $p$ orbitals in honeycomb lattices with ultracold atoms [11]. In a two-dimensional (2D) Hubbard model on a square lattice FM instability occurs at the van Hove singularity of the density of states [12–14]. It becomes relevant away from half filling when the band is flat due to the next neighbor hopping $t'$. This follows from a more general approach which predicts the FM instability by investigating the divergence of the uniform magnetic susceptibility.

Other factors which stabilize itinerant ferromagnetism in real materials go beyond the Hubbard model itself — these are: (i) direct intersite exchange coupling $|U|$, or (ii) band degeneracy with active Hund’s exchange coupling $|t_{HF}|$. The second mechanism is better known — it is responsible for ferromagnetism in transition metals Fe, Co and Ni which have rather large magnetic moments and FM states occur in a degenerate 3$d$ band where Hund’s exchange plays a prominent role [20]. Also here the Stoner parameter is strongly renormalized by the electron correlation effects [18], but the FM instability survives and is much easier to obtain than for the nondegenerate $s$ band [12]. FM states have been investigated for realistic transition metals using different methods including more recent studies with the Gutzwiller approximation [21]. This subject is interdisciplinary and itinerant ferromagnetism plays also a role in a ferromagnet/insulator/superconductor ballistic junction [22], while the essential role played in the onset of ferromagnetism by the orbital degeneracy was also demonstrated recently for the multiband Hubbard models on square and cubic lattices [23] relevant both for $p$-orbital bands with ultracold fermions in optical lattices and for electronic 3$d$-orbital bands in transition metal oxides.

Here we focus on the extended nondegenerate Hub-
The Fermi liquid interaction and the quasiparticle scattering amplitude on the Fermi surface in $\text{He}_3$ [24]. Further studies gave the Fermi liquid interaction and the quasiparticle scattering amplitude on the Fermi surface in $\text{He}_3$ [24]. The perturbative method predicts the change of sign of the Fermi liquid parameter $F_0$ in the 2D square lattice for small $U \simeq 2t$ [25], where $t$ is the hopping parameter. The calculation within the slave boson method in the doped 2D Hubbard model [26] does not confirm this result and gives a negative $F_0$ in the entire range of $U$ and its saturation with increasing $U$ towards a negative value larger than $-1$ and nearly independent of the doping. This behavior confirms the earlier result that the nondegenerate Hubbard model does not exhibit a FM instability even when $U$ is very large [4]. We remark that saturated ferromagnetism near half filling and at $U \to \infty$ which stems from the Nagaoka state is nevertheless not excluded, as shown by several studies [8, 27] including a slave boson approach [28]. This subject goes however beyond the scope of the present study.

The purpose of this paper is to derive and evaluate Fermi liquid Landau parameters for the metallic state in the extended Hubbard model. Despite of the above discussion on the FM instabilities, the influence of intersite Coulomb and exchange interactions on Landau parameters was not analyzed in the Hubbard model until now. We investigate the instabilities towards uniform FM and charge instabilities using the spin rotation invariant (SRI) representation of the Kotliar and Ruckenstein slave boson approach. We show analytically that weak FM intersite interactions are sufficient to trigger a divergence in the magnetic susceptibility expressed by the antisymmetric Landau parameter $F_0$ which implies that the FM instability occurs due to such interactions for any lattice. For a representative example of a three-dimensional (3D) cubic lattice we present also numerical analysis.

The paper is organized as follows: The extended Hubbard model is introduced in Sec. II together with its Kotliar and Ruckenstein SRI slave boson representation. In Sec. III we perform the saddle-point approximation and present the resulting system of coupled nonlinear equations. Fluctuations are captured within the one-loop approximation described in Sec. IV which allows one to determine analytically Fermi-liquid Landau parameter $F_0$ at half filling. Numerical results are presented and discussed in Sec. V where we address first the instabilities towards uniform spin polarization (ferromagnetism) and next consider charge order in Secs. VA and VB. The paper is summarized in Sec. VI.

II. EXTENDED HUBBARD MODEL

Numerous studies of correlated electrons have been devoted to the properties of the Hubbard model on a square lattice, especially after Anderson’s proposal that it represents a minimal model for the d electrons within the CuO$_2$ layers common to the high $T_c$ superconductors [29]. Yet the Hubbard model assumes a perfect screening of the long-range part of the Coulomb interaction. This may be questionable and the relevance of this approximation may be assessed by considering the extended Hubbard model that reads:

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i \left( n_{i\uparrow}^\dagger - \frac{1}{2} \right) \left( n_{i\downarrow}^\dagger - \frac{1}{2} \right)$$

$$+ \frac{1}{2} \sum_{i,j} V_{ij} (1 - n_{i\sigma})(1 - n_{j\sigma}) + \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j,$$

and includes intersite Coulomb $V_{ij}$ and exchange $J_{ij}$ interactions. Here $c_{i\sigma}^\dagger$ are electron creation operators at site $i$ with spin $\sigma$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $\vec{S}_i$ are spin operators. We consistently use the particle-hole symmetric form for both density-density interaction terms.

Since Mott insulating ground states are expected at half filling we perform our investigations in a framework which is able to capture interaction effects beyond the physics of Slater determinants. It is an extension of the Kotliar and Ruckenstein slave boson representation that reproduced the Gutzwiller approximation on the saddle-point level [30]. It entails the interaction driven Brinkman-Rice metal-to-insulator transition [31]. A whole range of valuable results have been obtained with Kotliar and Ruckenstein [30] and related slave boson representations. In particular they have been used to describe antiferromagnetic [32], ferromagnetic [28], spiral [35, 37] and striped [38, 41] phases. Furthermore, the competition between the latter two has been addressed as well [42]. The influence of the lattice geometry on the metal-to-insulator transition was discussed, too [43]. For instance, very good agreement with Quantum Monte Carlo simulations on the location of the metal-to-insulator transition of the honeycomb lattice has been demonstrated [44].

In the original Kotliar and Ruckenstein representation the spin interaction term remains a four-fermion term. This is no longer the case in the SRI representation [32, 33] which we therefore adopt and extend for our study. In this framework the Hamiltonian Eq. II may be represented as:

$$H = \sum_{i,j,\sigma} t_{ij} \sum_{\sigma\sigma’} z_{i\sigma}^\dagger f_{i\sigma}^\dagger f_{j\sigma’}^\dagger z_{j\sigma’}$$

$$+ U \sum_i \left[ d_{i\uparrow}^\dagger d_{i\downarrow} - \frac{1}{2} \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} + \frac{1}{4} \right]$$

$$+ \frac{1}{4} \sum_{i,j} V_{ij} \left[ (1 - \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma}) Y_j + Y_i \left( 1 - \sum_{\sigma} f_{j\sigma}^\dagger f_{j\sigma} \right) \right]$$
+ \frac{1}{2} \sum_{i,j} J_{ij} \sum_{\sigma' \sigma} \bar{\sigma}_{\sigma'} p_{i \sigma \sigma} \bar{p}_{i \sigma' \sigma'} \cdot \sum_{\rho \rho' \rho_1} \bar{\tau}_{\rho \rho'} p_{i \rho \rho_1} p_{j \rho_1 \rho'}, \tag{2}

where we introduced:

\[ z = e^l L M R p + \overline{p}^l L M R d, \tag{3} \]

with \( p = \frac{1}{2} \sum_{\mu=0}^3 p_{\mu} \bar{p}_{\mu} \) and \( \bar{p} \) being the Pauli matrices.

We further use \( \bar{p}_{\sigma' \sigma} \equiv \sigma' \bar{p}_{-\sigma',-\sigma}, \) and

\[ M = \left[ 1 + e^l + \sum_{\mu} p_{\mu} \bar{p}_{\mu} + d^l d' \right]^{\frac{1}{2}}, \]
\[ L = \left[ (1 - d^l d') \frac{1}{2} - 2 p^l \bar{p} \right]^{-\frac{1}{2}}, \]
\[ R = \left[ (1 - e^l) \frac{1}{2} - 2 p^l \bar{p} \right]^{-\frac{1}{2}}. \tag{4} \]

For more details see Ref. [41]. In Eq. (2) we used the mapping of the fermionic degrees of freedom onto bosons and expressed the hole doping operator as,

\[ Y_i = e^l e_i - d^l d_i, \tag{5} \]

and the spin operator as

\[ \bar{S}_i = \sum_{\sigma' \sigma} \bar{\sigma}_{\sigma' \sigma} p_{i \sigma \sigma} \bar{p}_{i \sigma' \sigma'}. \tag{6} \]

Since the auxiliary operators span an augmented Fock space, physically meaningful results may be obtained provided they satisfy local constraints. For each site they read:

\[ e^l e + \sum_{\mu} p_{\mu} \bar{p}_{\mu} + d^l d = 1, \tag{7} \]
\[ \sum_{\sigma} f_{\sigma} f_{\sigma} = \sum_{\mu} p_{\mu} \bar{p}_{\mu} + d^l d, \tag{8} \]
\[ \sum_{\sigma, \sigma'} f_{\sigma} \bar{\tau}_{\sigma' \sigma} f_{\sigma'} = \bar{p}_{0} \bar{p} + \bar{p}^l \bar{p}_{0} - i \bar{p}^l \times \bar{p}. \tag{9} \]

They may be enforced in path integral formalism.

We remark that any slave boson representation possesses an internal gauge symmetry group. In our case it may be made use of to simplify the problem and to gauge away the phases of the \( e \) and \( p_{\mu} \) bosons by promoting all constraint parameters to fields \( \overline{R}_{\mu} \), leaving us with radial slave bosons fields \( \bar{P}_{j} \). Their approximate values that are obtained in the saddle-point approximation may be viewed as an approximation to their exact expectation values that are generically non-vanishing [41]. The slave boson coordinate corresponding to double occupancy \( d \) has to remain complex however as emphasized by several authors [33, 48, 41].

Besides, the saddle-point approximation is exact in the large degeneracy limit, and the Gaussian fluctuations provide the \( 1/N \) corrections [32]. Moreover it obeys a variational principle in the limit of large spatial dimensions where the Gutzwiller approximation and the Gutzwiller wave function are identical [50]. One can infer from these formal properties that the approach captures characteristic features of strongly correlated electrons as the suppression of the quasiparticle residue and the Mott-Hubbard/Brinkman-Rice transition [31] to an insulating state at half filling with increasing on-site Coulomb interaction. Of particular relevance is the influence of the longer-ranged Coulomb interaction on the latter transition.

### III. SADDLE-POINT APPROXIMATION

 Though such functional integrals can be calculated exactly for the Ising chain [46] and some toy models [47], even with the Kotliar and Ruckenstein representation [51], this is unpractical on higher dimensional lattices. Here we rather resort to the saddle-point approximation. In the paramagnetic phase, the action at saddle-point reads (\( \beta = 1/k_B T \)):

\[ S = \beta L \left( S_B + S_F + \frac{1}{4} U \right), \tag{10} \]

with

\[ S_B = \alpha(e^2 + d^2 + \bar{p}_{0}^2 - 1) - \beta_0(p_0^2 + 2d^2) \]
\[ + U d^2 + \frac{1}{2} V_0 Y, \tag{11} \]
\[ S_F = -\frac{1}{\beta} \sum_{k, \sigma} \ln \left( 1 + e^{-\beta E_{k\sigma}} \right). \tag{12} \]

For the extended Hubbard model (1) the quasiparticle dispersion in Eq. (12) reads:

\[ E_{k\sigma} = z_0^2 t_k + \beta_0 - \frac{1}{2} U - \frac{1}{2} V_0 Y - \mu, \tag{13} \]

in which we introduced the Fourier transform of the intersite Coulomb repulsion,

\[ V_k = \frac{1}{L} \sum_{i,j} V_{ij} e^{-ik \cdot (\vec{R}_j - \vec{R}_i)}. \tag{14} \]

It is convenient to define the Fourier transform of the intersite exchange elements in a similar way,

\[ J_k = \frac{1}{L} \sum_{i,j} J_{ij} e^{-ik \cdot (\vec{R}_j - \vec{R}_i)}. \tag{15} \]

From Eq. (14) one obtains the following set of saddle-point equations:

\[ \frac{p_0^2}{2e} + e^2 + d^2 - 1 = 0, \]
\[ \frac{p_0^4}{2d} + 2d^2 = n, \]
\[ \frac{1}{2e} \frac{\partial^2}{\partial\bar{\varepsilon}} + \frac{1}{2} V_0(1 - n) \frac{1}{2e} \frac{\partial Y}{\partial e} = -\alpha, \]
\[ \frac{1}{2p_0} \frac{\partial^2}{\partial\bar{\varepsilon}} + \frac{1}{2} V_0(1 - n) \frac{1}{2d} \frac{\partial Y}{\partial d} = 2(\beta_0 - \alpha) + \alpha - U. \tag{16} \]
interaction $V$ has no influence on the Mott gap as discussed by Lavagna [52]. Furthermore, the double occupancy is in exact agreement with the Gutzwiller approximation as derived by Vollhardt, Wölfle and Anderson [53]. In the present case of a cubic lattice the double occupancy vanishes at half filling for $U_c = 16.0387t$. At this value of $U$ the effective mass $m^*$ vanishes and its inverse (being quasiparticle residue),

$$z^2 = \frac{m}{m^*},$$

(22)
diverges. Here $m$ is the electron mass and $z$ stands for the reduced jump in the electronic filling $\langle n_{\vec{k},\sigma} \rangle$ when the momentum $\vec{k}$ changes from inside to outside of the Fermi surface [4]. Solving the saddle-point equations (16) yields at half filling,

$$z^2 = 1 - \left( \frac{U}{U_c} \right)^2 .$$

(23)

Its doping dependence is universal in the extended Hubbard model, and is neither influenced by $V_{ij}$ nor by $J_{ij}$, see Fig. 1. The plot shows that only for filling $n > 0.8$ the Fermi liquid is substantially renormalized in the regime of large $U > U_c$.

**IV. ONE-LOOP APPROXIMATION TO THE RESPONSE FUNCTIONS**

Having mapped all degrees of freedom onto bosons allows us for directly evaluating the spin and charge response functions. Indeed, following Ref. [54], the spin and density fluctuations may be expressed as

$$\delta S = \sum_\sigma \delta n_{\sigma} = \delta (n_{\sigma} - \langle n_{\sigma} \rangle),$$

(24)

$$\delta N = \sum_\sigma \delta n_{\sigma} = \delta (n - \langle n \rangle),$$

(25)

in the SRI representation. The spin and charge autocorrelation functions can be written in terms of the slave boson correlation functions as:

$$\chi_s(k) = \sum_{\sigma,\sigma'} \langle \delta n_{\sigma}(-k) \delta n_{\sigma'}(k) \rangle = \langle \delta S(-k) \delta S(k) \rangle ,$$

(26)

$$\chi_c(k) = \sum_{\sigma,\sigma'} \langle \delta n_{\sigma}(-k) \delta n_{\sigma'}(k) \rangle = \langle \delta N(-k) \delta N(k) \rangle .$$

Here we use the notation $k \equiv (\vec{k}, \omega)$. Performing the calculation to one-loop order, one can make use of the propagator as given in the Appendix. The susceptibilities are given by the matrix elements of the inverse propagator as follows:

$$\chi_s(k) = 2 p_{0}^2 S_{77}^{-1}(k),$$

$$\chi_c(k) = 2 e^2 S_{11}^{-1}(k) - 4 e d S_{12}^{-1}(k) + 2 d^2 S_{22}^{-1}(k) .$$

(27)

As emphasized and analyzed by several authors, see e.g. Refs. [55, 56], the Fermi liquid behavior is obtained when
considering the above $\chi_s(k)$ and $\chi_c(k)$ in the long wavelength and low frequency limit. However, in contrast to the conventional random phase approximation (RPA) results, the obtained Landau parameters involve effective interactions, which differ in the spin channel and in the charge channel.

Explicitly the spin susceptibility reads:

$$\chi_s(k) = \frac{\chi_0(k)}{1 + A_k \chi_0(k) + B \chi_1(k) + C[\chi_1(k) - \chi_0(k)\chi_2(k)]},$$

where

$$A_k = \frac{\alpha - \beta \epsilon_0 z_0 \frac{\partial^2 z_{\uparrow}}{\partial p^2} + \epsilon_0 \left( \frac{\partial z_{\uparrow}}{\partial p} \right)^2}{2p_0^2} + \frac{1}{4} J_k,$$

$$B = \frac{z_0}{p_0} \left( \frac{\partial z_{\uparrow}}{\partial p} \right),$$

$$C = \left( \frac{z_0}{2p_0} \right)^2 \left( \frac{\partial z_{\uparrow}}{\partial p} \right)^2 .$$

Using

$$\frac{\partial z_{\uparrow}}{\partial p_3} = \sqrt{2} \left( e - d \right) \left( 1 - \delta^2 \right) - 2p_0^2 \delta(e + d) \left( 1 - \delta^2 \right)^{3/2},$$

$$\frac{\partial^2 z_{\uparrow}}{\partial p_3^2} = \sqrt{2} \frac{p_0}{1 - \delta^2} \left( 2(e + d) \left[ 1 - \delta^2 + 2p_0^2(1 + 2\delta^2) \right] - 4\delta(e - d)(1 - \delta^2) \right) .$$

together with the saddle-point Eqs. 10 yields the Landau parameter $F_a$ at half filling as:

$$F_a = 2\epsilon N_F \frac{u(1 - u)(2 + 2u) + (1 + u)(J_0/8\epsilon)}{(1 + u)^2(1 - u)},$$

where we have introduced the bare density of states at the Fermi energy $N_F^{(0)} = \rho(E_F)$. We decompose Eq. 34 into a regular and singular part,

$$F_a = 2N_F^{(0)} \left[ \frac{u(2 + u)}{(1 + u)^2} \frac{\epsilon}{81 - u^2} J_0 \right] ,$$

with the latter dependent on the exchange coupling $J_0$ 13. Spin and charge fluctuations separate at the one-loop order, and the intersite Coulomb elements in $V_0$ 14 have no effect on the value of $F_0^a$.

Equation 35 is the central analytic result obtained at half filling. Remarkably, the intersite exchange dominates over the Coulomb term near the metal-to-insulator transition. We have shown that introducing an arbitrarily weak exchange $J_0 \neq 0$ interaction results in a singular behavior in the vicinity of the Brinkman-Rice point $U_c$ ($u = 1$). This is in marked contrast to the known results for a flat band in the absence of inter site exchange:

$$F_0^a = -1 + \frac{1}{(1 + U/U_c)^2} .$$

While the simple form

$$F_0^a = \frac{U(2U_c - U)}{(U_c - U)^2} ,$$

could be derived in absence of Coulomb elements this is no longer the case when they are taken into account. Note that the property $F_0^a(U) = F_0^a(-U)$ can be derived on a more general ground 14.

V. NUMERICAL RESULTS

A. Ferromagnetic instability — $F_0^a$ parameter

In this Section we compute the Landau parameter $F_0^a$ for the cubic lattice to analyze its filling dependence. We first investigate half filling ($n = 1$), evaluating the obtained analytic expression Eq. 35 to demonstrate the divergent behavior at finite intersite exchange. The Hubbard model does not exhibit the FM instability in the metallic regime as $F_0^a > -1$, see Fig. 2. However, as anticipated above, an infinitesimal FM coupling $J_0$ generates an instability of the nonmagnetic state at half filling when the Coulomb interaction $U$ approaches $U_c$.

Although Eq. 35 is more general, we shall consider below the extended Hubbard model with nearest neighbor exchange interactions,

$$J_{ij} = \begin{cases} J & \text{for a bond } (ij) \text{ with } j \in \mathcal{N}(i) \\ 0 & \text{otherwise} \end{cases} ,$$

where $\mathcal{N}(i)$ stands for the set of nearest neighbors of site $i$. We have found that the model is unstable at half filling against the FM order near the metal-to-insulator transition. The location of the instability depends rather sensitively on the FM coupling, from $U_c$ for $J = 0^+$ down to 0.33$U_c$ for $J/U = -0.2$. Smaller values of $J/U$ are nonphysical and they are not considered below. On the contrary, a positive (AF) intersite exchange coupling $J_0 > 0$ suppresses the tendency towards ferromagnetism,
and the parameter $F_0^a$ becomes positive and large near the metal-to-insulator transition, see Fig. 2.

Since the Landau parameter $F_0^a$ is directly proportional to the product of the bare kinetic energy and the density of states at $E_F$, $\bar{\varepsilon} N_F^{(0)}$, it shows a lesser sensitivity to the band structure. For instance, one finds at half filling $\bar{\varepsilon} N_F^{(0)} = -0.5$ for a flat (rectangular) density of states (DOS), and $\bar{\varepsilon} N_F^{(0)} \simeq -0.57$ for the cubic lattice. This gives the value of $F_0^a \simeq -0.86$ at $J = 0$. We have verified that similar values are obtained for other typical DOSs at half filling, except for the 2D square lattice, where the van Hove singularity at $n = 1$ results in the FM instability at infinitesimal $U = 0^+$ disregarding the stronger AF instability following from nesting.

Next we consider the doping dependence of the Landau parameter $F_0^a$ in the Hubbard model, i.e., at $J_{ij} = 0$. As one can see in Fig. 3, $F_0^a$ reaches the critical value $F_0^a = -1$ for $U \approx 32t$ at $\delta = 0^+$, namely in the regime where Nagaoka ferromagnetism is expected. The critical $U$ increases linearly with doping. Furthermore, the cusp in the density of states for the cubic lattice at $n \simeq 0.43$ makes itself clearly visible in Fig. 3, with reduced values of $|F_0^a|$ at lower electron density.

Also away from half filling, finite FM exchange coupling $J_0 < 0$ triggers the FM instability $F_0^a = -1$ at significantly lower values of $U$. For instance, already $J/U = -0.01$ brings this instability down to the values of $U \sim 20t$ for the doping $\delta < 0.57$ (filling $n > 0.43$) where the DOS is almost independent of energy, see Fig. 4. When $J/U = -0.05$, the FM instability occurs at $U < 10t$ in the same doping regime, and comes down also for the lower electron fillings. For lower $J_0$ the FM instability occurs at even lower values of $U$. This is in contrast to the calculations to the two-band model, where the FM instability was only found in the doped Mott insulator regime [19]. In that case, no intersite FM coupling is
needed and the FM instability follows from Hund’s exchange.

On the contrary, an AF coupling suppresses the FM instability, and the value of $J_0 = 0.1$ totally removes ferromagnetism as shown in Fig. 5 For the small values of $U$ the Landau parameter $F^a_0$ is negative in the entire regime of $n$, but then changes sign when $U$ approaches $U_c$. The exception here is the regime of low filling $n < 0.2$, where $F^a_0 < 0$ for $U < U_c$. Larger AF exchange coupling $J_0/U = 0.2$ leaves only a narrow range of $F^a_0 < 0$ (not shown).

### B. Charge instability — $F^s_0$ parameter

The symmetric Landau parameter $F^s_0$ which stands for the charge response has to be evaluated numerically even at half filling, except for $V = 0$. As expected, $F^s_0$ vanishes both for $U = 0$ and for $n = 0$, as $F^s_0$ does. Otherwise, unlike the antisymmetric Landau parameter $F^a_0$ which decreases with increasing $U$ in the Hubbard model (at $V_0 = 0$), the symmetric parameter $F^s_0$ increases with $U$ in the entire regime of filling $0 < n < 1$. This increase is stronger near half filling, where $F^s_0 > 10$ for $U/U_c > 0.7$ in a range of small doping away from half filling, see Fig. 6. At half filling the value of the positive $F^s_0$ is given by Eq. 38. It rapidly increases and finally diverges at the metal-to-insulator transition (we recall that for the simple cubic lattice $U_c \approx 16.04t$). Away from $n = 1$ the increase of $F^s_0$ is moderate and it follows the same pattern as $1/z^2$ in Fig. 4 being another manifestation of strong electron correlations near half filling.

The increase of $F^s_0$ with increasing $U/U_c$ is enhanced by a positive intersite Coulomb repulsion in the extended Hubbard model. Here we also consider the case of nearest neighbor interactions,

$$V_{ij} = \begin{cases} V & \text{for a bond } (ij) \text{ with } j \in N(i) \\ 0 & \text{otherwise} \end{cases},$$

(39)

where we use the same notation as in Eq. 38. This case is particularly favorable for a charge instability near half filling, for instance in the form of a checkerboard state stable for large values of $V$ as then the cost of any intersite Coulomb energy $\propto V$ can be avoided. However, such a state does not occur as a consequence of the investigated instability of the uniform state. When $V > 0$, one finds even a stronger increase of $F^s_0$ near half filling, and finally it becomes even larger than $F^s_0 = 10$ in a broad range of filling $n > 0.6$ for the cubic lattice at $V = 0.2U$, see Fig. 7. The uniform charge distribution is therefore more robust in the regime of $n \simeq 1$, if $V/U > 0$.

We have found that the uniform charge distribution is destabilized by attractive charge interactions $V < 0$, particularly in the regime near quarter filling $n \simeq 0.5$. At $V = -0.2U$ the value of $F^s_0$ decreases with increasing $U$ for any filling $n$ and this decrease is fastest near quarter filling. For $U < U_c$ one finds the charge instability at $F^s_0 = -1$ in a broad range of $n \in (0.05, 0.96)$. This instability is related to the shape of the DOS and is easiest to realize at $n \simeq 0.42$, there the DOS has a van Hove singularity.

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**FIG. 6.** (Color online) Landau parameter $F^a_0$ for the Hubbard model on the cubic lattice. Here the white region stands for values $F^a_0 > 10$. No instability is found.

**FIG. 7.** (Color online) Landau parameter $F^a_0$ for the extended Hubbard model on the cubic lattice. Increase of $F^a_0$ with increasing $U/U_c$ is enhanced by positive $V/U = 0.2$; large values of $F^a_0 > 10$ are found for $n > 0.6$. 

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FIG. 8. (Color online) Landau parameter $F_0^s$ for the extended Hubbard model on the cubic lattice with attractive intersite interaction $V/U = -0.2$. Large values of $F_0^s > 3$ are found only near $n = 1$, while the charge instability $F_0^s = -1$ occurs for a broad range of $0.15 < n < 0.95$. The nearly vertical black line marks the divergence of $F_0^s$. Note that the instability line $F_0^s = -1$ does not extend to $n = 1$, but stops at $(n, U) \simeq (0.96, 0.79U_c)$.

The data of Figs. 7 and 8 suggest that in the case of charge response the regime near the metal-insulator transition at half filling is robust and the Landau parameter $F_0^s$ is here always enhanced, even for $V < 0$. This finding confirms that electrons are strongly correlated and the system properties change radically at the metal-to-insulator transition at $U_c$. Hence we inspect now the case $n = 1$ in more detail. We remark that the effect of finite $V$ first resembles somewhat that of finite $J$ for weak to moderate coupling: $F_0^s$ is reduced for attractive $V$ while it is enhanced for repulsive $V$, see Fig. 9. The reduction of $F_0^s$ occurs only for sufficiently large $-V$ and is visible in Fig. 8 for $V/U = -0.15$, and beyond. As a result a minimum in $F_0^s$ develops at $U \simeq 0.4U_c$, the minimal value of $F_0^s$ decreases with increasing $-V$, and a charge instability may be found at the critical value $V/U < -0.234$, see the inset in Fig. 9. The instability moves towards lower values of $U$ with decreasing $V$ when the minimum of $F_0^s$ becomes deeper with further decreasing $V$. Particularly interesting is the non-monotonic behavior of $F_0^s$ with increasing $U$ for $V < 0$. We therefore suggest that a sufficiently strong intersite Coulomb attraction $-V/U > 0.234$ is necessary to induce phase separation. The instability is absent for repulsive $V$, where the uniform charge distribution is locally stable.

FIG. 9. (Color online) Landau parameter $F_0^s$ for the extended Hubbard model on the cubic lattice at half filling ($n = 1$) for selected decreasing values of intersite Coulomb interaction $V$ from top to bottom: $V/U=0$ (black line), $V/U > 0$ (blue) — $V/U = 0.05$ (solid line), $V/U = 0.15$ (dotted) and $V/U = 0.25$ (dashed-dotted line), and $V/U < 0$ (red) — $V/U = -0.05$ (solid line), $V/U = -0.15$ (dotted) and $V/U = -0.25$ (dashed-dotted line). The inset shows the instability value $U_{\text{inst}}/U_c$ for $V/U \in [-1.0, -0.2]$. Its end point is marked by a solid circle.

VI. DISCUSSION AND SUMMARY

We have presented the consequences of finite intersite interactions: exchange $J_{ij}$ and Coulomb $V_{ij}$, and their impact on the instabilities of correlated electrons on a lattice in the nondegenerate band described by the extended Hubbard model. While the Hubbard model was originally introduced, inter alia, to explain the metallic ferromagnetism, this idea fails as it does not predict an instability of the metallic phase towards spin polarized (weakly ferromagnetic) states for the majority of lattices. Such an instability is expected in first place at half filling where electron correlation effects are strongest, so this case is of particular significance. However, it is well known that the metal-to-insulator transition happens typically for a lower value of $U$ than the ferromagnetic instability, given by the divergence of spin susceptibility when the antisymmetric Landau parameter takes the value $F_0^s = -1$.

The analytic result derived in this paper shows that intersite exchange interactions change radically the results for the metallic phase below the metal-to-insulator transition at $U_c$. If these interactions are globally ferromagnetic, a spin-polarized ground state occurs here before the system undergoes the metal-to-insulator transition.
This result could be of importance to decide about the properties of some compounds with strongly correlated electrons, for instance, heavy fermion systems.

Somewhat surprisingly we have found that the symmetric Landau parameter \( F_0^a \) has a rather rich behavior when intersite Coulomb interactions are included. Small interactions do not change the value of \( F_0^a \) significantly. Most unexpected is the absence of a charge instability at half filling for moderate intersite Coulomb interactions, independently of the sign of the intersite Coulomb interaction, as it takes a sufficiently large attractive Coulomb interactions \(-V/U > 0.234\) for a charge instability to take place. For smaller \(-V\), it develops in the intermediate regime of doping, i.e., 0.05 < \( n < 0.96\). It may be expected that the intersite Coulomb elements are repulsive except for systems with strong polaronic effects, which gives no charge instability. Whether or not such interactions could be sufficiently attractive to cause an instability is an experimental challenge for future studies.

Summarizing, we have shown that the Landau parameters \( F_0^a \) and \( F_0^b \) are both sensitive to different intersite elements — \( F_0^a \) is modified only by exchange elements, while \( F_0^b \) only by Coulomb elements. The derived analytic result for \( F_0^a \) at half filling Eq. (35) is very remarkable as it uncovers that the Hubbard model is at the verge of the ferromagnetic instability for any lattice, which is triggered by an infinitesimal globally ferromagnetic intersite exchange. This provides new context for the original idea of Kanamori who suggested the Hubbard model as the simplest model of itinerant ferromagnetism.

At the same time, interesting behavior of the symmetric Landau parameter \( F_0^b \) was found for attractive nearest neighbor Coulomb interactions. In contrast to \( F_0^a \), a more interesting result is found away from half filling, where attractive interactions lead to charge instabilities signaling a tendency towards phase separation. We also remark that we investigated here only instabilities towards uniform spin or charge order. Other instabilities may also occur at finite values of \( \bar{k} \) which is an interesting subject for future research.

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**Appendix: Inverse propagator matrix**

The derivation of the inverse propagator matrix for lattices with inversion symmetry follows the one by Zimmermann et al. To second order in the fluctuations the action \( S \) may be decomposed into two parts:

\[
S = S^{(\text{spin})} + S^{(\text{charge})},
\]

where

\[
S^{(\text{charge})} = \sum_{q,\mu,\nu} \delta \psi_{\mu}(-q) S_{\mu,\nu}^C(q) \delta \psi_{\nu}(q),
\]

with \( 1 \leq \mu, \nu \leq 6 \), and

\[
S^{(\text{spin})} = \sum_{q,\mu,\nu} \delta \psi_{\mu}(-q) S_{\mu,\nu}^S(q) \delta \psi_{\nu}(q),
\]

with \( 7 \leq \mu, \nu \leq 12 \) including the three spin components. We use the following sequence of boson fields: \( \psi_1 = e, \psi_2 = d, \psi_3 = d', \psi_4 = p_0, \psi_5 = b, \psi_6 = a, \psi_7 = p_x, \psi_8 = b_x, \psi_9 = p_y, \psi_10 = b_y, \psi_11 = p_z, \psi_12 = b_z \), after having introduced the short-hand notation \( d' = R(d) \) and \( d'' = 3(d) \).

Regarding the spin sector we find:

\[
S_{\tau,\tau}(k) = S_{9,9}(k) = S_{11,11}(k)
\]

\[
\equiv \alpha - \beta_0 + \frac{1}{2} j_{\bar{k}}^2,
\]

\[
+ \varepsilon_0 z_0 \frac{\partial^2}{\partial p_z^2} + \left[ 6 - \frac{1}{2} \delta_{z} \right] \left( \frac{\partial z}{\partial p_z} \right)^2,
\]

\[
S_{8,8}(k) = S_{10,10}(k) = S_{12,12}(k) \equiv - \frac{1}{2} \chi_0(k),
\]

\[
S_{7,8}(k) = S_{9,10}(k) = S_{11,12}(k) \equiv - p_0 - \frac{1}{2} \varepsilon_0 \chi_1(k) \frac{\partial z_0}{\partial p_z}.
\]

Here we used the Fourier transform \( j_{\bar{k}} \) Eq. (15) of the intersite exchange elements. Notably, regarding the spin sector, the only difference to the Hubbard model is the presence of \( J_{\bar{k}} \) in \( S_{7,7}(k) \).

Regarding the charge sector we obtain \( S^C = S + \tilde{S}(\bar{k}) \) with the non-vanishing matrix elements of \( S \):

\[
S_{1,1}(k) = \alpha + \frac{1}{2} \varepsilon_0 V_0,
\]

\[
S_{2,2}(k) = \alpha - 2 \beta_0 + U - \frac{1}{2} \varepsilon_0 V_0,
\]

\[
S_{3,3}(k) = \alpha - 2 \beta_0 + U - \frac{1}{2} \varepsilon_0 V_0,
\]

\[
S_{2,3}(k) = \omega_0,
\]

\[
S_{3,2}(k) = - \omega_0,
\]

\[
S_{4,4}(k) = \alpha - \beta_0,
\]

\[
S_{1,6}(k) = e = S_{6,1}(k),
\]

\[
S_{2,5}(k) = -2d = S_{5,2}(k),
\]

\[
S_{2,6}(k) = d = S_{6,2}(k),
\]

\[
S_{4,5}(k) = -p_0 = S_{5,4}(k),
\]

\[
S_{1,6}(k) = p_0 = S_{6,4}(k).
\]
We introduced above $\tilde{S}^{(l)}(k) = \tilde{S}(k) + \tilde{S}^{(V)}(k)$, with the non-vanishing matrix elements of $\tilde{S}(k)$ defined as:

\[
\tilde{S}_{\mu\nu}(k) = \frac{1}{2} \varepsilon_{\nu} \partial \mu \left[ \begin{array}{cc}
\varepsilon_k \partial z & \varepsilon_k \partial z \\
\varepsilon_k \partial \psi \partial \mu & \varepsilon_k \partial \psi \partial \mu
\end{array} \right] \gamma_{1,1}(k) \\
- \frac{1}{2} \varepsilon_0 \left[ \begin{array}{cc}
\varepsilon_k \partial z & \varepsilon_k \partial z \\
\varepsilon_k \partial \psi \partial \mu & \varepsilon_k \partial \psi \partial \mu
\end{array} \right] \gamma_{1,1}(k) \\
+ \partial z \partial \mu \gamma_{0,2}(k) + \partial z \partial \mu \gamma_{1,0}(k)
\] \\
\mu, \nu = 1, 2, 3, 4
\] 

(6)

\[
\tilde{S}_{\mu,5}(k) = \frac{1}{2} \varepsilon_0 \left[ \begin{array}{cc}
\varepsilon_k \partial z & \varepsilon_k \partial z \\
\varepsilon_k \partial \psi \partial \mu & \varepsilon_k \partial \psi \partial \mu
\end{array} \right] \gamma_{1,0}(k) \\
\tilde{S}_{5,\nu}(k) = \frac{1}{2} \varepsilon_0 \left[ \begin{array}{cc}
\varepsilon_k \partial z & \varepsilon_k \partial z \\
\varepsilon_k \partial \psi \partial \mu & \varepsilon_k \partial \psi \partial \mu
\end{array} \right] \gamma_{0,1}(k) \\
\mu, \nu = 1, 2, 3, 4
\]

(7)

These elements are defined in terms of:

\[
\chi_\alpha(p) = - \sum_{k,\sigma} (t_k + t_{k+p}) G_{0,\sigma}(kG_{0,\sigma}(k + p),
\gamma_{q,r}(p) = - \sum_{k,\sigma} (t_k)^q (t_{k+p})^r G_{0,\sigma}(kG_{0,\sigma}(k + p),
\varepsilon_k = \sum_{\tilde{p},\sigma} \tilde{G}_{0,\sigma}(p).
\]

(8)

For $p = 0$, the relation $\chi_\alpha(0) = (2t_F)^n \chi_0(0)$ may be established [54].

Explicitly, using $V_{-k} = V_k$ due to the inversion symmetry of the lattice, the relevant matrix elements of the hermitian matrix $\tilde{S}^{(V)}$ read:

\[
\tilde{S}_{1,1}^{(V)}(k) = \frac{1}{2} \left[ - e^z V_k^2 \chi_0(k) + 2 e \partial z \partial \psi \chi_1(k) - \partial \psi \right],
\]

\[
\tilde{S}_{1,1}^{(V)}(k) = \frac{1}{2} \left[ e^z V_k^2 \chi_0(k) + 2 e \partial z \partial \psi \chi_1(k) + \partial \psi \right],
\]

(9)

\[
\tilde{S}_{1,1}^{(V)}(k) = \frac{1}{2} e \partial \psi \chi_1(k),
\]

\[
\tilde{S}_{1,1}^{(V)}(k) = \frac{1}{2} e \partial \psi \chi_1(k),
\]

\[
\tilde{S}_{1,1}^{(V)}(k) = \frac{1}{2} e \partial \psi \chi_1(k),
\]

(10)

where we also introduced:

\[
\chi_1(p) = - \sum_{k,\sigma} (t_k - t_{k+p}) G_{0,\sigma}(kG_{0,\sigma}(k + p),
\varepsilon_V = V_0 n.
\]

(11)

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