Universal collective modes from strong correlations: Modified $1/N_f$ theory with application to high-$T_c$ cuprates

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A nonzero-temperature technique for strongly correlated electron lattice systems, combining elements of both variational wave function (VWF) approach and expansion in the inverse number of fermionic flavors ($1/N_f$), is developed. To the leading order, the combined VWF+$1/N_f$ scheme provides dynamical spin and charge response around the strongly-correlated VWF solution, whereas thermodynamic corrections to the saddle-point state arise systematically at consecutive orders. VWF+$1/N_f$ is used to evaluate dynamical response functions for the hole-doped Hubbard model and compared with available determinant quantum Monte-Carlo data, yielding a good overall agreement in the regime of coherent collective-mode dynamics. Emergence of well-defined spin and charge excitations from the incoherent continua is explicitly demonstrated, and a non-monotonic dependence of the charge-excitation energy on the interaction magnitude is found. The charge-mode energy saturates slowly when approaching the strong-coupling limit, which calls for a reevaluation of the $t$-$J$-model approach to charge dynamics. The results are also related to recent inelastic resonant $X$-ray scattering experiments for the high-$T_c$ cuprates.

I. INTRODUCTION

Strong electronic correlations in condensed matter systems support formation of exotic states of matter, such as high-temperature superconducting and pseudo-gap phases in doped layered copper oxides or heavy-fermion superconducting phase in $4f/5f$-electron systems. The simplest theoretical frameworks to study these phenomena are based on the Hubbard, $t$-$J$, $t$-$J$-$U$, and Anderson lattice models, with possible multi-orbital extensions. A number specific effects observed in high-$T_c$ superconductors and heavy-fermion systems have been satisfactorily interpreted within these models, using schemes specifically designed to incorporate the effects of strong local correlations, such as variational wave function (VWF) approach (in diagrammatic$^{[1]}$ or Monte-Carlo$^{[2]}$ form), or dynamical mean-field theory (DMFT)$^{[3]}$. However, new spectroscopic evidence$^{[4,5]}$ suggests that frameworks, based solely on local-correlation effects, are usually insufficient to provide a satisfactory account of magnetic and charge dynamics. Namely, resonant inelastic X-ray scattering (RIXS) and inelastic neutron scattering (INS) experiments have revealed well defined and universal magnetic excitations (paramagnons) in metallic phase of high-temperature (high-$T_c$) copper oxides$^{[6,7]}$ and iron pnictides$^{[8,9]}$, and in iridates$^{[10]}$. RIXS has also provided a detailed account of previously overlooked high-energy discrete charge modes in the cuprates that are currently under close scrutiny$^{[11,12]}$.

Regarding that weak-coupling theory predicts rapid overdamping of magnetic modes in the metallic state, in disagreement with experiment$^{[26]}$, an interplay between the long-wavelength collective excitations and local correlations becomes a factor that must be taken into account in order to successfully reproduce collective dynamics. Since none of the approximation schemes, mentioned above, captures local-correlations and long-wavelength collective excitations on the same footing, one is urged to resort to inherently unbiased techniques, such as determinant quantum Monte-Carlo (DQMC). The latter is, however, restricted to relatively small systems and suffers from the sign problem$^{[27]}$. Moreover, extracting real-time-dependent properties from imaginary-time DQMC results requires ill-conditioned analytic continuation of numerical data$^{[28]}$, limiting its accuracy in regard to the dynamical effects, particularly at higher temperature. Remarkably though, comparative studies of the Blankenbecler-Scalapino-Sugar quantum Monte-Carlo, DMFT, and cluster DMFT phase diagrams for the two-dimensional Hubbard model indicate that long-range fluctuations (such as paramagnons) are crucial for proper description of the metal-insulator transition, even in relatively small systems$^{[29]}$. As a step towards understanding the dynamics of strongly correlated materials, development of an alternative techniques, applicable in the thermodynamic limit and capable of describing local-correlations and collective-mode effects on the same footing, is thus highly needed.

In this paper, we present a new theoretical framework which is appropriate for strongly correlated lattice electron systems and combines variational wave function (VWF) method with field-theoretical expansion in inverse number of fermionic flavors ($1/N_f$), hereafter dubbed as VWF+$1/N_f$ approach. In the leading order, the VWF+$1/N_f$ method allows to study collective spin- and charge excitations around a correlated ground state and systematically include fluctuation-corrections to thermodynamics at higher orders, providing a way to generalize the Moriya-Hertz-Millis theory$^{[30,31]}$ to the situation with strongly-correlated fermions. At the same time, VWF+$1/N_f$ is relatively lightweight computationally and applicable to large systems ($>10^5$ orbitals), and also to broken-symmetry states. The price paid for those advantages is the accuracy loss due to inevitable truncation of the $1/N_f$ series and approximate diagrammatic treatment of variational wave functions. In a separate contribution$^{[32]}$, we already applied this method to hole-
doped cuprates and obtained a satisfactory agreement with the experimentally obtained paramagnon spectra across the hole-doped side of the phase diagram.

Both VWF and $1/N_f$ approaches, as treated separately, have received considerable attention so that their applicability range and limitations are well understood. The former provides a good description of local properties and static correlations for wide range of doping and interaction strength, by going beyond the renormalized mean-field theory. The latter allows to systematically evaluate dynamical response functions and thermodynamic fluctuation corrections in the weak- and intermediate-coupling regime. At strong coupling, the plain $1/N_f$ expansion is severely limited by Fierz ambiguity originating from multiple equivalent ways of Hubbard-Stratonovich decoupling of fermionic interaction vertices. This results in a problematic dependence of calculated phase diagrams on unphysical parameters.

For the common models, several physically motivated decoupling schemes have been developed over the years (see, e.g., Refs. 11-12), yet it is not clear how to systematically generalize them to arbitrary Hamiltonians. As one of the elements of VWF+$1/N_f$, we propose a conceptually different route to mitigate the Fierz problem by means of a specialized resummation of electronic interactions in the $1/N_f$ series. Finally, the construction of the combined VWF+$1/N_f$ is completed by carrying out a second resummation, ensuring that the large-$N_f$ (saddle point) free energy coincides with that obtained using VWF approach. This provides a systematic way to improve the plain VWF solution, as well as to calculate dynamical response functions to desired accuracy.

After setting up the formalism, we apply the VWF+$1/N_f$ approach to the hole-doped Hubbard model at the strong coupling $(U/t) = 8$ and compare both static and dynamics spin and charge susceptibilities against available DQMC data. The static spin susceptibility profiles agree semi-quantitatively for the two techniques if k-independent renormalization factor Z for large-$N_f$ VWF+$1/N_f$ susceptibilities is introduced in a direct analogy to the linear spin-wave theory calculations. We find that Z increases towards unity in hole-overdoped case, indicating a gradual loss multi-paramagnon scattering processes significance, as intuitively expected. The calculated energies of the charge and paramagnon excitations match quantitatively those obtained by DQMC as long as the width of those modes is not exceedingly large.

In the regime, where the collective excitations become highly incoherent, the VWF+$1/N_f$ and DQMC peak-intensity energies progressively diverge.

Finally, we demonstrate explicitly the gradual emergence of coherent quasiparticles from the particle-hole continuum as the system evolves from the non-interacting Fermi sea to strongly correlated metal with increasing onsite Coulomb repulsion. This progressive development is of basic interest in the context of the robust paramagnon and charge modes observed in variety of correlated compounds, but it is difficult to describe within $1/N_f$ expansions developed previously. This is because those techniques are constructed based on Hubbard operators and thus intended for strongly-coupled ($t$-$J$-model) limit. In effect, the impact of the finite-$U$ effects on charge dynamics has not received anticipated attention so far. By employing the particle-hole non-symmetric Hubbard model to reproduce the fermiology of high-$T_c$ superconductors, we find a sharp crossover behavior manifesting itself as a non-monotonic dependence of charge mode energy on the magnitude of electronic interactions. For overdoped system ($\delta = 20\%$), charge mode hardens with increasing interaction for $U \lesssim 0.5W$ (where $W$ is the bare bandwidth) and exhibits gradual softening above this threshold. Additionally, in the crossover regime, a sharp peak in charge response emerges from the continuum as a consequence of single-particle bandwidth renormalization due to strong correlations. We also demonstrate that the charge mode energy undergoes large renormalization (by a factor of $\sim 2$) as the interaction increases from $U \sim W$ to $U = \infty$. The charge-mode dynamics thus turns out to be governed, to a large extent, by finite-$U$ effects, which calling for reconsideration of the strong-coupling ($t$-$J$ model limit) approaches to as a tool to quantitatively study charge excitations in the cuprates in favor of more general $t$-$J$-$U$ and $t$-$J$-$U$-$V$ models. This is one of the principal findings of the present VWF+$1/N_f$ analysis. The spin-excitation peak-intensity energy, on the other hand, decreases systematically as $U$ is increased, with a resonance-like feature building up on top of the continuum.

The paper is organized as follows. In Sec. II we overview the Diagrammatic Expansion of the Gutzwiller Wave Function (DE-GWF) formulation of the VWF technique, that combines well with the $1/N_f$ expansion and is applicable also at non-zero temperature. In Sec. III we propose a resummation scheme for $1/N_f$ expansion, based on two-channel Hubbard-Stratonovich decoupling of the interaction term. In Sec. IV we construct hybrid VWF+$1/N_f$ technique, combining the developments of Secs. II and III. In Sec. V we apply the VWF+$1/N_f$ to the Hubbard model at various doping levels and compare calculated spin- and charge static and dynamic susceptibilities with available DQMC data. In Sec. VI we discuss the emergence of robust spin and charge excitations from the incoherent continuum. Finally, in Sec. VII we provide summary and discussion. Technical details and supplementary analysis are shifted to Appendices A-B.

II. VARIATIONALLY OBTAINED STATE AS THE SADDLE-POINT SOLUTION

The starting point of the VWF+$1/N_f$ technique is variational wave function $|\Psi_{\text{var}}\rangle \equiv \hat{P}(\lambda)|\Psi_0\rangle$, where $\hat{P}$ is an operator dependent on the vector of parameters, $\lambda$, and $|\Psi_0\rangle$ is an “uncorrelated” wave function that is defined as the ground state of a tight-binding Hamiltonian, i.e., $H_{\text{eff}}|\Psi_0\rangle = E|\Psi_0\rangle$ and is also adjusted variationally...
by selecting $\hat{H}_{\text{eff}}$. The precise form of $\hat{H}_{\text{eff}}$ is not specified at this point and hence, the effective Hamiltonian becomes a variational object itself. Numerous physically motivated choices for $\hat{P}$ are possible including those of Gutzwiller and Jastrow type.

The plain VWF method reduces to minimization of the energy functional

$$E_{\text{var}} \equiv \langle \hat{H} \rangle_{\text{var}} = \frac{\langle \Psi_{\text{var}} | \hat{H} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle}$$

with respect of both $\lambda$ and $\hat{H}_{\text{eff}}$, under the constraint $\langle \hat{N}_e \rangle_{\text{var}} \equiv N_e$. The operator $\hat{H}$ is the model Hamiltonian, whereas $\hat{N}_e$ and $N_e$ denote particle number operator and total electron number, respectively. We have also introduced correlated variational averages, marked by the subscript “var”. With the use of Wick’s theorem, both the numerator and denominator can be factorized in terms of two-point correlation functions (“lines”) of the form $P_{\alpha\beta} \equiv \langle \hat{c}_{\alpha} \hat{c}_{\beta} \rangle_0 \equiv \langle \Psi_0 | \hat{c}_{\alpha} \hat{c}_{\beta} | \Psi_0 \rangle$, where $\alpha, \beta$ are indices combining lattice-site position and local degrees of freedom (e.g., spin and orbital). A vector composed of all lines will be hereafter denoted as $\mathbf{P}$. In turn, the energy functional depends on line- and correlator-parameter vectors, $E_{\text{var}} = E_{\text{var}}(\mathbf{P}, \lambda)$. The variational problem reduces to minimization of $E_{\text{var}}$ over $\mathbf{P}$ and $\lambda$ under the constraints $P_{\alpha\beta} \equiv \langle \Psi_0 | \hat{c}_{\alpha} \hat{c}_{\beta} | \Psi_0 \rangle$ and $\langle \hat{N}_e \rangle_{\text{var}} \equiv N_e$. As we show below, for computational reasons it is customary to restrict further the correlator variational space by means of a vector composing the constraints, $\mathbf{C}(\mathbf{P}, \lambda) \equiv 0$.

The plain VWF method, outlined above, is a zero-temperature formalism that cannot account for the thermal effects and phase transitions. In the following we employ its more refined finite-temperature extension that reduces to the plain VWF solution in the $T \to 0$ limit. The starting point of the improved approach is the effective Landau functional of the form

$$\mathcal{F}(\lambda, \mathbf{P}, \xi, \rho, \mu) = -\frac{1}{\beta} \ln \text{Tr} \exp \left( -\beta E_{\text{var}}(\mathbf{P}, \lambda) + i\beta \sum_{\alpha\beta} \xi_{\alpha\beta}^* (P_{\alpha\beta} - \hat{c}_{\alpha}^\dagger \hat{c}_{\beta}) + i\beta \rho^T \cdot \mathbf{C}(\mathbf{P}, \lambda) + \beta \mu \left( \sum_{\alpha} P_{\alpha\alpha} - N_e \right) \right),$$

where $\xi$ and $\rho$ are vectors composed of Lagrange multipliers to be defined subsequently, trace is taken over electronic degrees of freedom, and $\beta \equiv (k_B T)^{-1}$ is the inverse temperature. The chemical potential, $\mu$, ensures that the total number of electrons in the system equals to $N_e$.

The methodology of the approach is as follows. We start from the model Hamiltonian (Hubbard, t-J, t-J-U, etc.) so that $E_{\text{var}}$ is given by Eq. (1). To assure that the quantities calculated self-consistently, i.e., the Bogoliubov theorem is fulfilled as shown earlier, we supplement $E_{\text{var}}$ determination with the Lagrange constraints (the last three terms). The Langrange multipliers have to be determined self-consistently (cf. also Appendix A). Finally, the nonzero temperature is included through inclusion of fluctuations of the physical quantities contained on the right-hand-side of Eq. (2). The physical free energy is determined as the saddle-point of the functional (2), leading to the set of equations

$$i\xi_{\alpha\beta}^* = \frac{\partial E_G(\mathbf{P}, \lambda)}{P_{\alpha\beta}} - i\rho^T \cdot \frac{\partial \mathbf{C}(\mathbf{P}, \lambda)}{\partial P_{\alpha\beta}} - \mu \delta_{\alpha\beta}, \quad (3)$$

$$\mathbf{C}(\mathbf{P}, \lambda) = 0, \quad (4)$$

$$P_{\alpha\beta} = \frac{\text{Tr} \hat{c}_{\alpha}^\dagger \hat{c}_{\beta} \exp(-\hat{H}_{\text{eff}})}{\text{Tr} \exp(-\hat{H}_{\text{eff}})} \quad (5)$$

$$\hat{H}_{\text{eff}} = \sum_{\alpha\beta} i\xi_{\alpha\beta}^* \hat{c}_{\alpha}^\dagger \hat{c}_{\beta}, \quad (6)$$

$$\sum_{\alpha} P_{\alpha\alpha} = N_e \quad (7)$$

The free energy may be then written as

$$F = -\frac{1}{\beta} \ln \mathcal{F}(\lambda, \mathbf{P}, \xi, \rho, \mu)|_{\text{at saddle point}} = E_G(\mathbf{P}, \lambda) - \sum_{\alpha\beta} \hat{H}_{\text{eff}}^{\alpha\beta} P_{\alpha\beta} - \frac{1}{\beta} \ln \text{Tr} \exp(-\hat{H}_{\text{eff}}) = E_G(\mathbf{P}, \lambda) - TS \quad (8)$$

where all the variables acquire the saddle-point values defined by Eqs. (3)-(7), and the entropy reads

$$S = -k_B \sum_l n_l \ln n_l - k_B \sum_l (1 - n_l) \ln (1 - n_l) \quad (9)$$
where index \( l \) runs over the complete set of eigenvalues of \( \mathcal{H}_{\text{eff}} \). At \( T = 0 \), the free energy \( \mathcal{H}_{\text{eff}} \) reduces thus to the minimum of the variational energy, as stated above. It is essential to note that eigenenergies are obtained by diagonalization of the effective single-particle Hamiltonian \( \mathcal{H}_{\text{eff}} \), defined by Eq. (4), and describes the interaction-renormalized Landau quasiparticles. For a detailed discussion of \( \mathcal{H}_{\text{eff}} \) as the object controlling effective quasi-particle dynamics, see Refs. [39,47]. The structure of the free energy thus implies that the variational technique, formulated above, incorporates single-particle excitations around the correlated ground-state, but lacks the collective mode contribution to thermodynamics. The aim of the next two sections is to provide an extension of the variational scheme which becomes capable of describing those excitations (fluctuations).

### A. Linked cluster expansion of the correlated energy functional

The main difficulty involved in a variational procedure is evaluation of the correlated energy functional \( E_{\text{var}}(\mathbf{P}, \lambda) \). In the following we restrict ourselves to the intra-orbital correlator in the form \( \hat{P} = \hat{P}_{\mathcal{G}} = \prod_I \hat{P}_{\mathcal{G},I} \), for which efficient computational schemes have been developed[48]. Here “\( I \)” and “\( P \)” run over lattice-site positions and orbital indices, respectively. For brevity, we have introduced also joint position and orbital index, \( I \equiv (i, l) \). The correlated expectation values, evaluated using \( \hat{P}_{\mathcal{G}} \), will be indicated by the subscript “\( \mathcal{G} \)”. To make sure that the VWF solution interfaces well with the fluctuation extensions introduced in Sec. [IV] already at this stage one needs to ensure that the employed correlator is compatible with the spin rotational symmetry. In particular, spin quantization axis cannot be arbitrarily fixed as this would discard the spin precession associated with spin-wave propagation that are active at low-energies. Violating this symmetry requirement at the correlator level typically results in breakdown of the Goldstone’s theorem in magnetically ordered states. We thus consider \( \hat{P}_{\mathcal{G},I} \) in the rotationally-invariant form

\[
\hat{P}_{\mathcal{G},I} = \lambda_{il}^0 |0 \rangle_I \langle 0 | + \lambda_{il}^{\uparrow \downarrow} | \uparrow \rangle_I \langle \downarrow | + \lambda_{il}^{\downarrow \uparrow} | \downarrow \rangle_I \langle \uparrow | + \lambda_{il}^{\uparrow \uparrow} | \uparrow \rangle_I \langle \uparrow | + \lambda_{il}^{\downarrow \downarrow} | \downarrow \rangle_I \langle \downarrow | + \lambda_{il}^{\uparrow \downarrow} | \uparrow \rangle_I \langle \downarrow | + \lambda_{il}^{\downarrow \uparrow} | \downarrow \rangle_I \langle \uparrow | + \lambda_{il}^{\uparrow \uparrow} | \uparrow \rangle_I \langle \uparrow | .
\]

(10)

Additionally, we require require that \( \hat{P}_{\mathcal{G},I} \) is Hermitian, which implies the relation \( \lambda_{il}^{\uparrow \downarrow} = \lambda_{il}^{\downarrow \uparrow} \). The terms \( \propto \lambda_{il}^{\uparrow \uparrow} \) and \( \propto \lambda_{il}^{\downarrow \downarrow} \) are necessary for rotational symmetry and are usually discarded in static variational calculations for paramagnetic and magnetic states with specified spin quantization axis. In the correlator \( \mathcal{G} \) we have disregarded doublon creation and annihilation terms \( \propto \langle 0 | \uparrow \rangle_I \langle \uparrow \downarrow | 0 \rangle_I \) and \( \propto \langle \uparrow \downarrow | \uparrow \rangle_I \langle 0 | 0 \rangle_I \) so that there are six independent correlator parameters per orbital.

The problem of evaluating the correlated expectation value \( \mathcal{G} \) simplifies substantially (cf. Ref. [48] and Appendix [B]) if the subsidiary condition

\[
\hat{P}_{\mathcal{G},I}^2 = 1 + x_l \hat{d}_I,
\]

(11)

is imposed. In Eq. (11)

\[
\hat{d}_I \equiv \hat{n}_I - n_I \hat{n}_I - \hat{n}_I \hat{n}_I + S_I^+ \hat{S}_I^- + S_I^+ \hat{S}_I^- + n_I \hat{n}_I - S_I^+ \hat{S}_I^-.
\]

(12)

is the modified double-occupancy operator with \( \hat{d}_I \equiv \hat{n}_I - n_I \hat{n}_I \), \( n_I \equiv \langle \Psi_0 | \hat{n}_I | \Psi_0 \rangle \), \( S_I^+ \equiv \langle \Psi_0 | \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \downarrow} | \Psi_0 \rangle \), \( S_I^- \equiv \langle \Psi_0 | \hat{c}_{I \downarrow} \hat{c}_{I \uparrow} | \Psi_0 \rangle \), and \( x_l \) denotes a free parameter. Requirement (11) along with the definitions (10) and (12) imposes five conditions for six \( \lambda \) variables, leaving out one only parameter per orbital,

\[
x_l \equiv \frac{\lambda_{l0}^2 - 1}{n_I \hat{n}_I - S_I^+ S_I^-}.
\]

(13)

Instead of working directly with the condition (11), hereafter we employ five constraints

\[
C^1_I \equiv \langle \hat{P}_{\mathcal{G},I}^2 \rangle_0 = 1,
\]

(14)

\[
C^2_I \equiv \langle \hat{P}_{\mathcal{G},I} \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \uparrow} \hat{P}_{\mathcal{G},I} \rangle_0 - \langle \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \uparrow} \rangle_0 = 0,
\]

(15)

\[
C^3_I \equiv \langle \hat{P}_{\mathcal{G},I} \hat{c}_{I \downarrow}^\dagger \hat{c}_{I \downarrow} \hat{P}_{\mathcal{G},I} \rangle_0 - \langle \hat{c}_{I \downarrow}^\dagger \hat{c}_{I \downarrow} \rangle_0 = 0,
\]

(16)

\[
C^4_I \equiv \text{Re} (\langle \hat{P}_{\mathcal{G},I} \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \downarrow} \hat{P}_{\mathcal{G},I} \rangle_0 - \langle \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \downarrow} \rangle_0) = 0,
\]

(17)

\[
C^5_I \equiv \text{Im} (\langle \hat{P}_{\mathcal{G},I} \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \downarrow} \hat{P}_{\mathcal{G},I} \rangle_0 - \langle \hat{c}_{I \uparrow}^\dagger \hat{c}_{I \downarrow} \rangle_0) = 0,
\]

(18)

which may be given a transparent physical interpretation (cf. Secs. [II A 1] and [II A 2] below) and imply (11), as shown in Appendix [A].

If one restricts to one- and two-site contributions in the Hamiltonian, which already encompasses most of the commonly used lattice models, evaluation of the correlated energy functional \( E_{\mathcal{G}} \) reduces to the computing of two kinds of averages: \( \langle A_I \rangle_{\mathcal{G}} \) and \( \langle A_I B_J \rangle_{\mathcal{G}} \), where \( A_I \) and \( B_J \) are operators acting on orbitals \( I \) and \( J \), respectively (\( I \neq J \) is assumed). A specialized version of linked-cluster theorem (see Appendix [B]) may be used to efficiently evaluate them. One obtains
\begin{equation}
\langle \hat{A}_I \rangle_G = \langle \hat{A}_I \rangle_0 + \sum_{k=0}^{\infty} \sum_{J_1 \ldots J_k} \frac{x_{J_1} \ldots x_{J_k}}{k!} \langle \left( \hat{A}_I - \langle \hat{A}_I \rangle_0 \hat{P}_{G,I}^2 \right) \cdot \hat{d}_{J_1} \ldots \hat{d}_{J_k} \rangle_0^c,
\end{equation}

(19)

where the superscript “c” in the averages means that only the diagrams, in which all operators entering \( \hat{d}_{J_k} \) are connected to external vertices at positions \( I/J \), are retained. We have defined “primed,” locally-correlated operators \( \hat{A}'_I \equiv \hat{P}_{G,I} \hat{A}_I \hat{P}_{G,I} \) and \( \hat{B}'_J \equiv \hat{P}_{G,J} \hat{B}_J \hat{P}_{G,J} \). Primed summations indicate that \( J_1, \ldots, J_k \) are restricted to be all different and also distinct from the external indices, \( I \) and \( J \).

Equations (19)-(20) constitute the basis for the diagrammatic expansion of the Gutzwiller wave function method (DE-GWF), developed elsewhere. Since the variational state serves only as a saddle-point solution within our expansion scheme, we restrict to two basic approximations to, detailed below. Incorporation of high-order diagrammatic contributions should be discussed separately.

1. Local-diagram approximation

Within the local-diagram (LD) approximation, only the operators, acting on the same sites as the terms of the original Hamiltonian, are retained. Disregarding all non-local contributions allows us to evaluate all expectation values contributing to the variational energy, \( E_{\text{var}} \), in a closed form. Namely, one arrives at

\begin{equation}
\langle \hat{A}_I \rangle_G \approx \langle \hat{A}'_I \rangle_0,
\end{equation}

(21)

\begin{equation}
\langle \hat{A}_I \hat{B}_J \rangle_G \approx \langle \hat{A}'_I \rangle_0 \langle \hat{B}'_J \rangle_0 + \langle \left( \hat{A}'_I - \langle \hat{A}'_I \rangle_0 \hat{P}_{G,I}^2 \right) \cdot \hat{B}_J \rangle_0,
\end{equation}

(22)

where the latter useful property is generally invalidated by higher-order diagrammatic contributions.

2. \( d = \infty \) (Gutzwiller) approximation

An approximation, providing expressions simpler than those given by LD approximation [cf. Eqs. (21)-(22)], is based on the formal assumption of large spatial dimensionality \( d \to \infty \) so that \( 1/d \) plays the role of small parameter. For a single-orbital model, such as the Hubbard model, it can be argued \(^{20}\) that \( d = \infty \) condition is implemented by adopting the following simplifications

\begin{equation}
\langle \hat{A}_I \rangle_G \approx \langle \hat{P}_{G,I} \hat{A}_I \hat{P}_{G,I} \rangle_0,
\end{equation}

(23)

\begin{equation}
\langle \hat{c}^\dagger_{J_o} \hat{c}_{J_o'} \rangle_G \approx \langle \hat{P}_{G,I} \hat{c}^\dagger_{J_o} \hat{P}_{G,I} \hat{P}_{G,J} \hat{c}_{J_o'} \hat{P}_{G,J} \rangle_0 \text{ one line},
\end{equation}

(24)

\begin{equation}
\langle \hat{S}_I \hat{S}_J \rangle_G \approx \langle \hat{P}_{G,I} \hat{S}_I \hat{P}_{G,I} \hat{P}_{G,J} \hat{S}_J \hat{P}_{G,J} \rangle_0 \text{ two lines},
\end{equation}

(25)

\begin{equation}
\langle \hat{n}_I \hat{n}_J \rangle_G \approx \langle \hat{P}_{G,I} \hat{n}_I \hat{P}_{G,I} \hat{P}_{G,J} \hat{n}_J \hat{P}_{G,J} \rangle_0 \text{ two lines},
\end{equation}

(26)

where we list explicitly only selected expectation values of interest. The substrates “one line” and “two lines” mean that one should retain only the diagrams containing no more than one and two non-local lines, respectively (non-local are those connecting sites \( I \) and \( J \)). The \( d = \infty \) approximation may be thus viewed as a truncated version of the local-diagram calculation, where the diagrams with the largest number of loops are discarded. Gutzwiller approximation inherits thus the property \( \langle \hat{c}^\dagger_{J_o} \hat{c}_{J_o'} \rangle_G = \langle \hat{c}^\dagger_{J_o} \hat{c}_{J_o'} \rangle_0 \).

III. RESUMMED 1/\( N_f \) EXPANSION AND FIERZ AMBIGUITY

Closed-form approximations for the free energy and dynamical structure factors of the collective modes may be obtained by extending the number of fermionic flavors from one to \( N_f \gg 1 \) and treating \( 1/N_f \) as a (formal) small parameter. This is effectively implemented by Hubbard-Stratonovich (HS) decoupling of the
fermionic interaction Hamiltonian in terms of auxiliary fields. The latter procedure is, however, the source of notorious Fierz-ambiguity problem (cf. Sec. I), which in the leading expansion order may also result in violating the symmetry-related properties, such as the Goldstone’s theorem. The former issue may be, to some extent, mitigated by inclusion of subleading terms in $1/N_f$ expansion or via renormalization-group procedure.[21] The latter, on the other hand, may be cured by careful selection of the decoupling scheme or applying specialized symmetrization procedures.[22] Importantly, by properly selecting the exact form of the standard Hubbard-Stratonovich decoupling, Gaussian-order fluctuations can be brought to the form consistent with the weak-coupling random-phase-approximation (RPA) results in selected scattering channels, but at the cost of disrupting the agreement in the other. An explicit example of the spin-rotationally-symmetric Hubbard-Stratonovich decoupling that leads to correct weak-coupling behavior of spin susceptibilities, but yields unphysical degeneracy between the masses of spin- and charge modes, is discussed in [23]. Also, alternative ways to avoid the Fierz ambiguity have been proposed very recently in the context of the dynamical mean-field theory extension, and are based either on cluster calculations.[24] or multi-channel decouplings.[25] In this section, we develop a variant of the Hubbard-Stratonovich transformation which results in an unbiased $1/N_f$ expansion and, at weak-coupling, reduces to the RPA results in all particle-hole scattering channels at the same time. As is shown in Sec. IV this decoupling may be also naturally extended to the regime of strong correlations.

A. Unbiased Hubbard-Stratonovich transformation

We consider a general normal-ordered Hamiltonian with four-fermion interactions only, i.e.,

$$\hat{H} = \hat{T} + \hat{V} = \sum_{\alpha \beta} (t_{\alpha \beta} - \delta_{\alpha \beta \mu}) \hat{c}_\alpha^\dagger \hat{c}_\beta + \frac{1}{2} \sum_{\alpha \beta \gamma \rho} V_{\alpha \beta \gamma \rho} \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\rho \hat{c}_\gamma,$$  (27)

where the Greek indices $\alpha$, $\beta$, $\gamma$, $\rho$ accommodate all degrees of freedom for given model (lattice, spin, orbital, etc.), and $\mu$ is chemical potential. By hermiticity, the coefficients the conditions $t_{\alpha \beta} = t_{\beta \alpha}^*$ and $V_{\alpha \beta \gamma \rho} = V_{\gamma \rho \alpha \beta}^*$. We have explicitly decomposed the Hamiltonian into the hopping and interaction parts, $\hat{T}$ and $\hat{V}$, respectively.

We define uncorrelated kinetic and potential energies in the form

$$E_{0,\text{kin}} = \langle \hat{T} \rangle_0 = \sum_{\alpha \beta} (t_{\alpha \beta} - \delta_{\alpha \beta \mu}) \langle \hat{c}_\alpha^\dagger \hat{c}_\beta \rangle_0$$  (28)

and

$$E_{0,\text{int}} = \langle \hat{V} \rangle_0 = \frac{1}{2} \sum_{\alpha \beta \gamma \rho} V_{\alpha \beta \gamma \rho} \langle \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\rho \hat{c}_\gamma \rangle_0$$

respectively. The symmetrized vertex $V_{\alpha \beta \gamma \rho} \equiv (V_{\gamma \rho \alpha \beta} + V_{\gamma \beta \rho \alpha} - V_{\gamma \rho \alpha \beta})/2$ satisfies the condition $\langle V_{\gamma \rho \alpha \beta} \rangle^* = V_{\alpha \beta \gamma \rho}$. The interaction matrix may be also written in manifestly hermitian form $V_{\alpha \beta \gamma \rho} = \partial_{\alpha \rho} \partial_{\beta \gamma} E_0$. It is also useful to define the total uncorrelated energy functional $E_0 \equiv E_{0,\text{kin}} + E_{0,\text{int}}$. The subindex "0" in the averages means that they are evaluated in an uncorrelated (Hartree-Fock-type) state $|\Psi_0\rangle$ so that Wick’s theorem holds. The fact that $T = 0$ averages are used to define $E_{0,\text{kin}}, E_{0,\text{int}}$ and $E_0$ may suggest that the resulting approach is limited to zero temperature, which is not the case. Below we demonstrate that VWF+$1/N_f$ is applicable at $T > 0$ as well.

We now propose the following transformation

$$\exp \left( - \int d\tau \hat{H}(\eta, \nu, \mu) \right) \propto \lim_{\epsilon \to 0} \int D\mathbf{P} D\mathbf{P}^\dagger \exp \left( - \int d\tau E_{0,\text{kin}}(\mathbf{P}, \mu) - \frac{1}{2} \int d\tau E_{0,\text{int}}(\mathbf{P}) + i \epsilon \mathbf{P}^\dagger \mathbf{P} - \frac{\epsilon}{2} \int d\tau \mathbf{P}^\dagger \mathbf{P} \right),$$  (30)

where $\eta_\alpha$ and $\nu_\alpha$ are the Grassmann fields. On the right-hand side, we have introduced Grassmann bilinears $P_{\alpha \beta} \equiv \eta_\alpha \nu_\beta$, as well as the complex fields $P_{\alpha \beta}^* \equiv \eta_\alpha^\dagger \nu_\beta^\dagger$ and $\xi_{\alpha \beta}$ being fluctuating line-fields and Lagrange multipliers enforcing that the line fluctuations are compatible with Hamiltonian dynamics, respectively. The last term, proportional to infinitesimal positive $\epsilon$, is introduced to regularize the integral. In the following, $P_{\alpha \beta}$ and $P_{\beta \alpha}$ are not considered to be independent variables, but we impose identities $P_{\alpha \beta} \equiv P_{\beta \alpha}^*$, in accordance with the symmetry properties of their Grassmann correspondents, $P_{\alpha \beta}$. In particular, the “diagonal” lines $P_{\alpha \alpha}$ are manifestly real. We have introduced a vector notation $\mathbf{P} = (P_{\alpha \beta})$ for all values of $\alpha$ and $\beta$; the remaining fields are handled in an analogous manner. In particular, $\xi \mathbf{P} \equiv \sum_{\alpha \beta} \xi_{\alpha \beta} P_{\alpha \beta} = \sum_{\alpha \beta} P_{\alpha \beta}^* \xi_{\alpha \beta} = \mathbf{P}^\dagger \xi$. The kinetic and potential energy functionals, entering Eq. (30), may be now written explicitly as $E_{0,\text{kin}}(\mathbf{P}) \equiv \sum_{\alpha \beta} \xi_{\alpha \beta} P_{\alpha \beta}$ and $E_{0,\text{int}}(\mathbf{P}) = \frac{1}{2} \sum_{\alpha \beta \gamma \rho} P_{\alpha \beta}^* V_{\alpha \beta \gamma \rho} P_{\gamma \rho}$. Remarkably, the interaction energy functional $E_{0,\text{int}}$ enters Eq. (30) with factor $\frac{1}{2}$. This is necessary to compensate for the double counting due to two inequivalent Wick contractions [cf. Eq. (28)]. Decomposition (30) is derived in Appendix C.

A methodological remark is in order at this point. The interaction energy functional, $E_{0,\text{int}}$, is generally
not positive definite, even for the simplest models. For the Hubbard Hamiltonian with on-site repulsive interaction, $U$, one gets $E_{0,\text{int}} = U \sum_i \langle n_i \sigma | n_i \sigma \rangle = U \sum_i \langle n_i \sigma | n_i \sigma \rangle$ with $n_i \sigma \equiv \langle \hat{n}_i \sigma \rangle$ and $S_i^\sigma \equiv \langle \hat{c}_i \hat{c}_i \rangle_0$, $S_i^\sigma \equiv S^\sigma +$, which is clearly not bounded from below for unrestricted line values. The order of integration in Eq. (30) thus matters and care should be taken to integrate out $\xi$ variables before integrating over $P$-fields whenever ambiguities arise. This effectively enforces constraint for $P$-field integration.

Making use of decoupling (30), the generating functional for the model (27) may be written as

$$Z[J] = \int \mathcal{D}\eta \mathcal{D}\bar{\eta} \exp \left( -\int d\tau \left\{ \hat{\eta} + \bar{\eta} \partial_\tau \eta - J^\dagger \hat{P} \right\} \right) \propto \lim_{\epsilon \to 0^+} \int \mathcal{D}\eta \mathcal{D}P \mathcal{D}\xi \exp (-S) \quad (31)$$

with the system action defined by

$$S = \int d\tau \bar{\eta} \partial_\tau \eta + \int d\tau E_{0,\text{kin}}(P, \mu) + \frac{1}{2} \int d\tau E_{0,\text{int}}(P) + i\xi^\dagger (P - \bar{P}) + \frac{\epsilon}{2} \int d\tau \xi \xi - \int d\tau J^\dagger \hat{P}, \quad (32)$$

with $J$ being the auxiliary current taken to define the generating functional, $Z[J]$.

**B. Resummed $1/N_f$ expansion**

We now turn to the $1/N_f$ expansion for the model Hamiltonian (27), starting from the action (32). For that sake, we introduce fermionic flavor index, $s = 1, \ldots, N_f$ and formally create $N_f$ copies of Grassmann fields, $\eta \to \eta^s$. The interaction matrix elements, $V_{\alpha\beta\gamma\mu}$, are rescaled accordingly by the factor $C_{N_f} \equiv \frac{2N_f-1}{N_f}$ to make the solution non-trivial in the large-$N_f$ limit. The prescription $\hat{V} \to \hat{V}_{N_f} \equiv C_{N_f} \hat{V}$ ensures that $\hat{V}_{N_f}$ interpolates smoothly between $\hat{V}_{N_f} \sim \hat{V}/N_f$ for $N_f \gg 1$ and $\hat{V}_{N_f} \sim 1/\hat{V}$ for $N_f = 1$, and distinguishes our approach from usual choice $C_{N_f} = 1/N_f$ (see, e.g., Ref. 54). At the same time, we may rescale the dummy Hubbard-Stratonovich fields as $P \to N_f P$ and infinitesimal term $\epsilon \to \epsilon/N_f$. Since kinetic- and potential energy functional are homogeneous functions of $P$-fields of degree one and two, respectively, we have a simple rescaling $E_{0,\text{kin}} \to N_f E_{0,\text{kin}}$ and $E_{0,\text{int}} \to N_f^2 C_{N_f} E_{0,\text{int}}$. In effect, we arrive at the action

$$S = \int d\tau \bar{\eta} \left( \partial_\tau + (i\xi^\dagger - J^\dagger) \hat{O} \right) \eta^s + \int d\tau \left( N_f E_{0,\text{kin}}(P, \mu) + N_f^2 \frac{C_{N_f}}{2} E_{0,\text{int}}(P) - i\xi^\dagger P + \frac{\epsilon}{2} \xi \xi \right) = \int d\tau \bar{\eta} \left( \partial_\tau + (i\xi^\dagger - J^\dagger) \hat{O} \right) \eta^s - \frac{1}{2} \int d\tau E_{0,\text{int}}(P) + N_f \int d\tau \left( E_0(P, \mu) - i\xi^\dagger P + \frac{\epsilon}{2} \xi \xi \right), \quad (33)$$

where we have introduced vector of matrices $\hat{O}$, with entries $\hat{O}_{\alpha\beta} \equiv (\bar{\eta} \bar{\eta}_{\alpha\beta} \eta)$. The present formulation has two desired properties: (i) it ensures that for physical case of $N_f = 1$ the Hubbard-Stratonovich decoupling reproduces exactly the original Hamiltonian (this becomes apparent after comparing Eq. (33) with Eq. (32) for $N_f = 1$), and (ii) in the regime of small interaction, the large-$N_f$ solution is consistent with the RPA calculation. Moreover, by construction, the proposed decoupling is unbiased as it does not favor any of the fermionic scattering channels. Since the introduced rescaling factor $C_{N_f}$ involves both $O(N_f^{-1})$ and $O(N_f^{-2})$ terms, it may be physically viewed as a resummation of the interaction analogous to those performed in hot quantum field theories. The $O(1/N_f^2)$ is not included at the level of the saddle-point solution, but it generates a two-point interaction vertex in the next-leading order, affecting the structure of expansion at all consecutive orders.

By integrating over fermions fields, the effective action (33) reduces to

$$S_{\text{eff}} = -N_f \text{Tr} \ln \left( -\partial_\tau - (i\xi^\dagger - J^\dagger) \hat{O} \right) + \frac{1}{2} \int d\tau \left( E_0(P, \mu) - i\xi^\dagger P + \frac{\epsilon}{2} \xi \xi \right) - \frac{1}{2} \int d\tau E_{\text{int}}(P). \quad (34)$$

The large-$N_f$ solution is found as a saddle point of the first two terms on the right-hand-side of Eq. (34) with external currents $J$ set to zero and the last $O(1)$ term discarded. The saddle point equations must be supplemented with the requirement that the total number of electrons is equal to $N_e$, providing the condition for chemical potential, $\mu$. In turn, one obtains

$$P_{\alpha\beta}^{(0)} = \tilde{c}^\beta_\alpha (0^-), \quad (35)$$

$$\eta_{\alpha\beta}^{(0)} = \frac{\partial E_0(P^{(0)}, \mu)}{\partial P^{(0)}_{\alpha\beta}}, \quad (36)$$

$$\sum_\alpha P_{\alpha\alpha} = N_e, \quad (37)$$
which is equivalent to the Hartree-Fock solution. We have used the superscript “(0)” to mark large-\(N_f\) value and introduced bare imaginary-time Green’s function

\[
\hat{G}_0^{\alpha \beta} (\tau - \tau') = \frac{-\text{Tr} \mathcal{T}_\tau \hat{c}_\alpha (\tau) \hat{c}^\dagger_{\beta} (\tau') \exp(-\hat{H}_\text{eff})}{\text{Tr} \exp(-\hat{H}_\text{eff})}, \quad (38)
\]

defined through the effective quasiparticle Hamiltonian

\[
\hat{H}_\text{eff} = \sum_{\alpha \beta} i \varepsilon^{\alpha (0)} c^\dagger_{\alpha} \hat{c}_\beta = \sum_{\alpha \beta} \frac{\partial E_0 (\mathbf{P}(0), \mu)}{\partial P^{\alpha \beta}} \hat{c}^\dagger_{\alpha} \hat{c}_\beta. \quad (39)
\]

The right-hand-side of Eq. \([39]\) has been obtained with the use of the saddle-point condition \([36]\).

Thermodynamic corrections to the saddle point may now be systematically studied by decomposing the fields into the static saddle-point and dynamic fluctuation parts as \(\xi (\tau) \rightarrow \xi^{(0)} + \delta \xi (\tau), \mathbf{P} (\tau) \rightarrow \mathbf{P}(0) + \delta \mathbf{P} (\tau)\), and expanding the action to quadratic terms in fluctuations and currents. One arrives at

\[
S_{\text{eff}} = N_f S_{\text{eff}}^{(0)} + \frac{N_f}{2} \int d\tau d\tau' (\delta \mathbf{P}^{\dagger}, \delta \xi^{(0)}) \left( \begin{array}{cc} \hat{V}(\tau - \tau') & -i \delta(\tau - \tau') \\ -i \delta(\tau - \tau') & \epsilon (\tau - \tau') + \hat{\chi}_0 (\tau, \tau') \end{array} \right) \left( \begin{array}{c} \delta \mathbf{P} \\ \delta \xi \end{array} \right) - \frac{N_f}{2} \int \mathbf{J}^{\dagger} \hat{\chi}_0 \mathbf{J}, \quad (40)
\]

where

\[
S_{\text{eff}}^{(0)} = -\sum_{\alpha} \text{tr} \ln \hat{G}(i\omega_n)^{-1} + \beta \left( E(\mathbf{P}(0)) - i \xi^{(0)} \mathbf{P}(0) + \frac{\epsilon}{2} \xi^{(0)} \xi^{(0)} \right) \quad (41)
\]

is the saddle-point action and

\[
\hat{\chi}^{\alpha_1 \beta_1 \alpha_2 \beta_2}_0 (\tau, \tau') = \langle T \hat{r}^{\alpha_1}_\tau (\tau) \hat{c}^{\dagger}_{\beta_1} (\tau') \hat{c}_{\alpha_2} (\tau') \hat{c}_{\beta_2} (\tau) \rangle_0 = -G^{\alpha \beta}_0 (\tau - \tau') G^{\alpha_2 \beta_1}_0 (\tau' - \tau) \quad (42)
\]

is the Lindhard susceptibility. Finally, by integrating out the Gaussian fluctuations and taking \(\epsilon \rightarrow 0^+\) limit, one arrives at the final form of the effective action

\[
S_{\text{eff}} = N_f S_{\text{eff}}^{(0)} + \frac{1}{2} \sum_n \text{tr} \ln \left( 1 + \hat{\mathcal{V}} \hat{\chi}_0 (i\omega_n) \right) - \frac{\beta}{2} E_{\text{int}} (\mathbf{P}(0)) - \frac{N_f}{2\beta} \sum_n \mathbf{J}^{\dagger} (i\omega_n) (1 + \hat{\chi}_0 (i\omega_n) \hat{\mathcal{V}})^{-1} \hat{\chi}_0 (i\omega_n) \mathbf{J} (i\omega_n)
\]

\[
- N_f \mathbf{J}^{\dagger} (i\omega_n = 0) \mathbf{P}(0) \quad (43)
\]

to the order \(\mathcal{O}(1)\). We have introduced Fourier-transformed fields and susceptibilities as

\[
\mathbf{J}(i\omega_n) = \int d\tau e^{i\omega_n \tau} \mathbf{J}(\tau), \quad (44)
\]
\[
\hat{\chi}_0 (i\omega_n) = \int d(\tau - \tau') e^{i\omega_n (\tau - \tau')} \hat{\chi}_0 (\tau, \tau'). \quad (45)
\]

The term \(\propto \text{Tr} \ln \) in the first line of Eq. \([43]\) is the thermodynamic correction due to collective excitations, whereas \(\frac{\beta}{2} E_{\text{int}} (\mathbf{P}(0))\) originates from our resummation procedure and is absent in standard \(1/N_f\) expansion. The term \(\propto \mathbf{J}^{\dagger} (i\omega_n = 0) \mathbf{P}(0)\) represents elastic (Bragg) contribution that disappears if the saddle-point value of the line is zero, i.e., \(\mathbf{P}(0) = 0\).

## IV. VARIATIONAL WAVE FUNCTION APPROACH COMBINED WITH \(1/N_f\) EXPANSION

We are now in position to introduce VWF+1/\(N_f\) approach, combining diagrammatic VWF method with resummed 1/\(N_f\) expansion, outlined in Secs. \(\text{II}\) and \(\text{III}\) respectively. The idea is based on performing the second resummation, in addition to that discussed in Sec. \(\text{III}\) so
that the resulting expansion fulfill the following conditions: (i) it agrees with the VWF solution at the saddle-point level, (ii) is not biased in favor of any of the scattering channels, (iii) reproduces the exact generating functional \([31]\) for the model Hamiltonian \(\hat{\mathcal{H}}\) in the physical \(N_f = 1\) limit, (iv) is capable of describing correlated collective excitations (e.g., charge, spin) already in the leading non-trivial order, and (v) it reduces to RPA at weak coupling.

We argue that \(1/N_f\) expansion based on the modified action

\[
S_{\text{var}}[\mathbf{P}, \xi, \rho, \bar{\eta}, \eta, \mathbf{J}, \mu] = \int d\tau \bar{\eta}^a \left( \partial_\tau + (i\xi^I - J^I) \hat{\mathcal{O}} \right) \eta^a + N_f \int d\tau \left( E_{\text{var}}(\mathbf{P}, \lambda, \mu) - i\xi^I \mathbf{P} \right) + \int d\tau E_{0,\text{kin}}(\mathbf{P}, \mu) + \frac{1}{2} \int d\tau E_{0,\text{int}}(\mathbf{P}) - \int d\tau E_{\text{var}}(\mathbf{P}, \lambda, \mu) - iN_f \int d\tau \rho^T \mathbf{C}(\mathbf{P}, \lambda) + \frac{N_f}{2} \kappa \int d\tau \mathbf{C}(\mathbf{P}, \lambda)^T \mathbf{C}(\mathbf{P}, \lambda) - \ln \left| \det \frac{\partial \mathbf{C}}{\partial \lambda} \right| \tag{46}
\]

fulfills the requirements (i)-(v). For brevity of notation, in the above action we have deliberately omitted the \(e\)-terms that should be reintroduced whenever necessary. The structure of the first two lines of Eq. \(46\) is reminiscent of the uncorrelated action of Eq. \(33\), albeit with two modifications. First, in the \(O(N_f)\) block, the uncorrelated energy functional \(E_0(\mathbf{P}, \mu)\) has been substituted with the correlated one, \(E_{\text{var}}(\mathbf{P}, \lambda, \mu)\). To proof the concept, here we restrict to calculations for the Gutzwiller functional, \(E_{\text{var}} \equiv E_G\). Second, the resummed \(O(1)\) terms [second line of Eq. \(46\)] have been adjusted accordingly so that the action \(32\) is retrieved for \(N_f = 1\). Now, since the correlated energy depends not only on the line-fields \(\mathbf{P}\), but also on the correlator parameter vector, \(\lambda\), the constraints introduced in Section \(\S 1\) need to be incorporated at the dynamical level. This is implemented in the third line of Eq. \(46\) by means of an additional set of time-dependent Lagrange-multiplier fields, \(\rho\). The unconventional term \(\propto \kappa \int d\tau \mathbf{C}^T \mathbf{C}\) in the last line, controlled by a positive parameter \(\kappa\), is of no physical significance due to the constraints \(\mathbf{C} = 0\), but it regularizes the series expansion, as elaborated below. Finally, the \(\ln \left| \det \frac{\partial \mathbf{C}}{\partial \lambda} \right|\) term, with \(\frac{\partial \mathbf{C}}{\partial \lambda}\) being the Jacobian of the constraints, is necessary to compensate for unphysical interaction terms generated by the fluctuations of the correlator parameters. This contribution is highly non-linear and it may be equivalently represented as a functional integral over Faddeev-Popov ghost fields \(\xi^I\) to facilitate calculations beyond the leading order. As a formal requirement (allowing to make the approach rigorous), we demand additionally that the \(\lambda\)-fields have no own dynamics, i.e. they passively adjust to fluctuations of the line-fields, \(\mathbf{P}\). The number of constraints must thus match number of \(\lambda\)-fields. Moreover, uniqueness of the solution is assumed (this can be always achieved by proper choice of constraints). In Sec. \(\S 1\) we have already constructed five constraints for six \(\lambda\) parameters per orbital. As an additional, sixth constraint, we will hereafter consider consider either (i) \(C_\lambda^I = \lambda_{d,I} - \bar{\lambda}_{d,I}\) or (ii) \(C_\lambda^I = (n_I n_{1I} - S_I^+ S_I^-) x_I - (\lambda_{10}^2 - 1)\), where \(\lambda_{d,I}\) and \(x_I\) are understood to be time-independent variational parameters to be determined by minimization of the free energy functional. The choices (i) and (ii) define two different resummation schemes and their selection should be made based on physical arguments and benchmarks against other techniques. The variant (i) is based on assumption that the dynamics in the doublon sector is much faster than that of the collective excitations, whereas (ii) is generalization of the tadpole cancellation condition \(12\) to the dynamical level. Our benchmark calculations reveal that, up to moderate coupling, the large-\(N_f\) solutions obtained within both schemes are quantitatively consistent, whereas the first one (i) provides more reliable charge dynamics at strong coupling. Summary of the approximation schemes and acronyms used throughout the paper is shown in Table \(\S 1\). A formal derivation and extended discussion of Eq. \(46\) are deferred to Appendix \(\S D\).

### A. Correlated large-\(N_f\) limit

We now proceed to analyze the saddle-point (large-\(N_f\)) VWF+1/\(N_f\) solution by retaining only the leading \(O(N_f)\) terms and those involving Grassmann variables, in the full analogy to the discussion of Sec. \(\S 1\). After integrating out fermions, one arrives at the correlated effective action

\[
S_{\text{var,eff}}[\mathbf{P}, \xi, \rho, \mathbf{J}, \mu] = N_f \int d\tau \left\{ E_{\text{var}}(\mathbf{P}, \lambda, \mu) - i\xi^I \mathbf{P} - i\rho^T \mathbf{C}(\mathbf{P}, \lambda) + \frac{\kappa}{2} \mathbf{C}(\mathbf{P}, \lambda)^T \mathbf{C}(\mathbf{P}, \lambda) \right\} - N_f \kappa \ln \left[ \text{det} \left( \frac{\partial \mathbf{C}}{\partial \lambda} \right) \right] + \mathcal{O}(1) \tag{47}
\]
so that the large-$N_f$ saddle point equations read

\[ \begin{align*}
\mathbf{P}^{(0)}_{\alpha\beta} &= \hat{G}^{\alpha\beta}_{0}(0), \\
\mathbf{C}^{(0)}_{\alpha\beta}\mathbf{C}^{(0)}_{\alpha\beta} &= 0,
\end{align*} \]

(48)

(51)

(52)

Equations (48)-(50) resemble those for the uncorrelated expansion [Eqs. (35)-(37)]. The essential difference is that the correlated energy $E_{\text{var}}$ rather than $E_0$ is used in Eq. (50). The Green’s function in Eq. (48) is defined in the same manner as in the uncorrelated case, but using the correlated effective Hamiltonian

\[ \hat{H}_{\text{corr}} = i\xi^\dagger \mathbf{P} = \sum_{\alpha\beta} \left( \frac{\partial E_{\text{var}}}{\partial P_{\alpha\beta}} - i\rho_T \frac{\partial \mathbf{C}}{\partial \mathbf{P}^{(0)}_{\alpha\beta}} \right) c^\dagger_{\alpha} \hat{c}_{\beta}. \]

(53)

Note that, for general $E_{\text{var}}$, the left-hand-side of Eq. (50) for the chemical potential cannot be evaluated explicitly as in the uncorrelated case. Nonetheless, for the truncated series expansions, described in IIA1 and IIA2, Eq. (50) becomes identical to Eq. (37). For the Gutzwiller energy functional ($E_{\text{var}} = E_G$), Eqs. (48)-(52) constitute the set of integral equations that are equivalent to those solved within the DE-GWF method.

B. Effective scattering matrix and correlated collective modes

The collective excitations around the correlated ground state may be studied by employing the procedure, analogous to that described in Sec. III for the Hartree-Fock saddle-point. This leads to the Gaussian-fluctuation action

\[ S_{\text{var,eff}} \approx N_f S_{\text{var,eff}}^{(0)} + \frac{N_f}{2} \int d\tau (\delta \mathbf{P}^4 \delta \lambda^4 \delta \rho^4) \left( \begin{array}{cccc} \tilde{\mathcal{V}}_{\lambda\alpha\beta} & \kappa \tilde{\mathcal{V}}_{\alpha\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} \\
\kappa \tilde{\mathcal{V}}_{\alpha\beta} & \kappa \tilde{\mathcal{V}}_{\alpha\beta} & \kappa \tilde{\mathcal{V}}_{\alpha\beta} & \kappa \tilde{\mathcal{V}}_{\alpha\beta} \\
\kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} \\
\kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} & \kappa \tilde{\mathcal{V}}_{\lambda\beta} \end{array} \right) \left( \begin{array}{c} \delta \mathbf{P} \\
\delta \lambda \\
\delta \rho \\
\delta \rho \end{array} \right) - \frac{N_f}{2} \int d\tau \mathbf{J}^4 (\mathbf{P}^{(0)}) + \mathcal{O}(1), \]

(54)

where

\[ \tilde{\mathcal{V}}_{\alpha\beta} = \partial_{\alpha\beta} \partial_{\lambda\rho} (E_G - i\rho T \mathbf{C}) \]

are scattering matrix elements, reflecting interactions between fluctuation fields. As before, the subscript “0” indicates that the derivatives are evaluated at the saddle point.

The problem, given by Eq. (54), can be simplified by introducing the concept of effective scattering matrix, $\mathcal{V}_{\text{eff}}$, describing residual interactions between correlated quasi-particle excitations, which is obtained by integrating out the $\lambda$ and $\rho$ fields. As is demonstrated in Appendix D, the resulting $\mathcal{V}_{\text{eff}}$ is independent on $\kappa$. Inclusion of the terms $\propto \kappa$ may be thus regarded as a gauge transformation that ensures convergence while evaluating the integral over $\mathbf{A}$-fields. Explicitly, we obtain (Appendix D)

\[ \tilde{\mathcal{V}}_{\text{eff}} = \tilde{\mathcal{V}}_{\rho\rho} - (\tilde{\mathcal{V}}_{\rho\rho}, i\tilde{\mathcal{V}}_{\rho\rho}) \left( \begin{array}{cc} \tilde{\mathcal{V}}_{\lambda\lambda} & i\tilde{\mathcal{V}}_{\lambda\rho} \\
i\tilde{\mathcal{V}}_{\rho\lambda} & 0 \end{array} \right)^{-1} \left( \begin{array}{c} \tilde{\mathcal{V}}_{\lambda\lambda} \\
i\tilde{\mathcal{V}}_{\rho\lambda} \end{array} \right), \]

(60)

so that now

\[ S_{\text{var,eff}} = N_f S_{\text{var,eff}}^{(0)} + \frac{N_f}{2} \int d\tau \delta \mathbf{P}^4 \mathcal{V}_{\text{eff}} \delta \mathbf{P} - i \int d\tau \delta \xi^4 \mathcal{P} - \frac{N_f}{2} \int d\tau d\tau' \left( i\delta \xi^4 (\mathbf{J}^4 (\mathbf{P}^{(0)})) \chi (\mathbf{J}^4 (\mathbf{P}^{(0)})) \right) - \frac{N_f}{2} \int d\tau d\tau' \left( i\delta \xi^4 (\mathbf{J}^4 (\mathbf{P}^{(0)})) \chi (\mathbf{J}^4 (\mathbf{P}^{(0)})) \right), \]

(61)

This action may be used directly to construct the generating functional as discussed in Sec. III. The final large-$N_f$ form for the correlated case is thus
\[
Z[\mathbf{J}] \approx \exp \left( -N_f S^{(0)}_\text{eff} + \frac{N_f}{2\beta} \sum_n J^{(i\omega_n)}_n \chi(i\omega_n) J(i\omega_n) - N_f \int d\tau J^{(0)} \right),
\]

where the correlated dynamical susceptibility matrix reads

\[
\tilde{\chi}(i\omega_n) = (1 + \tilde{\chi}_0(i\omega_n) \tilde{V}_{\text{eff}})^{-1} \tilde{\chi}_0(i\omega_n).
\]

In Eq. (63), \( \tilde{\chi}_0(i\omega_n) \) represents correlated Lindhard susceptibility evaluated using single-particle excitations governed by the correlated effective Hamiltonian \[\text{[53]}\].

This completes the technical overview of the VWF+1/\( N_f \) method. Below, we discuss the applications of the leading-order formula (62) to the one-band Hubbard model.

V. COMPARISON WITH DETERMINANT QUANTUM MONTE-CARLO

The techniques providing quantitatively reliable description of the dynamics for large-sized strongly-correlated fermionic systems are scarce. To benchmark our VWF+1/\( N_f \) approach, here we resort to available determinant quantum Monte-Carlo (DQMC) data as a reference point. It should be emphasized though that DQMC and VWF+1/\( N_f \) have different use cases and regimes of applicability. Namely, VWF+1/\( N_f \) is an approximate tool for exploring real-time dynamics in the thermodynamic-limit, possibly in a broken-symmetry state. DQMC, on the other hand, provides a numerically exact description of the imaginary-time correlations for small systems (tens of sites) in the disordered state. Since analytic continuation of the Monte-Carlo data introduces poorly controlled errors (see, e.g., Ref. [25]), such a benchmark accounts to comparison between two sets of approximate data points.

Before turning attention to dynamical quantities, we address first the static magnetic response that does not rely on analytic continuation. We employ particle-hole-symmetric Hubbard model at strong-coupling (only nearest-neighbor hopping, \( t \), is retained and the on-site repulsion is set to \( U/|t| = 8 \)). In Fig. 1(a)-(b) we display renormalized paramagnetic-state SGA\( \lambda_d+1/N_f \) and DQMC results of Ref. [59] by green circles and blue diamonds, respectively (for the definition of the SGA\( \lambda_d+1/N_f \), see Table I). Panels (a) and (b) correspond to overdoped (\( \delta = 0.40 \)) and undoped (\( \delta = 0 \)) system, respectively. The temperature has been set to \( k_B T = |t|/3 \) for DQMC, whereas \( k_B T = 0.333|t| \) and \( k_B T = 0.35|t| \) has been used for SGA\( \lambda_d+1/N_f \) in panels (a) and (b), respectively. The reason for selecting such a high temperature is twofold: (i) within DQMC it improves the statistics by reducing the sign problem and (ii) it allows to say clear of the spurious low-temperature broken-symmetry states within SGA\( \lambda_d+1/N_f \) [cf. Appendix [E]].

As is apparent from Fig. 1, the SGA\( \lambda_d+1/N_f \) closely follows the DQMC susceptibility profile along the representative \( \Gamma-X-M-\Gamma \) \( k \)-space contour (green circles and blue diamonds, respectively), yet it overestimates it quantitatively in a systematic manner. This behavior is expected within large-\( N_f \) calculation, since the effects magnetic spectral-weight redistribution due to magnon (multi-paramagnon) excitations that are not included in the leading order. The latter tend to reduce static susceptibility and may be systematically calculated as \( 1/N_f \) corrections within the framework of the model [46]. This goes beyond the scope of the present contribution; we take another route by introducing spin-susceptibility renormalization factor, \( \chi_s \rightarrow Z\chi_s \). The latter procedure is fully analogous to that employed in Fig. 1. Static spin susceptibilities of the particle-hole symmetric, two-dimensional Hubbard model with only nearest-neighbor hopping included, and the on-site repulsion \( U/|t| = 8 \). Hole doping level is set to \( \delta = 0.40 \) [panel (a)] and at half-filling [panel (b)]. Lattice size is taken as \( 10 \times 10 \). Blue diamonds represent determinant quantum Monte-Carlo data of Ref. [59] at temperature \( k_B T = |t|/3 \), whereas green circles represent corresponding paramagnetic-phase SGA\( \lambda_d+1/N_f \) results for \( k_B T = 0.333|t| \) [panel (a)] and \( k_B T = 0.35|t| \) [panel (b)]. Red crosses are SGA\( \lambda_d+1/N_f \) scaled by respective renormalization factors \( Z = 0.80 \) for panel (a) and \( Z = 0.61 \) for panel (b) (cf. discussion in the text). Cyan symbols represent correlated bare (Lindhard) susceptibilities, \( \tilde{\chi}_0(k, \omega = 0) \). Lines are guides to the eye.
FIG. 2. Comparison of imaginary parts of the dynamical charge- and spin susceptibilities (top and bottom panels, respectively) obtained within the SGA$\delta + 1/N_f$ and DQMC methods for undoped ($\delta = 0$), near-optimally-doped ($\delta = 0.15$), and overdoped ($\delta = 0.40$) 300 × 300 square-lattice Hubbard model. The model parameters are: $t < 0$, $t' = 0.3|t|$, $U = 8|t|$, temperature $k_B T = |t|/3$ (DQMC), $k_B T = 0.35|t|$ (SGA$\delta + 1/N_f$ at $\delta = 0$), and $k_B T = 0.333|t|$ (SGA$\delta + 1/N_f$ at $\delta > 0$). Color maps illustrate imaginary parts of SGA$\delta + 1/N_f$ dynamical susceptibilities, whereas red lines follow maximal values of intensities for given wave vector. Yellow symbols are the corresponding maximum-intensity frequencies for analytically continued 64-site DQMC data of Ref. 60. For definition of SGA$\delta + 1/N_f$, cf. Table I. Analytic continuation was performed as $i\omega_n \to w + i\epsilon$ with $\epsilon = 0.02|t|$.

linear spin-wave theory calculations, where the values of renormalization factors are known. We have found $Z \approx 0.61$ for undoped system ($\delta = 0$) and $Z \approx 0.80$ for the overdoped case ($\delta = 0.40$). The SGA$\delta + 1/N_f$ result, rescaled by respective renormalization factors, $Z$, is marked in Fig. 1 by red crosses, yielding semi-quantitative agreement with DQMC data. The renormalization factors for undoped case can be directly compared with available square-lattice Heisenberg model results, where spin-wave-theory calculation provides $Z_x = 0.4844$ [88] whereas within the series expansion method $Z_x = 0.52$ [89] is obtained. Both results are consistent with our estimate for $\delta = 0$ within $< 30\%$ margin, even though we consider magnetically-disordered state at finite temperature and for finite Hubbard-$U$ rather than the Néel state at $T = 0$ and strong-coupling. As to the overdoped case, where reference results from spin-models are not available, an increase of $Z$ is observed. This is expected behavior and we attribute it to reduction of the nonlinear fluctuation corrections due to loss of the spin-coherence deep in metallic state. Finally, magenta symbols represent the correlated Lindhard susceptibility, $\chi_0(k, \omega)$, evaluated at $\omega = 0$ [cf. Eq. (63)], which is featureless for both doping levels, in disagreement with the DQMC data. The residual scattering is thus a driving force for substantial magnetic response enhancement.

We now proceed to collective-mode dynamics. In Fig. 2, we compare the SGA$\delta + 1/N_f$ results (cf. Table I) with DQMC for the Hubbard model with nearest- and next-nearest-neighbor hopping at strong-coupling. The set of parameters, common for both methods, is $t < 0$, $t' = 0.3|t|$, $U = 8|t|$, and temperature $k_B T = |t|/3$ (DQMC), $k_B T = 0.35|t|$ (SGA$\delta + 1/N_f$ at $\delta = 0$), and $k_B T = 0.333|t|$ (SGA$\delta + 1/N_f$ at $\delta > 0$). Remarkably, for this parameter range, the weak-coupling RPA approach fails outright as it does not yield a locally-stable paramagnetic state. In previous RPA studies, this problem was bypassed by taking nonphysically small $U \sim 1.5|t|$ [90]. The top panels of Fig. 2 show imaginary part of the dynamical charge susceptibility along $\Gamma$-$X$ and $\Gamma$-$M$ lines, evaluated for three hole-doping levels [undoped $\delta = 0$ for (a)-(b), near-optimally-doped $\delta = 0.15$ for (c)-(d), and overdoped $\delta = 0.40$ for (e)-(f)]. The color map represents the paramagnetic-state SGA$\delta + 1/N_f$ intensity obtained for a $300 \times 300$ lattice, whereas red lines follow maximum values of calculated intensities. Yellow symbols are the corresponding DQMC maximum-intensity frequencies obtained for a 64-site lattice [90]. Lower panels represent longitudinal spin susceptibilities, obtained using the same set of parameters as the corresponding top panels (note different energy scales for charge- and spin excitations).

As follows from Fig. 2(a)-(f), the characteristic charge excitation energies agree well between the two techniques, with the exception of $\Gamma$-$X$ direction for undoped systems [panel (a)] and $\Gamma$-$M$ direction for overdoped case [panel (f)]. To understand those discrepancies at both ends, one should take into consideration not only the peak po-
sitions, but also widths of the features in the dynamic charge susceptibilities. By inspecting DQMC intensity profiles [Fig. 3(d1)-(d2) of Ref. 60], it is apparent that the energy-width of charge excitations increases with doping along the nodal $\Gamma$-$M$ direction, whereas the opposite tendency is seen for the anti-nodal $\Gamma$-$X$ axis. In turn, panels (a) and (f), correspond precisely to the situation, where charge modes are incoherent and not well defined. A detailed analysis of the charge-mode lineshapes across the Brillouin zone for both techniques is thus needed to make a robust comparison at those doping levels. Interestingly, SGA $\lambda_\delta+1/N_f$ method yields sharp peaks in the charge susceptibility for undoped and intermediately-doped systems (yet considerable damping appears for the overdoped case), in contrast to relatively broad features in DQMC profiles at all doping levels. It is not obvious at this point whether the latter discrepancy should be interpreted as an artifact of a large-$N_f$ limit, or an inaccuracy related to analytic continuation that may smear-out or miss sharp spectral features (see, e.g., Ref. 28).

Panels (g)-(l) of Fig. 2 show calculated imaginary parts of the dynamical longitudinal spin susceptibility for the same doping levels as the top panels, (a)-(f). Whereas semi-quantitative agreement between SGA $\lambda_\delta+1/N_f$ and DQMC data is observed for the anti-nodal ($\Gamma$-$X$) direction at all hole concentrations [panels (g), (i), and (k)], notable differences occur for the nodal ($\Gamma$-$M$) line. For the intermediate- and highly-doped cases the discrepancies along $\Gamma$-$M$ line may be, once again, interpreted in terms of broad DQMC line shapes. Indeed, by inspecting Fig. 2(d1)-(d2) of Ref. 60 we find out that the features in the magnetic response along the nodal direction become extremely broad for $\delta > 0.1$, with widths by far exceeding peak energies. The anti-nodal paramagnons, on the other hand, retain their coherence up to overdoped regime. Once again, matching of the peak positions alone is thus not an authoritative benchmark along $\Gamma$-$M$ direction for doped systems. On the other hand, the discussion for the $G$-$X$ direction, where both approaches yield well-defined paramagnons is more reliable in this context. Parenthetically, such strongly-anisotropic damping, revealed by both techniques, is consistent with recent experiments on high-$T_c$ cuprates (cf. Sec. 1) and may be semi-quantitatively described within the present VWF+1/$N_f$ approach 29 As to the undoped ($\delta = 0$) case, the SGA $\lambda_\delta+1/N_f$ overestimates the paramagnon damping which leads to underestimated paramagnon energies. Remarkably though, a non-monotonic behavior of the intensity maximum in Fig. 2(h) and (j), seen within DQMC, is also observed within SGA $\lambda_\delta+1/N_f$. This is related to strong antiferromagnetic correlations that cause transfer of the magnetic spectral weight to lower energies near the $M$ point.

In Fig. 3 we perform a similar analysis of the maximum-intensity profiles for the particle-hole symmetric Hubbard model ($t' = 0$) and compare the results with the DQMC data of Ref. 59. The model parameters are taken as $U = 8|t|$, $k_B T = |t|/3$ (DQMC), $k_B T = 0.333|t|$ (SGA $\lambda_\delta+1/N_f$ for $\delta > 0$), and $k_B T = 0.35|t|$ (SGA $\lambda_\delta+1/N_f$ for $\delta = 0$). The slightly elevated temperature for $\delta = 0$ is necessary to avoid an instability toward antiferromagnetic state. Since Ref. 59 provides dynamic structure factor

$$S(k, \omega) = -\frac{2}{\exp(-\omega/k_B T) - 1} \chi''(k, \omega) \tag{64}$$

that differs from the imaginary part of dynamical spin susceptibility by detailed balance factor, here we compute this quantity as well. Fig. 3 shows the comparison of $S(k, \omega)$, obtained within SGA $\lambda_\delta+1/N_f$ with the DQMC result for three doping levels, $\delta = 0$ [panels (a)-(b)], $\delta = 0.2$ [panels (c)-(d)], and $\delta = 0.4$ [panels (e)-(f)]. In full analogy to the particle-hole asymmetric case, the agreement between maximum-intensity profiles along $\Gamma$-$X$ direction is semi-quantitative. Both methods yield systematic hardening of magnetic excitations with increasing doping, more pronounced than for particle-hole non-symmetric case ($t' \neq 0$). This is a counter-intuitive result originating from strong electronic correlations. In the $\Gamma$-$M$ direction, SGA $\lambda_\delta+1/N_f$ structure factors for undoped and intermediately-doped case [panels (d) and (e)] exhibit features indicative of the close proximity to antiferromagnetic instability, which is not as pronounced in DQMC. This results in a transfer of the SGA $\lambda_\delta+1/N_f$ magnetic spectral weight to low energies, which is further enhanced by the detailed balance factor, divergent for $\omega \to 0$, cf. Eq. (64). In effect, close to half-filling, the SGA $\lambda_\delta+1/N_f$ intensity exhibits maxima for near-zero energies, in contrast to DQMC yielding substantially softened, yet non-zero peak-energies. For the overdoped system [panel (f)] both methods exhibit consistent step-like feature along the $\Gamma$-$M$ line.

VI. EMERGENCE OF ROBUST COLLECTIVE EXCITATIONS AT STRONG COUPLING

Experimental observation of robust propagating spin- and charge excitations in several families of correlated materials calls for identification of the mechanism leading to the enhanced coherence of the collective-modes. Present semi-analytic techniques that have been successful in describing those excitations are based on Hubbard operators and thus apply mostly to the strong-coupling ($t$-$J$-model) limit 13 Our VWF+1/$N_f$ approach covers both Hubbard- and $t$-$J$-type models on the same footing and may be directly used to study the evolution of collective excitations from weak- to strong-coupling. In this section we perform such an analysis, employing Hubbard model with $t < 0$, $t' = 0.3|t|$, $k_B T = 0.35|t|$ hole-doping $\delta = 0.2$, and variable on-site Coulomb repulsion, $U$. We also compare the characteristics of various truncation schemes, listed in Table 1 as a function of interaction strength.
In Fig. 3 we plot calculated imaginary parts of dynamical spin- and charge susceptibilities at the antinodal X point (panels (a) and (b), respectively) for $U/|t| = 0.1, 4, 12, \infty$. At weak-coupling, magnetic response in panel (a) is broad and featureless, but it systematically acquires coherence as $U$ is increased. Around $U = |8t|$, a resonance-like feature emerges from particle-hole continuum and shifts toward lower energies for $U \to \infty$ (already at $U/|t| = 4$, an emerging mode with energy $\sim |t|$ may be noticed). This can be related to well-defined paramagnons in metallic state of high-$T_c$ copper oxides. In Ref. [26] we have been able to semi-quantitatively reproduce RIXS data for $La_{2−x}Sr_xCuO_4$ and $(Bi,Pb)_{2}(Sr,La)_3CuO_{6+\delta}$ with the VWF$+1/N_f$ framework. In contrast to paramagnons, the peak-energy of charge excitations [panel (b)] exhibits a non-monotonic dependence on the interaction strength. For small values of $U$, charge dynamics is incoherent with the peak intensity shifting upward with increasing $U$. Already at intermediate interaction strengths, a sharp charge mode emerges form the continuum. With further increase of the Hubbard $U$, the charge mode energy decreases in order to finally saturate at finite value for $U \to \infty$. This behavior is not observed in weak-coupling calculations and thus should be interpreted as a footprint of strong electronic correlations. Note that the substantial downward shift of charge mode energies in the range $U/|t| = 12$ and $U/|t| = \infty$ (solid green- and red dash-dot lines in panel (b), respectively). The finite-$U$ effects are thus not negligible which calls for reexamination of the applicability of the $t$-$J$-model to the description of charge-modes in high-$T_c$ copper oxides in favor of more general models, e.g. $t$-$J$-$U$-$V$ [13].

In Fig. 4 we plot calculated imaginary parts of dynamical spin- and charge susceptibilities as a function of the on-site Coulomb repulsion, $U$, for the Hubbard model with non-zero next- and next-nearest neighbor hopping, taken at the X point in the Brillouin zone. The employed model parameters are: $t < 0$, $t' = 0.3|t|$, $k_BT = 0.35|t|$, and hole-doping $\delta = 0.2$. The calculations have been performed for a $300 \times 300$ square lattice using SGA$+1/N_f$ approximation (cf. Table I).
other. This indicates that neither way the doublon excitations are treated nor the additional diagrams included in within LD + 1/N_f affect noticeably spin dynamics. In panel (b), SGA_{\lambda_d+1/N_f} and LD_{\lambda_d+1/N_f} provide nearly the same charge-mode energies that decrease with U at strong coupling and saturate for U \to \infty. This is consistent with previous results for the charge dynamics in the t-J model within Hubbard-operator large-N_f limit. The situation becomes qualitatively different for the case of SGA_{x+1/N_f} and LD_{x+1/N_f} that both yield an abrupt jump of charge mode energy scale and monotonically increasing peak energies in the strong-coupling regime. The discontinuous evolution is a consequence of a shoulder building up at the threshold of particle-hole continuum that rapidly grows in intensity for U/|t| \gtrsim 2. The monotonic increase of mode energy for SGA_{x+1/N_f} and LD_{x+1/N_f} at strong coupling is likely an unphysical behavior that we attribute to poor handling of the doublon excitations within SGA_{x+1/N_f} and FD_{x+1/N_f} truncation schemes. Physically, doublon dynamics is expected to occur on much faster timescale then the collective charge mode which may be effectively accounted for by freezing-out \lambda_d Lagrange-multiplier. This is achieved within \lambda_d \equiv \lambda_d condition of SGA_{\lambda_d+1/N_f} and FD_{\lambda_d+1/N_f}, but not SGA_{x+1/N_f} and FD_{x+1/N_f} truncations. The choice detailed expansion scheme does not matter as the model is solved exactly, but it generates notable differences at the saddle-point and Gaussian-fluctuation levels. Finally, it is reassuring that, in all cases, the higher-order diagrams included in LD approximation only marginally affect the collective mode energy relative to simpler SGA approach. As is shown in Appendix D those additional diagrams lead to enhancement of the magnetic susceptibility value.

**FIG. 5.** Comparison of the peak energies for spin- [panel (a)] and charge [panel (b)] dynamical susceptibilities for the Hubbard model as a function of the Hubbard U, evaluated at the X point. The remaining parameters are: t < 0, t' = 0.3|t|, k_B T = 0.35|t|, hole doping \delta = 0.2, and lattice size is taken as 300 \times 300. All susceptibilities are evaluated at the X point as a function of energy, and four symbols described in the legend correspond to four truncation schemes listed in Table I. Lines are guides to the eye.

VII. DISCUSSION AND OUTLOOK

Several qualitative comments may be formulated based on the analysis Secs. V-VI. As is apparent from Figs. 2 and 3, the agreement between VWF + 1/N_f and available DQMC data is quantitative in the experimentally relevant case of coherent collective-mode dynamics. Second, the position of the peak-maxima in dynamical susceptibilities, as obtained within the two methods, tend to differ quantitatively for the doping levels and Brillouin-zone contours, for which collective modes become excessively broad. In the latter situation, simple benchmark should be considered overly simplified though. Basing on the available simulations and experimental data for the cuprates, on can infer that SGA_{\lambda_d+1/N_f} calculation tends to overestimate paramagnon damping in the regime of incoherent magnetic dynamics.

Also, a remark should be made on the reported collective-mode energies values. The peak energies for the dynamical susceptibilities that are commonly presented in DQMC studies as a characteristic scale, do not generally reflect the energy of a collective mode, either spin or charge. This problem has been addressed in detail recently in the context of extracting paramagnon energies from RIXS experiments. For that sake, one should carefully distinguish between several frequency scales appearing in the problem. Assuming a harmonic-oscillator model, dynamical susceptibilities may be decomposed as

\[ \chi''(k, \omega) \propto \frac{\gamma(k)\omega}{(\omega^2 - \omega_0(k)^2)^2 + 4\gamma(k)^2\omega^2} + \chi''_{\text{incoh}}(k, \omega). \]

(65)

The above expression depends on wave-vector-dependent damping rate, \gamma(k), and the frequency, \omega_0(k) that. Yet another energy appears naturally as the maximum of \chi''(k, \omega) for given k, which may be approximately identified with \omega_0(k) for \gamma \ll \omega_0. In the above, \chi''_{\text{incoh}} accommodates all incoherent and non-resonant contributions, such as particle-hole and multi-magnon continua. Whereas \omega_0(k) appears explicitly in the formula (65), the energy scale of physical relevance is the so-called propagating frequency, \omega_p(k) = \sqrt{\omega_0^2(k) - \gamma(k)^2} for \gamma < \omega_0 and \omega_p(k) = 0 otherwise. The value \omega_p(k) reflects the real part of the collective quasiparticle pole and is of physical significance. In effect, the mode may turn
out to be overdamped even if $\omega_0(k)$ is large. Ideally, comparing various techniques should thus be based on the propagating energies rather than peak energies. The value of $\omega_0(k)$ may be estimated based on VWF+$1/N_f$ calculation,\cite{footnote9} yet we are not aware of a quantitative study of propagating frequencies within DQMC for the Hubbard model. The discrepancies between propagating and bare frequencies are most pronounced in the physically interesting case of intermediately- and highly-doped systems.

We now discuss the relation of our VWF+$1/N_f$ technique to variety of other approaches, with which is shares common elements. The first is Koltiar-Ruckenstein (KR) slave-boson method that takes Gutzwiller approximation as the saddle point,\cite{footnote10} and may be systematically supplemented with the fluctuation effects at higher expansion orders.\cite{footnote10} The KR method has been successfully applied to model Hamiltonians (see, e.g., \cite{footnote11}), yet this approach requires careful treatment of emerging gauge symmetry and, akin to the plain $1/N_f$ expansion, suffers from ambiguities that need to be handled on case by case basis.\cite{footnote12} The essential advantage of our VWF+$1/N_f$ over slave-bosons is that it allows to go beyond Gutzwiller approximation ($d=\infty$ case) already at the saddle-point level. This is done by diagrammatically incorporating higher-order diagrammatic corrections (cf. Sec. [I]). Since the $d=\infty$ solution is known to exhibit artifacts that are not present at finite dimensions, such as Brinkman-Rice transition,\cite{footnote13} this is a qualitative rather than technical improvement. Here we have restricted ourselves to the lowest-order non-trivial extension beyond $d=\infty$ limit that we dub “local diagrammatic” approximation (cf. Table [I]). Non-local diagrammatic contributions are more technically demanding\cite{footnote14, footnote15} and should be analyzed separately.

Another family of approximations that may be connected to VWF+$1/N_f$ relies on Hubbard-operator representation of the Hamiltonian, for which specialized diagrammatic techniques has been developed.\cite{footnote16, footnote17} Resummation of diagrams leads to generalized random-phase approximation.\cite{footnote18} Also, a different approach based on path-integral $1/N$ treatment of Hubbard operators has been recently applied to the extended $t$-$J$ models to study charge modes in high-$T_c$ cuprates.\cite{footnote19, footnote20} The technique provides good agreement with RIXS charge-mode energies if interlayer hopping and long-range Coulomb interactions are included in the Hamiltonian. In this context, a qualitative advantage of VWF+$1/N_f$ is that it is straightforwardly applicable both to the $t$-$J$ model and finite-$U$ Hubbard-type models on the same footing, whereas Hubbard-operator-based techniques become excessively complex in the latter case. As we demonstrated in Sec. [V] finite-$U$ effects have non-negligible impact on the charge mode. Also, it has been long understood that finite-$U$ effects affect substantially the high-energy magnetic excitations in Hubbard-type models, particularly at the magnetic Brillouin-zone boundary.\cite{footnote21} The magnetic dispersion along those contours may be accurately reproduced by taking $U/t \lesssim 8$, which is far from the $t$-$J$ limit. Even though it is possible to describe high-energy spin-wave dispersion using $t$-$J$ Hamiltonians, the long-range exchange interactions and cyclic exchange terms need to be then incorporated into the Hamiltonian suggesting that strong-coupling limit is not an adequate starting point to address high-energy paramagnons.

Yet another relevant technique is time-dependent Gutzwiller approximation\cite{footnote22} (dubbed Gutzwiller + random-phase-approximation, GA+RPA), which has been applied to study dynamics in lattice systems.\cite{footnote23, footnote24} An extension of this concept by means of adaptive canonical transformation has been proposed recently.\cite{footnote25, footnote26} The VWF+$1/N_f$ and GA+RPA methods are similar in the sense that both are a dynamical extension of the variational wave function, but the realization of this goal is achieved in different manner. VWF+$1/N_f$ is a path-integral method applicable at finite-temperature, whereas GA+RPA is a $T=0$ formalism based on the equations of motion for the density-matrix. Also, in contrast to GA+RPA, VWF+$1/N_f$ provides a small parameter (1/$N_f$) that allows for a systematic incorporation of higher-order thermodynamic corrections, e.g., those due to multi-paramagnon effects. The latter renormalize various characteristics of the and become increasingly important as half-filling is approached, which we pointed out in Sec. [V]. It is not clear how to construct such systematic extension for GA+RPA.

Finally, we elaborate on the limitations of VWF+$1/N_f$. First of all, $1/N_f$ expansion at high orders is computationally demanding as it relies on evaluating of high-dimensional loop integrals. Here we have limited ourselves to discussion of the dynamical susceptibilities around correlated large-$N_f$ limit. With an efficient implementation, the $O(1)$ fluctuation corrections to thermodynamics should be still accessible without major supercomputing. Including the latter should allow to eliminate spurious ordered phases at high temperatures, and to explore the regime of low temperatures down to $T=0$. Second, VWF+$1/N_f$ suffers from rapid proliferation of number of lines, $P_{n\beta}$, both as a consequence of including diagrammatic corrections to the variational energy and including longer-range hopping and Coulomb integrals into the Hamiltonian. The effective scattering matrix becomes thus a substantial object. Finally, in the present contribution we have completely disregarded superconducting fluctuations, represented by anomalous lines $S_{n\alpha \beta} \propto \langle c_{\alpha \beta} c_{\alpha \beta} \rangle$.\cite{footnote27} The latter may be incorporated by appropriate generalization of the Hubbard-Stratonovich transformation, introduced in Sec. [III]. This would, however, lead to doubling the dimension of the effective Hamiltonian and further proliferation of lines. Therefore, VWF+$1/N_f$ may be expected to be applicable to relative small (few-orbital) superconducting lattice systems. This extension should be the subject of a separate study.
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Appendix A: Representation of the constraints

Here we show that the constraints (14)-(18) enforce the tadpole-cancellation condition (11). First, we will argue that in Eqs. (15)-(18) one can commute $\hat{P}_G$ to the left, i.e., those equations may be represented as

$$\langle \hat{P}_{G,I}^2 \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \rangle_0 = \langle \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \rangle_0. \quad (A1)$$

For the extended off-diagonal correlator, considered here, this is a non-trivial statement since $\hat{P}_{G,I}$ does not commute with $\hat{c}_{\sigma}^\dagger \hat{c}_{\sigma}$ in general. Yet, one can perform a unitary transformation $\hat{c}_{\sigma} \rightarrow \hat{U}_{\sigma\sigma'} \hat{c}_{\sigma'}$, so that $\langle \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \rangle_0 = \delta_{\sigma\sigma'} \langle \hat{n}_{\sigma} \rangle_0$. Eqs. (15)-(18) may be then jointly written as $\langle \hat{P}_{G,I}^2 \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \hat{P}_G \rangle_0 = \delta_{\sigma\sigma'} \langle \hat{n}_{\sigma} \rangle_0$. For the off-diagonal terms, one gets

$$\langle \hat{P}_{G,I}^2 \hat{c}_{\sigma}^\dagger \hat{n}_{\sigma} \rangle_0 = \langle \hat{c}_{\sigma}^\dagger \hat{n}_{\sigma} \rangle_0 \cdot \langle \hat{P}_G \rangle_0 = \langle \hat{c}_{\sigma} \rangle_0 \cdot \langle \hat{n}_{\sigma} \rangle_0.$$

where the rotated correlator parameters $\tilde{\lambda}_{\sigma\sigma'}$ are obtained from the condition

$$\langle \hat{P}_{G,I} \rangle_0 \equiv \tilde{\lambda}^\dagger_{0\sigma} \langle \hat{n}_{\sigma} \rangle_0 = \tilde{\lambda}^\dagger_{\sigma\sigma'} \langle \hat{n}_{\sigma} \rangle_0 = \tilde{\lambda}^\dagger_{\sigma\sigma'} \langle \hat{n}_{\sigma} \rangle_0.$$

As long as the electron density is non-zero and (as we have assumed) $\tilde{\lambda}_\sigma > 0$ the expression in the bracket is positive and we have $\tilde{\lambda}_{\sigma\sigma} = 0$. The density matrix and $\lambda_{\sigma\sigma'}$ are thus simultaneously diagonalizable for field configurations satisfying the constraints. In that diagonal basis ($\lambda_{\sigma\sigma} = 0$ and $\langle \hat{c}_{\sigma}^\dagger \hat{c}_{\sigma} \rangle_0 = 0$) it is easy to verify that $\hat{P}_{G,I}$ may be commuted to the left. Finally, Eq. (A1) along with Eq. (14) effectively enforces (11). This can be seen on diagrammatic level, where it implies that diagrams with a single tadpole attached to $\hat{P}_{G,I}^2$ cancel out and $\langle \hat{P}_{G,I}^2 \rangle_0 = 1$. We have also checked directly in simulations that the constraints (14)-(18) and (11) lead to the same saddle-point values of $\lambda$-parameters.

Appendix B: Linked cluster theorem for rotationally-invariant correlators

Here we justify the decomposition of Eqs. (19) and (20), employing arguments analogous to those developed in Ref. [18], carefully generalized to the rationally invariant off-diagonal correlators and general (either isotropic or broken-symmetry) states. For brevity, we introduce joint position and orbital indices, $I \equiv (i,l)$, and locally-correlated operators $\hat{A}_I^{(\alpha)} = \hat{P}_{G,I}^{(\alpha)} \hat{P}_G$, indexed by $\alpha = 1, \ldots, n$. The starting point is the partial result that under the assumption $\langle \hat{A}_I^{(\alpha)} \rangle_0 = 0$ for each $\alpha$, one has

$$\langle \hat{P}_G \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \hat{P}_G \rangle_0 = \sum_{k=0}^{\infty} \sum_{J_1 \ldots J_k} \langle \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \rangle_0 \hat{J}_1 \cdots \hat{J}_n \rangle_0, \quad (B1)$$

where the superscript “c” indicates that only the diagrams with all internal vertices $\hat{J}_n$ connected to the external vertices, $\hat{A}_I^{(\alpha)}$, are retained in the Wick’s decomposition. Primed summation means that the indices $J_a$ are constrained to be all different and also take values distinct from $I_1, \ldots, I_n$. To show Eq. (B1), we transform the numerator of the left-hand-side

$$\langle \hat{P}_G \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \hat{P}_G \rangle_0 = \langle \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \rangle_0 \prod_{j \neq I_1, \ldots, I_n} \hat{P}_{G,j} \rangle_0 = \sum_{k=0}^{\infty} \sum_{J_1 \ldots J_k} \langle \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \rangle_0 \hat{J}_1 \cdots \hat{J}_n \rangle_0, \quad (B2)$$

where we have made use of the correlator property $\hat{P}_{G,I}^2 = 1 + x_I \hat{d}_I$. Importantly, the summation restrictions in the second line of Eq. (B2) may be relaxed if diagrammatic expansion is slightly altered, i.e.,

$$\langle \hat{P}_G \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \hat{P}_G \rangle_0 = \sum_{k=0}^{\infty} \sum_{J_1 \ldots J_k} \langle \hat{A}_I^{(1)} \cdots \hat{A}_I^{(n)} \rangle_0 \hat{J}_1 \cdots \hat{J}_n \rangle_0 \text{modified}, \quad (B3)$$
where the subscript “modified” means that, in the Wick’s expansion, we reject diagrams involving local loops with a leg attached to internal vertices $\hat{d}_{I_1}$ (loops attached solely to external vertices $\hat{A}^{(\alpha)}_{\bar{I}_n}$ are allowed). Note lack of “primed” double-occupancy operators and primed summation in Eq. (B3).

At this point it may be clarified why the assumption $\langle \hat{A}^{(\alpha)}_{\bar{I}_n} \rangle_0 = 0$ is needed. Namely, this condition ensures that all “modified” diagrams involving the new operators $\hat{d}_{I_1}, \ldots, \hat{d}_{I_n}$, inserted at the sites already occupied by external vertices, cancel out automatically. To show that, we point out that $\langle \hat{A}^{(\alpha)}_{\bar{I}_n} \rangle_0 = 0$ implies that non-zero contributions originate solely from diagrams in which $\hat{A}^{(\alpha)}_{\bar{I}_n}$ is connected to some other operator by at least one fermionic line. The expectation values of the type $\langle \hat{A}^{(\alpha)}_{\bar{I}_n}, \hat{A}^{(\alpha)}_{\bar{I}_n} \rangle_0$ then vanish identically if any of the indices $I_1, \ldots, I_n,$ is equal to an external vertex position (in the range $I_1, \ldots, I_n$). Indeed, without loss of generality, let us assume that $J_1 = I_1$ so that $\langle \hat{A}^{(\alpha)}_{\bar{I}_n} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \rangle_0$ (other operators)${}^{\text{modified}}$. In the wick decomposition of this expression one always encounters pairs of truncations of the type

\[
\langle \hat{A}^{(\alpha)}_{\bar{I}_n} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \rangle_0^{\text{modified}}
\]

and

\[
\langle \hat{A}^{(\alpha)}_{\bar{I}_n} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \hat{c}_{I_1\dagger} \hat{c}_{I_1} \rangle_0^{\text{modified}}
\]

that cancel each other. For the sake of argument, we have assumed that the line connects the operator $\hat{c}_{I_1}$ in $\hat{A}^{(\alpha)}_{\bar{I}_n}$; other cases may be handled in an analogous manner. Note that operator $\hat{c}_{I_1}$ in $\hat{A}^{(\alpha)}_{\bar{I}_n}$ cannot be directly connected to $\hat{c}^\dagger_{I_1}$ in $\hat{d}_{I_1}$ due to modified prescription of diagrammatic expansion.

Now, since each diagram in (B3) may be unambiguously separated into part connected to external vertices and the remaining one (disconnected component), one obtains

\[
\langle \hat{P}_\bar{G} \hat{A}^{(1)}_{\bar{I}_1} \cdots \hat{A}^{(n)}_{\bar{I}_n} \hat{P}_\bar{G} \rangle_0 = \sum_{k=0}^{\infty} \sum_{I_1 \ldots I_k} \frac{x_{J_1} \cdots x_{J_k}}{k!} \sum_{l=0}^{k} \left( \begin{array}{c} k \\ k - l \end{array} \right) \langle \hat{A}^{(1)}_{\bar{I}_1} \cdots \hat{A}^{(1)}_{\bar{I}_n} \hat{d}_{I_1} \cdots \hat{d}_{I_k} \rangle_0^{\text{modified}} \cdot \langle \hat{d}_{I_{k+1}} \cdots \hat{d}_{I_n} \rangle_0^{\text{modified}} = \\
\left( \sum_{k=0}^{\infty} \sum_{I_1 \ldots I_k} \frac{x_{J_1} \cdots x_{J_k}}{k!} \langle \hat{A}^{(1)}_{\bar{I}_1} \cdots \hat{A}^{(1)}_{\bar{I}_n} \hat{d}_{I_1} \cdots \hat{d}_{I_k} \rangle_0^{\text{modified}} \right) \cdot \left( \sum_{k=0}^{\infty} \sum_{I_1 \ldots I_k} \frac{x_{J_1} \cdots x_{J_k}}{k!} \langle \hat{d}_{I_{k+1}} \cdots \hat{d}_{I_n} \rangle_0^{\text{modified}} \right) .
\]

In the second line of Eq. (B6), the last term in bracket is equal to $\langle \hat{P}_\bar{G}^2 \rangle_0$ and thus is canceled by denominator of the left-hand side of Eq. (B1). As the final step, one should reintroduce restriction summations in Eq. (B6) in order to restore usual diagrammatic expansion. This yields Eq. (B1).

**Expansion for one-site operators**

We now consider general operator $\hat{A}_I$ and corresponding $\hat{A}_I' \equiv \hat{P}_\bar{G} \hat{A}_I \hat{P}_\bar{G}$ with not necessarily vanishing expectation value, i.e., $\langle \hat{A}_I' \rangle_0 \neq 0$. One then has

\[
\langle \hat{A}_I' \rangle_0 \equiv \frac{\langle \hat{P}_\bar{G} \hat{A}_I \hat{P}_\bar{G} \rangle_0}{\langle \hat{P}_\bar{G} \hat{P}_\bar{G} \rangle_0} = \langle \hat{A}_I' \rangle_0 + \frac{\langle \hat{P}_\bar{G} (\hat{A}_I - \langle \hat{A}_I' \rangle_0) \hat{P}_\bar{G} \rangle_0}{\langle \hat{P}_\bar{G} \hat{P}_\bar{G} \rangle_0} = \\
\langle \hat{A}_I' \rangle_0 + \sum_{k=0}^{\infty} \sum_{I_1 \ldots I_k} \frac{x_{J_1} \cdots x_{J_k}}{k!} \langle \left( \hat{A}_I - \langle \hat{A}_I' \rangle_0 \hat{P}_\bar{G}^2 \right) \cdot \hat{d}_{I_1} \cdots \hat{d}_{I_k} \rangle_0
\]

which is equivalent to Eq. (19). Note that the linked cluster expansion (B1) can be applied here since $\langle \hat{A}_I' - \langle \hat{A}_I' \rangle_0 \hat{P}_\bar{G}^2 \rangle_0 = 0$. Analogous procedure may be used to derive Eq. (20).
Appendix C: Path integral decomposition of the interaction term

Here we will prove the Hubbard-Stratonovich decomposition, employed in Sec. III, i.e.

$$\exp\left(-\mathcal{F}(\hat{\mathbf{P}})\right) = \lim_{\epsilon \to 0^+} \int \mathcal{D}\hat{\mathbf{P}} \mathcal{D}\xi \exp \left( - \int d\tau \mathcal{F}(\hat{\mathbf{P}}) - i \int d\tau \xi^\dagger (\hat{\mathbf{P}} - \mathbf{P}) - \frac{\epsilon}{2} \int d\tau \xi^T \xi \right),$$  \hspace{1cm} (C1)

where $\hat{\mathbf{P}}$ are Grassmann bilinears, and $\mathbf{P}$ and $\xi$ are corresponding fields (real for the “diagonal”, $P_{\alpha\alpha}/\xi_{\alpha\alpha}$, and complex for “off-diagonal”, $P_{\alpha\beta}/\xi_{\alpha\beta}$, entries; here $\alpha \neq \beta$). In physical terms, the imaginary-time-dependent vector $\xi$ ensure that those excitations are consistent with Hamiltonian dynamics. The infinitesimal term $\epsilon$ has been introduced to make the integral over $\xi$-fields convergent. Also, it should be possible to bound the functional $\mathcal{F}$ from below by a quadratic form in $\mathbf{P}$-fields to make the integral over $\mathbf{P}$ well-defined for sufficiently small $\epsilon$. This is always the case for models with only quartic fermion-fermion interactions, such as that given by the Hamiltonian (27), but might not be satisfied if the uncorrelated energy functional $E_{\text{var}}(\mathbf{P}, \mu)$ is substituted with $E_{\text{var}}(\mathbf{P}, \mathbf{A}, \mu)$, as is done within the VWF+$1/N_f$ method (cf. Sec. IV). In the latter case $\mathcal{F}$, one can introduce a modified functional $\mathcal{F}_\eta = \mathcal{F} + \eta \mathcal{F}^2$ and take $\eta \to 0^+$ limit at the end of calculation.

We first switch to real representation by means of the unitary transformation, $\hat{\mathbf{P}} = \hat{\Gamma}\mathbf{P}$, defined as follows:

$$\begin{align*}
\hat{P}_{\alpha\beta}' &= P_{\alpha\beta} & \text{for} \ \alpha = \beta, \\
\hat{P}_{\alpha\beta}' &= \frac{1}{\sqrt{2}} (P_{\alpha\beta} + P_{\alpha\beta}^*) & \text{for} \ \alpha \neq \beta,
\end{align*}$$  \hspace{1cm} (C2)

where $\hat{P}_{\alpha\beta}'$ are manifestly real fields. Note that the imaginary components, $P_{\alpha\alpha}$ are identically zero. In the following, we understand that $\hat{\mathbf{P}}$ is a vector composed of all fields $P_{\alpha\alpha}', P_{\alpha\beta}'$, and $P_{\alpha\beta}''$ for $\alpha \neq \beta$. Similarly, we define $\hat{\xi} \equiv \hat{\Gamma}\xi$ and $\hat{\mathbf{P}} \equiv \hat{\Gamma}\mathbf{P}$.

Using Eq. (C2), one gets

$$\int d\tau \mathcal{F}(\mathbf{P}) + i \int d\tau \xi^\dagger (\hat{\mathbf{P}} - \mathbf{P}) + \frac{\epsilon}{2} \int d\tau \xi^T \xi = \int d\tau \mathcal{F}(\hat{\mathbf{P}}) + i \int d\tau \xi^\dagger \hat{\mathbf{P}} - \mathbf{P} + \frac{\epsilon}{2} \int d\tau \xi^T \xi \hspace{1cm} (C3)$$

which can be used to transform the right-hand side (RHS) of Eq. (C1) as

$$\text{RHS} = \lim_{\epsilon \to 0^+} \int \mathcal{D}\hat{\mathbf{P}} \mathcal{D}\xi \exp \left( - \int d\tau \mathcal{F}(\hat{\mathbf{P}}) - i \int d\tau \xi^\dagger \hat{\mathbf{P}} - \mathbf{P} - \frac{\epsilon}{2} \int d\tau \xi^T \xi \right) \propto$$

$$\lim_{\epsilon \to 0^+} \int \mathcal{D}\hat{\mathbf{P}} \exp \left( - \int d\tau \mathcal{F}(\hat{\mathbf{P}}) - \frac{1}{2\epsilon} \int d\tau (\hat{\mathbf{P}} - \mathbf{P})^T (\hat{\mathbf{P}} - \mathbf{P}) \right) =$$

$$\lim_{\epsilon \to 0^+} \exp \left( - \frac{1}{2\epsilon} \int d\tau \hat{\mathbf{P}}^T \hat{\mathbf{P}} \right) \sum_{i_1, \ldots, i_M = 0}^\infty \int \mathcal{D}\hat{\mathbf{P}} \left( \int d\tau_1 \hat{P}_{1\dagger} \hat{P}_1 \right)^{i_1} \cdots \left( \int d\tau_M \hat{P}_{M\dagger} \hat{P}_M \right)^{i_M} \exp \left( - \int d\tau \mathcal{F}(\hat{\mathbf{P}}) - \frac{1}{2\epsilon} \int d\tau \hat{\mathbf{P}}^T \hat{\mathbf{P}} \right),$$  \hspace{1cm} (C4)

where the $M$ is the total number of scalar field components. The transition from the second to the third line of Eq. (C4) has been performed by Taylor-expanding the exponential term

$$\exp \left( \frac{1}{\epsilon} \int d\tau \hat{\mathbf{P}} \cdot \hat{\mathbf{P}} \right) = \exp \left( \frac{1}{\epsilon} \sum_{i=1}^M \int d\tau_i \hat{P}_i \cdot \hat{P}_i \right).$$  \hspace{1cm} (C5)

The integral in the last term of Eq. (C4) can be evaluated by introducing the generating functional
\[ Z[J] = \int \mathcal{D}\hat{\Phi} \exp \left( -\int d\tau \mathcal{F}(\hat{\Phi}) - \frac{1}{2} \int d\tau \hat{\Phi}^T \hat{\Phi} + \frac{1}{\epsilon} \int d\tau \hat{\Phi}^T \hat{\Phi} \right) \times \]
\[ \int \mathcal{D}\hat{\Phi} \exp \left( -\int d\tau \mathcal{F}(\epsilon \hat{\Phi}^\dagger \hat{\Phi} + \hat{\Phi}^\dagger J) - \frac{\epsilon}{2} \int d\tau \hat{\Phi}^T \hat{\Phi} + \frac{1}{2\epsilon} \int d\tau \hat{\Phi}^T \hat{\Phi} \right), \tag{C6} \]

where the last line has been obtained by a change of variables, \( \hat{\Phi} \rightarrow e^{\hat{\Phi}} + \hat{J} \). One thus gets

\[ \text{RHS} \propto \lim_{\epsilon \rightarrow 0^+} \exp \left( -\int d\tau E_{0,\text{kin}}(\hat{\Phi}) - \frac{1}{2} \int d\tau E_{0,\text{int}}(\hat{\Phi}) - i \int d\tau \hat{\Phi}^T \hat{\Phi} - \frac{\epsilon}{2} \int d\tau \hat{\Phi}^T \hat{\Phi} \right) \times \]
\[ \int \mathcal{D}\hat{\Phi} \exp \left( -\int d\tau E_{0,\text{kin}}(\hat{\Phi}) - \frac{1}{2} \int d\tau E_{0,\text{int}}(\hat{\Phi}) - i \int d\tau \hat{\Phi}^T \hat{\Phi} - \frac{\epsilon}{2} \int d\tau \hat{\Phi}^T \hat{\Phi} \right) \times \exp \left( -\int d\tau \hat{\Phi}^T \hat{\Phi} \right) \rightarrow \exp \left( -\mathcal{F}(\hat{\Phi}) \right), \tag{C7} \]

which concludes the reasoning.

One can now use Eq. (C1) to derive Eq. (30) by taking \( \mathcal{F}(\hat{\Phi}) = E_{0,\text{kin}}(\hat{\Phi}) + \frac{1}{2} E_{0,\text{int}}(\hat{\Phi}) \). Indeed, we get

\[ \lim_{\epsilon \rightarrow 0^+} \int \mathcal{D}\Phi \mathcal{D}\xi \exp \left( -\int d\tau E_{0,\text{kin}}(\hat{\Phi}) - \frac{1}{2} \int d\tau E_{0,\text{int}}(\hat{\Phi}) - i \int d\tau \hat{\Phi}^T \hat{\Phi} - \frac{\epsilon}{2} \int d\tau \hat{\Phi}^T \hat{\Phi} \right) \times \]
\[ \exp \left( -\int d\tau E_{0,\text{kin}}(\hat{\Phi}) - \frac{1}{2} \int d\tau E_{0,\text{int}}(\hat{\Phi}) \right) = \exp \left( -\int d\tau \hat{\Phi}^T \hat{\Phi} \right). \tag{C8} \]

The last inequality in Eq. (C8) follows directly from the structure of the Hamiltonian. For the kinetic part, one obtains \( E_{\text{kin}}(\hat{\Phi}) = \sum_{\alpha\beta} t_{\alpha\beta} \hat{\Phi}_{\alpha\beta} = \sum_{\alpha\beta} t_{\alpha\beta} \bar{\eta}_{\alpha} \eta_{\beta} \). In a similar manner, the potential-energy part may be transformed as

\[ E_{\text{int}}(\hat{\Phi}) = \frac{1}{2} \sum_{\alpha\gamma\rho} \hat{\Phi}_{\alpha\beta} \hat{\Phi}_{\gamma\rho} = \frac{1}{2} \sum_{\alpha\gamma\rho} \bar{\eta}_{\alpha} \bar{\eta}_{\beta} \eta_{\gamma} \eta_{\rho} = \sum_{\alpha\beta\gamma\rho} V_{\alpha\beta\gamma\rho} \bar{\eta}_{\alpha} \bar{\eta}_{\beta} \eta_{\gamma} \eta_{\rho} = 2 \cdot \hat{V}[\hat{\eta}], \tag{C9} \]

where we have made use of the definition of the summarized vertex, \( V_{\alpha\beta\gamma\rho} \equiv (-V_{\beta\rho\alpha} + V_{\beta\gamma\rho} + V_{\gamma\beta\rho} - V_{\gamma\rho\beta})/2 \).

Finally, one gets \( \int d\tau E_{0,\text{kin}}(\hat{\Phi}) + \frac{1}{2} \int d\tau E_{0,\text{int}}(\hat{\Phi}) = \int d\tau \hat{\Phi}^T \hat{\Phi} \). The apparent double counting of interaction after substituting Grassmann bilinears into \( E_{0,\text{int}} \) originates from unbiased (all-channel) version of Hubbard-Stratonovich decomposition, as discussed in detail in Sec. [III].

**Appendix D: Action for correlated 1/\( N_f \) expansion and effective scattering matrix**

Here we show that after integrating out the fields \( \lambda \) and \( \rho \), the action (46) becomes equivalent to the resummed 1/\( N_f \) action (51). For \( N_f = 1 \), the action (46) reproduces thus faithfully the thermodynamics of the original model, defined by the Hamiltonian \( \hat{H} \) so that our approach provides a systematic route to improvement of the VWF technique by incorporating consecutive 1/\( N_f \) corrections around the correlated saddle point solution.

The proof is performed by consecutively integrating out the \( \rho, \lambda, \xi, \Phi \). By taking the action (46) with \( N_f = 1 \), one arrives at

\[ Z[J] = \int \mathcal{D}\hat{\eta} \mathcal{D}\eta \mathcal{D}\Phi \mathcal{D}\xi \mathcal{D}\lambda \mathcal{D}\rho \exp (-S_{\text{var}}[\Phi, \xi, \lambda, \rho, \eta, \eta, J, \mu]) \times \]
\[ \int \mathcal{D}\hat{\eta} \mathcal{D}\eta \mathcal{D}\Phi \mathcal{D}\xi \mathcal{D}\lambda \exp (-S[\Phi, \xi, \eta, J, \mu]) \delta(C(\Phi, \lambda)) \left| \det \frac{\partial C}{\partial \lambda} \right| \exp \left( -\frac{1}{2} \int d\tau C^T C \right) \times \]
\[ \int \mathcal{D}\hat{\eta} \mathcal{D}\eta \mathcal{D}\Phi \mathcal{D}\xi \exp (-S[\Phi, \xi, \eta, J, \mu]) \times \]
\[ \int \mathcal{D}\hat{\eta} \mathcal{D}\eta \exp \left( \int d\tau \hat{\eta}^T \hat{\eta} - \int d\tau \hat{\Phi}^T \hat{\Phi} \right), \tag{D1} \]
where $S_{\text{var}}$ is the VWF $+1/N_f$ action [Eq. (46)], $S$ denotes the “uncorrelated” action [Eq. (33)], and $\hat{H}[\eta, \eta, \mu]$ is the Hamiltonian expressed in terms of Grassmann fields. The Dirac delta imposing $C = 0$ in the second line originates from integration over $\rho$ fields. As a consequence, the term $\propto \kappa$ is equal to zero, making the observables generated based on $Z[J]$ independent on $\kappa$, as stated in the main text. Finally, the $O(1)$ constraint Jacobian term allows to explicitly evaluate enteral over $\lambda$ without generating any artifact $P$-field interactions. The $\lambda$-fields evolution is then fully determined by line-fields, $\mathbf{P}$, and may be determined by solving the equations $\mathbf{C} = 0$. The transition between the last two lines of Eq. (D1) has been performed based on the results of Sec. III and Appendix C. The model thus reproduces the thermodynamics of the model, given by $\hat{H}$.

We now derive the effective scattering matrix, given by Eq. (60), taking the Gaussian-fluctuation action [51] as the departure point. First, for the reasons that will be made clear below, it is essential to switch to real representation with the use of $\tilde{C}$2. By transforming the quadratic part, one obtains

$$S_{\text{quadratic}} = \frac{N_f}{2} \int d\tau \left( \frac{\delta^T \delta \lambda^T \delta \rho^T}{\delta \rho^T} \right) \begin{pmatrix} \hat{V}_{\rho \rho} + \kappa \hat{V}_{\rho \rho} \hat{V}_{\rho \rho} & \hat{V}_{\lambda \rho} + \kappa \hat{V}_{\lambda \rho} \hat{V}_{\lambda \rho} \\ i\hat{V}_{\rho \lambda} & i\hat{V}_{\lambda \rho} \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta \lambda \end{pmatrix} = \frac{N_f}{2} \int d\tau \left( \frac{\delta^T \delta \lambda^T \delta \rho^T}{\delta \rho^T} \right) \begin{pmatrix} \hat{V}_{\rho \rho} + \kappa \hat{V}_{\rho \rho} \hat{V}_{\rho \rho} & \hat{V}_{\lambda \rho} + \kappa \hat{V}_{\lambda \rho} \hat{V}_{\lambda \rho} \\ i\hat{V}_{\rho \lambda} & i\hat{V}_{\lambda \rho} \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta \lambda \end{pmatrix} \equiv \left( \delta^T \delta \lambda^T \delta \rho^T \right) \hat{V}(2) \left( \delta \rho \right), \quad (D2)$$

where $\delta \mathbf{P}$, $\delta \lambda$, and $\delta \rho$ are real and the transformed scattering matrix, $\hat{V}(2) = \hat{V}(2)^T + i\hat{V}(2)^T$, is complex symmetric. We have also explicitly restored the infinitesimal term $\frac{N_f}{2} \int d\tau \delta \rho^T \delta \rho$ with $\epsilon_\rho > 0$ that we deliberately discarded in Sec. [V] for brevity of notation.

Let us begin the derivation by representing $S_{\text{quadratic}}$ as

$$S_{\text{quadratic}} = \frac{N_f}{2} \int d\tau \delta^T \mathbf{P} \left( \hat{V}_{\rho \rho} + \kappa \hat{V}_{\rho \rho} \hat{V}_{\rho \rho} \right) \mathbf{P} + \frac{N_f}{2} \int d\tau \left( \delta^T \delta \lambda^T \delta \rho^T \right) \begin{pmatrix} \hat{V}_{\lambda \rho} + \kappa \hat{V}_{\lambda \rho} \hat{V}_{\lambda \rho} \\ i\hat{V}_{\lambda \rho} \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta \lambda \end{pmatrix} + \frac{N_f}{2} \int d\tau \left( \delta^T \delta \rho^T \hat{V}_{\lambda \rho} \right) \begin{pmatrix} \delta \lambda \\ \delta \rho \end{pmatrix} \left( \begin{pmatrix} \hat{P} + \kappa \hat{V}_{\rho \rho} \hat{P} \\ i\hat{V}_{\rho \rho} \end{pmatrix} \right), \quad (D3)$$
and integrating out $\delta \tilde{\lambda}$ and $\delta \tilde{\rho}$ fields. It is essential to argue that one can apply the standard formula for evaluating Gaussian path integrals to the present case, based on completing the square and functional determinant. This is difficult to prove in the complex-field representation of Eq. (D2), since the involved matrix is complex and non-symmetric. On the other hand, by employing the real representation of Eq. (D3), this can be rigorously shown by making an additional assumption that the real-part of the scattering matrix between $\lambda$ and $\rho$ fields,

$$
\tilde{\mathcal{V}}^{(2)} = \begin{pmatrix}
\hat{\mathcal{V}}_{\lambda\lambda} + \kappa \hat{\mathcal{V}}_{\lambda\rho} \hat{\mathcal{V}}_{\rho\lambda} & i \hat{\mathcal{V}}_{\lambda\rho} \\
i \hat{\mathcal{V}}_{\rho\lambda} & \epsilon_ho
\end{pmatrix},
$$

(D4)
is positive definite. Recall that $\hat{\mathcal{V}}_{\lambda\rho}$ is the Jacobian of the constraints ($C = 0$) [cf. Eq. (59)], being a real square matrix since the number of constraints equal to the number of $\lambda$ fields, as demanded in Sec. IV. Moreover, we demand that the constraints $C = 0$ locally determine $\lambda$-fields (cf. Sec. IV), which is implemented by the condition $\det \hat{\mathcal{V}}_{\lambda\rho} \neq 0$. Under those circumstances, to make the real part of $\hat{\mathcal{V}}^{(2)}$ positive definite is sufficient to assure that its left-upper block $\hat{\mathcal{V}}_{\lambda\lambda} + \kappa \hat{\mathcal{V}}_{\lambda\rho} \hat{\mathcal{V}}_{\rho\lambda}$ is positive definite (here $\hat{\mathcal{V}}_{\lambda\lambda}$ denotes real-part of the matrix $\hat{\mathcal{V}}_{\lambda\lambda} \equiv \hat{\mathcal{V}}_{\lambda\lambda} + i \hat{\mathcal{V}}^\prime_{\lambda\lambda}$). The latter condition is always met if sufficiently large positive $\kappa$ is taken, thus $\kappa$-parameter needs to be introduced to ensure convergence.

By employing the above assumptions, $\hat{\mathcal{V}}^{(2)}$ may be brought to diagonal form by congruence as $\hat{\mathcal{V}}^{(2)} = \hat{K}(1 + i \hat{D})\hat{K}^T$, where $\hat{1}$ is identity matrix, $\hat{K}$ is real, and $\hat{D}$ is diagonal. This can be seen by application of Cholesky factorization to the real-part, $\hat{\mathcal{V}}^{(2)} = \hat{L}\hat{L}^T$, and orthogonally diagonalizing the symmetric matrix $\hat{L}^{-1}\hat{\mathcal{V}}^{(2)}(\hat{L}^{-1})^T = \hat{Q}\hat{D}\hat{Q}^T$. Then one gets $\hat{K} = \hat{L}\hat{Q}$. Using this decomposition, it is straightforward to show that the Gaussian integral factorizes into a product of Gaussian integrals for which it is the usual formulas for integration hold.

Integrating out $\delta \tilde{\lambda}$ and $\delta \tilde{\rho}$ fields by completing to the square, which yields effective contribution depending only on the fluctuation of $\mathcal{P}$-fields, i.e.,

$$
\mathcal{S}_{\text{quadratic}} \to \mathcal{S}_{\text{quadratic,eff}} = \frac{N_f}{2} \int d\tau \delta \hat{\mathcal{P}}^T \hat{\mathcal{V}}_{\text{eff}} \hat{\mathcal{P}} + \mathcal{O}(1),
$$

(D5)

where $\mathcal{O}(1)$ terms originate from the determinant generated by evaluation of the Gaussian integral. In Eq. (D5) we have introduced effective $\kappa$-dependent scattering matrix

$$
\hat{\mathcal{V}}_{\text{eff}} = \hat{\mathcal{V}}_{\mathcal{P}\mathcal{P}} + \kappa \hat{\mathcal{V}}_{\mathcal{P}\mathcal{P}} \hat{\mathcal{V}}_{\mathcal{P}\mathcal{P}} - \left( \hat{\mathcal{V}}_{\mathcal{P}\lambda} + \kappa \hat{\mathcal{V}}_{\mathcal{P}\rho} \hat{\mathcal{V}}_{\rho\lambda}, i \hat{\mathcal{V}}_{\mathcal{P}\rho} \right) \left( \hat{\mathcal{V}}_{\lambda\lambda} + \kappa \hat{\mathcal{V}}_{\lambda\rho} \hat{\mathcal{V}}_{\rho\lambda} i \hat{\mathcal{V}}_{\lambda\rho} \epsilon_ho \right)^{-1} \left( \hat{\mathcal{V}}_{\lambda\rho} + \kappa \hat{\mathcal{V}}_{\lambda\rho} \hat{\mathcal{V}}_{\rho\rho} \right).
$$

(D6)

Equation (D6) resembles Eq. (60) of the main text, but it seemingly depends on the unphysical gauge parameter, $\kappa$. We now show that all contributions $\propto \kappa$ actually cancel out exactly in Eq. (D6), so that this expression is gauge-invariant. Note that, whereas independence of the exact generating functional $Z[J]$ on $\kappa$ follows directly from the series of transformations (D1), the statement that $\kappa$-dependence is lost at the leading order of $1/N_f$ expansion requires further justification. Provided that the determinant of the Jacobian $\det \hat{\mathcal{V}}_{\lambda\rho} \neq 0$, the inverse of $\hat{\mathcal{V}}^{(2)}$ on the right-hand-side of Eq. (D6) exists and may be evaluated using the block-matrix inverse formula as

$$
\left( \begin{array}{cc}
\hat{\mathcal{V}}^{\prime}_{\lambda\lambda} + \kappa \hat{\mathcal{V}}^{\prime}_{\lambda\rho} \hat{\mathcal{V}}^{\prime}_{\rho\lambda} & i \hat{\mathcal{V}}^{\prime}_{\lambda\rho} \\
i \hat{\mathcal{V}}^{\prime}_{\rho\lambda} & \epsilon_ho
\end{array} \right)^{-1} = \left( \begin{array}{cc}
0 & -i \hat{\mathcal{V}}^{\prime \dagger}_{\rho\rho} \\
i \hat{\mathcal{V}}^{\prime \dagger}_{\lambda\rho} & \hat{\mathcal{V}}^{\prime \dagger}_{\lambda\lambda} \hat{\mathcal{V}}^{\prime \dagger}_{\lambda\rho} + \kappa
\end{array} \right),
$$

(D7)

where we have already taken $\epsilon_ho \to 0^+$ limit. By working out the structure of Eq. (D6) using Eq. (D7) it becomes apparent that all the terms proportional to $\kappa$ cancel out, and Eq. (D6) becomes equivalent Eq. (60) if the fields and matrices are rotated-back to the complex representations with the use of transformation $\hat{\Gamma}$ (see Appendix C). This concludes the derivation of the scattering matrix.

**Appendix E: Stability of the paramagnetic state against fluctuations**

In this Appendix, we discuss the stability of $\text{SGA}_{\lambda_d} + 1/N_f$ paramagnetic state against both charge- and spin excitations for model parameters employed in $\text{SGA}_{\lambda_d}$.
FIG. 7. Calculated SGA$\lambda_f+1/N_f$ static spin [panels (a)-(f)] and charge [panels (g)-(l)] susceptibility ($\chi'_s(k, \omega = 0)$ and $\chi'_c(k, \omega = 0)$, respectively) for the Hubbard model with the same parameters as those used to generate Fig. 3 i.e., $t < 0$, $t' = 0$, $U = 8|t|$, lattice size $500 \times 500$, and doping levels $\delta = 0, 0.2$, and 0.4. The temperature has been set to $k_BT = 0.35|t|$ for $\delta = 0$, and $k_BT = 0.35|t|$ for $\delta = 0.2$ and $\delta = 0.2$. Hole concentration are provided inside the panels.

In Fig. 8 we show the calculated dependence of the static spin susceptibility on the on-site Coulomb repulsion, $U$, for the Hubbard model. We plot only the data for the point $M$ as the representative one in the context of magnetic instability. Model parameters are the same parameters as those employed to generate Fig. 3. Blue- and yellow point correspond to SGA$\lambda_f+1/N_f$ and LD$\lambda_f+1/N_f$, respectively. Lines are guides to the eye.
$U \sim 8|t|$ of the order of bare bandwidth. The paramagnetic is thus locally stable against antiferromagnetic...
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