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Emergent Bloch excitations in Mott matter

Abstract

We develop a unified theoretical picture for excitations in Mott systems, portraying both the heavy quasiparticle excitations and the Hubbard bands as features of an emergent Fermi liquid state formed in an extended Hilbert space, which is nonperturbatively connected to the physical system. This observation sheds light on the fact that even the incoherent excitations in strongly correlated matter often display a well-defined Bloch character, with pronounced momentum dispersion. Furthermore, it indicates that the Mott point can be viewed as a topological transition, where the number of distinct dispersing bands displays a sudden change at the critical point. Our results, obtained from an appropriate variational principle, display also remarkable quantitative accuracy. This opens an exciting avenue for fast realistic modeling of strongly correlated materials.

Disciplines

Condensed Matter Physics

Emergent Bloch excitations in Mott matterNicola Lanatà,¹ Tsung-Han Lee,¹ Yong-Xin Yao,² and Vladimir Dobrosavljević¹¹*Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA*²*Ames Laboratory-U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

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We develop a unified theoretical picture for excitations in Mott systems, portraying both the heavy quasiparticle excitations and the Hubbard bands as features of an emergent Fermi liquid state formed in an extended Hilbert space, which is nonperturbatively connected to the physical system. This observation sheds light on the fact that even the incoherent excitations in strongly correlated matter often display a well-defined Bloch character, with pronounced momentum dispersion. Furthermore, it indicates that the Mott point can be viewed as a topological transition, where the number of distinct dispersing bands displays a sudden change at the critical point. Our results, obtained from an appropriate variational principle, display also remarkable quantitative accuracy. This opens an exciting avenue for fast realistic modeling of strongly correlated materials.

DOI: [10.1103/PhysRevB.96.195126](https://doi.org/10.1103/PhysRevB.96.195126)**I. INTRODUCTION**

The physical nature of the excited states in strongly interacting quantum systems has long been a subject of much controversy and debate. Deeper understanding was achieved by Landau, more than half a century ago [1], who realized that in systems of fermions the Pauli principle provides a spectacular simplification. He showed that many properties of Fermi systems can be understood in terms of weakly interacting quasiparticles (QPs), allowing a precise and detailed description of strongly correlated matter. Modern experiments provide for even more direct evidence of such QP excitations, for example from using angle-resolved photoemission spectroscopy (ARPES) [2] or scanning-tunneling microscopy (STM) methods [3].

The Fermi liquid paradigm, however, describes only the low-energy excitations. At higher energies, the physical properties are often dominated by incoherent processes, which do not conform to the Landau picture. The task to provide a simple and robust theoretical description of such incoherent excitations has therefore emerged as a central challenge of contemporary physics. An intriguing apparent paradox is most evident around the Mott point. Here, ARPES and STM experiments provide often clear evidence of additional well-defined high-energy excitations (Hubbard bands), which, while being fairly incoherent, still display relatively well-defined Bloch character with pronounced momentum dispersion, see, e.g., Ref. [4]. As a matter of fact, it is often difficult experimentally to even distinguish the Hubbard bands found in Mott insulators from ordinary Bloch bands found at high energy in conventional band insulators. While such behavior can be already numerically reproduced by some modern many-body approximations [5,6], a simple conceptual picture for the apparent Bloch character of such high-energy charge excitations is not still available. In particular, variational methods such as the Gutzwiller approximation (GA) [7], which are often able to reproduce the numerical results in a much simpler semianalytical fashion, generally capture only the low-lying QP features on the metallic side, but cannot provide

a description of charge excitations around the Mott point and in the insulating regime.

The goal of this paper is to write an appropriate variational wave function able to capture the main features of both the (low-energy) QP bands and the (high-energy) Hubbard bands, within the same theoretical framework. A particularly interesting fact emerging from our theory is that many key attributes of both types of excitations are encoded in the bare density of states (DOS) of the uncorrelated system and a few renormalization parameters—in a similar fashion as for the QP excitations in Landau theory of Fermi liquids. This is accomplished, similarly as in many other theories for many-body systems, see, e.g., Refs. [8–10], by enlarging the Hilbert space by introducing auxiliary “ghost” degrees of freedom. In particular, this construction sheds light on the physical origin of the “hidden” Bloch character of the Hubbard bands mentioned above. Our calculations of the single-band Hubbard model, which are benchmarked against the dynamical mean-field theory (DMFT) [5,6] solution, show that the new wave function quantitatively captures not only the dispersion of the QP but also of the Hubbard bands. Furthermore, our theory enables us to describe the Mott transition and the coexistence region between the metallic and the Mott-insulator phases.

II. GHOST-GA THEORY

For simplicity, our theory will be formulated here for the single-band Hubbard model

$$\hat{H} = \sum_{RR'} \sum_{\sigma} t_{RR'} c_{R\sigma}^{\dagger} c_{R'\sigma} + \sum_{R\sigma} U \hat{n}_{R\uparrow} \hat{n}_{R\downarrow} \quad (1)$$

at half-filling. The generalization to arbitrary multiorbital Hubbard Hamiltonians is straightforward [11].

In order to construct the ghost-GA theory we are going to embed the physical Hamiltonian of the system [Eq. (1)] within an extended Hilbert space obtained by introducing auxiliary Fermionic “ghost” degrees of freedom not coupled with the physical orbitals, see Fig. 1. Let us represent \hat{H} within the

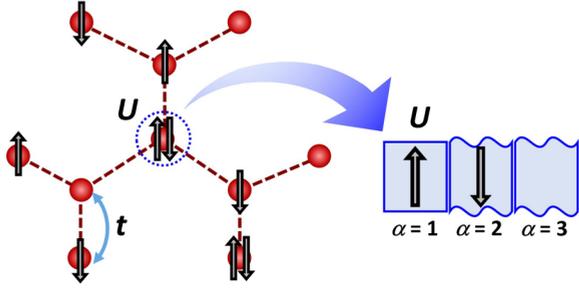


FIG. 1. Representation of a lattice including two ghost orbitals ($\alpha = 2, 3$). The Hamiltonian of the system acts as 0 over the auxiliary ghost degrees of freedom. The Hubbard interaction U acts only on the physical orbital $\alpha = 1$.

extended Hilbert space mentioned above as follows:

$$\begin{aligned}\hat{H} &= \sum_{RR'} \sum_{\alpha\beta\sigma} \tilde{t}_{RR'}^{\alpha\beta} c_{R\alpha\sigma}^\dagger c_{R'\beta\sigma} + \sum_R U \hat{n}_{R1\uparrow} \hat{n}_{R1\downarrow} \\ &= \sum_k \sum_{\alpha\beta\sigma} \tilde{\epsilon}_k^{\alpha\beta} c_{k\alpha\sigma}^\dagger c_{k\beta\sigma} + \sum_R U \hat{n}_{R1\uparrow} \hat{n}_{R1\downarrow},\end{aligned}\quad (2)$$

where $\tilde{t}_{RR'}^{11} = t_{RR'}$ are the physical hopping parameters, $\tilde{\epsilon}_k^{11} = \epsilon_k$ are the eigenvalues of the first term of \hat{H} , $\tilde{t}_{RR'}^{\alpha\beta} = \tilde{\epsilon}_k^{\alpha\beta} = 0 \forall (\alpha, \beta) \neq (1, 1)$ and σ is the spin.

Our theory consists in applying the ordinary multiorbital GA theory [14–18] to Eq. (2). In other words, the expectation value of \hat{H} is optimized variationally with respect to a Gutzwiller wave function represented as $|\Psi_G\rangle = \hat{\mathcal{P}}_G |\Psi_0\rangle$, where $|\Psi_0\rangle$ is the most general Slater determinant, $\hat{\mathcal{P}}_G = \prod_R \hat{\mathcal{P}}_R$, and $\hat{\mathcal{P}}_R$ acts over all of the local degrees of freedom labeled by R —including the ghost orbitals $\alpha > 1$ —and commutes with the total number operator $\sum_{\alpha\sigma} c_{R\alpha\sigma}^\dagger c_{R\alpha\sigma}$. The variational wave function is restricted by the following conditions:

$$\langle \Psi_0 | \hat{\mathcal{P}}_R^\dagger \hat{\mathcal{P}}_R | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle \quad (3)$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_R^\dagger \hat{\mathcal{P}}_R c_{R\alpha\sigma}^\dagger c_{R\beta\sigma} | \Psi_0 \rangle = \langle \Psi_0 | c_{R\alpha\sigma}^\dagger c_{R\beta\sigma} | \Psi_0 \rangle, \quad (4)$$

which are commonly called “Gutzwiller constraints”. Furthermore, the so-called “Gutzwiller approximation” [7], which is exact in the limit of infinite dimensions (where DMFT is exact), is employed. The minimization of the variational energy will be performed by employing the algorithms derived in Ref. [19]. Note that extending the Hilbert space by introducing the ghost orbitals does not affect the physical Hubbard Hamiltonian \hat{H} , as all of its terms involving ghost orbitals are multiplied by 0, see Eq. (2).

The advantage of enlarging the Hilbert space arises from the fact that the resulting ghost-GA variational wave function is substantially richer with respect to the ordinary GA [11]. In particular, $|\Psi_0\rangle$ is variationally allowed to be any multiorbital Slater determinant lying within the whole extended Hilbert space, i.e., to display entanglement between physical and auxiliary degrees of freedom. However, as proven explicitly in the Supplemental Material [11], the Gutzwiller local operator $\hat{\mathcal{P}}_G = \prod_R \hat{\mathcal{P}}_R$, which is also variationally determined, maps $|\Psi_0\rangle$ into a physical correlated wave function $|\Psi_G\rangle = \hat{\mathcal{P}}_G |\Psi_0\rangle$,

i.e., into a many-body state disentangled from the auxiliary ghost space (consistently with the fact that \hat{H} depends exclusively on the physical degrees of freedom). Thus, the benefit of enlarging the Hilbert space is that it enables us to extend the ordinary GA variational space, while retaining the mathematical structure of the conventional GA theory.

We point out that the ghost-GA variational construction outlined above presents insightful formal and physical analogies with the theories of matrix product states (MPS) and projected entangled pair states (PEPS) [9,10], which are also variational schemes involving virtual entanglement and local maps from an auxiliary extended Hilbert space into the physical space [20].

III. EXCITATIONS

As shown in previous works, see, e.g., Refs. [16], the variational energy minimum of \hat{H} is realized by a wave function $|\Psi_G\rangle = \hat{\mathcal{P}}_G |\Psi_0\rangle$ where $|\Psi_0\rangle$ is the ground state of a quadratic multiband Hamiltonian represented as

$$\hat{H}_{\text{qp}} = \sum_{k\alpha\sigma} [\tilde{\mathcal{R}} \tilde{\epsilon}_k \tilde{\mathcal{R}}^\dagger + \tilde{\lambda}]_{ab} f_{k\alpha\sigma}^\dagger f_{k\beta\sigma} = \sum_{k\alpha\sigma} \tilde{\epsilon}_{kn}^* \psi_{k\alpha\sigma}^\dagger \psi_{k\alpha\sigma}, \quad (5)$$

where $f_{k\alpha\sigma}$ are related to $c_{k\alpha\sigma}$ by a proper unitary transformation [14,16], the matrices $\tilde{\mathcal{R}}$ and $\tilde{\lambda}$ are determined variationally, and $\tilde{\epsilon}_{kn}^*$ and $\psi_{k\alpha\sigma}^\dagger$ are the eigenvalues and eigenoperators of \hat{H}_{qp} , respectively. The states $|\Psi_{Gkn\sigma}^p\rangle = \hat{\mathcal{P}}_G \psi_{k\alpha\sigma}^\dagger |\Psi_0\rangle$ and $|\Psi_{Gkn\sigma}^h\rangle = \hat{\mathcal{P}}_G \psi_{k\alpha\sigma} |\Psi_0\rangle$ represent excited states of \hat{H} [11,21,22].

The energy-resolved Green’s function of the physical degrees of freedom ($\alpha = 1$) can be evaluated in terms of the excitations mentioned above [11] and represented as

$$\begin{aligned}G(\epsilon_k, \omega) &= \left[\tilde{\mathcal{R}}^\dagger \frac{1}{\omega - (\tilde{\mathcal{R}} \tilde{\epsilon}_k \tilde{\mathcal{R}}^\dagger + \tilde{\lambda})} \tilde{\mathcal{R}} \right]_{11} \\ &= [\omega - \epsilon_k - \Sigma(\omega)]^{-1},\end{aligned}\quad (6)$$

where the subscript “11” indicates that we are interested only in the physical component $\alpha = \beta = 1$ of the Green’s function. As we are going to see, the ghost-GA approximation to the physical self-energy $\Sigma(\omega)$, see Eq. (6), is generally a nonlinear function of ω [11,23,24]—while it is linear by construction within the ordinary GA theory. Note also that the poles of $G(\epsilon_k, \omega)$ coincide with the eigenvalues $\tilde{\epsilon}_{kn}^*$ of \hat{H}_{qp} , see Eqs. (5) and (6).

IV. APPLICATION TO THE SINGLE-BAND HUBBARD MODEL

Below we apply our approach to the Hubbard Hamiltonian [Eq. (2)] at half-filling assuming a semicircular DOS [25], which corresponds, e.g., to the Bethe lattice in the limit of infinite connectivity, where DMFT is exact [5]. The half-bandwidth D will be used as the unit of energy. The extended ghost-GA scheme will be applied following the procedure of Ref. [19], utilizing up to two ghost orbitals.

In Fig. 2 is shown the evolution as a function of the Hubbard interaction strength U of the ghost-GA total energy, the local double occupancy and the QP weight z . Our results are shown

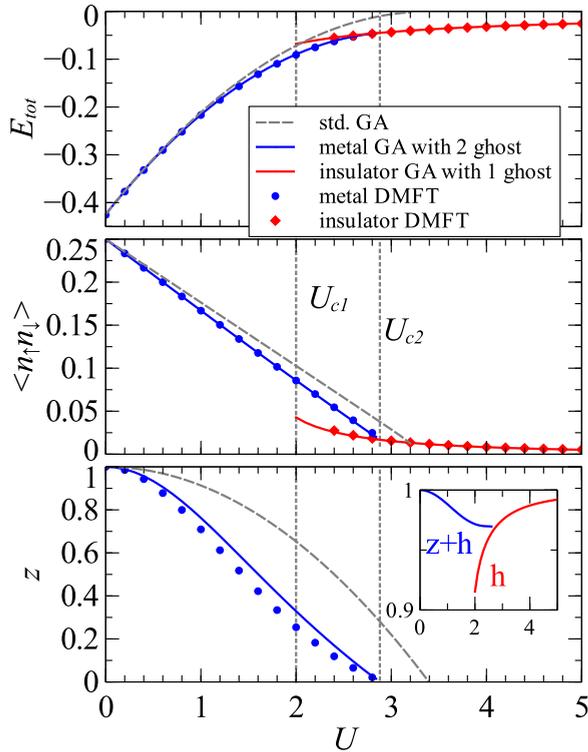


FIG. 2. Evolution of (top) total energy, (middle) local double occupancy, and (bottom) QP weight as a function of the Hubbard interaction strength U for the single-band Hubbard model with semicircular DOS at half-filling. The ghost-GA results are shown in comparison with the ordinary GA and with DMFT+NRG. The ghost-GA boundaries of the coexistence region U_{c1}, U_{c2} are indicated by vertical dotted lines. Inset: Integral of ghost-GA local spectral weight over all frequencies (see discussion in main text).

in comparison with the ordinary GA theory and with DMFT in combination with numerical renormalization group (NRG). In particular, we employed the “NRG Ljubljana” impurity solver [26].

The agreement between ghost-GA and DMFT is quantitatively remarkable. In particular, the ghost-GA theory enables us to account for the coexistence region of the Mott and metallic phases, which is not captured by the ordinary GA theory. The values of the boundaries of the coexistence region $U_{c1} \simeq 2$, $U_{c2} \simeq 2.88$ are in good agreement with the DMFT results available in the literature [27–30], i.e., $U_{c1} \simeq 2.39$, $U_{c2} \simeq 2.94$. The ghost-GA value of U_{c2} , which is the actual Mott transition point at $T = 0$, is particularly accurate. The method also gives a reasonable value for the very small energy scale characterizing the coexistence region, which we can estimate as $T_c \simeq E_{\text{ins}}(U_{c1}) - E_{\text{met}}(U_{c1}) \simeq 0.02$, consistently with both DMFT and experiments [31,32]. We point out also that, as shown in the second panel of Fig. 2, the ghost-GA approach captures the charge fluctuations in the Mott phase, while this is approximated by the simple atomic limit (which has zero double occupancy) within the Brinkman-Rice scenario [33].

Interestingly, while at least two ghost orbitals are necessary to obtain the data illustrated above for the metallic solution, one ghost orbital is sufficient to obtain our results concerning the

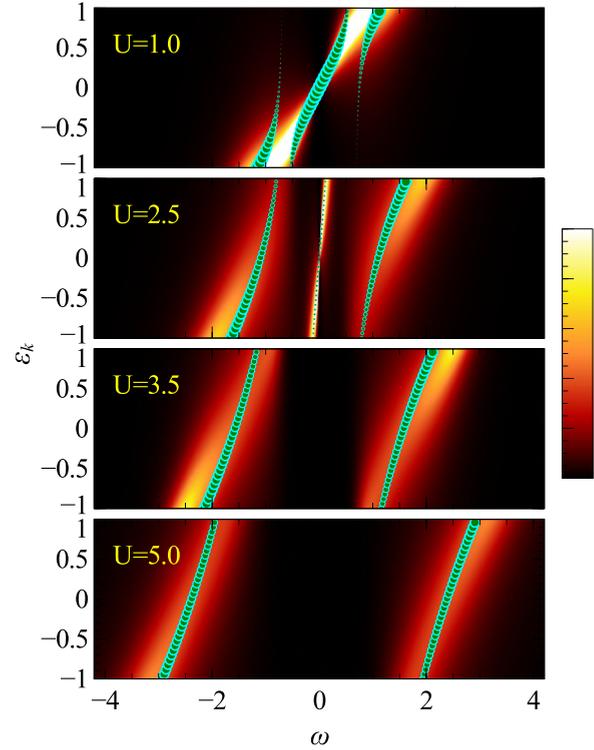


FIG. 3. Poles of the ghost-GA energy-resolved Green’s function (bullets), see Eq. (6), in comparison with DMFT+NRG. The size of the bullets indicates the spectral weights of the corresponding poles. Metallic solution for $U = 1, 2.5$ and Mott solution for $U = 3.5, 5$.

Mott phase. Increasing further the number of ghost orbitals does not lead to any appreciable difference [11]. As we are going to show, this is connected with the fact that the electronic structures of the Mott and the metallic phases are topologically distinct.

Let us now analyze the ghost-GA single-particle Green’s function $G(\epsilon, \omega)$, see Eq. (6). In Fig. 3 is shown the ghost-GA energy-resolved spectral function $A(\epsilon, \omega) = -\frac{1}{\pi} \text{Im} G(\epsilon, \omega)$ in comparison with DMFT [34]. Although the broadening of the bands (scattering rate), is not captured by our approximation (as it is not captured by the ordinary GA), the positions and the weights of the poles of the ghost-GA spectral function encode most of the DMFT features, not only at low energies (QP excitations), but also at high energies (Hubbard bands). In order to analyze how the spectral properties of the system emerge within the ghost-GA theory, it is particularly convenient to express the QP Hamiltonian [Eq. (5)] in a gauge where $\tilde{\lambda}$ is diagonal [35].

In the metallic phase, an explicit ghost-GA calculation obtained employing two ghost orbitals shows that the matrices $\tilde{\mathcal{R}}$ and $\tilde{\lambda}$ are represented as follows:

$$\tilde{\lambda}_{ij} = l \delta_{ij} (\delta_{2i} - \delta_{3i}) \quad (7)$$

$$\tilde{\mathcal{R}}_{ij} = \delta_{j1} (\sqrt{z} \delta_{i1} + \sqrt{h} (\delta_{i2} + \delta_{i3}) / \sqrt{2}), \quad (8)$$

where δ_{ij} is the Kronecker delta, and l, z and h are real positive numbers determined numerically as in Ref. [19]. The

corresponding self-energy, see Eq. (6), is [36]:

$$\Sigma(\omega) = \frac{\omega}{1 + \frac{1}{z - \frac{\omega^2 - l^2 + 2h\omega^2}{\omega^2 - l^2}}} = -\frac{1-z}{z}\omega + o(\omega^2). \quad (9)$$

Thus, the variational parameter z of Eq. (8) represents the QP weight, whose behavior was displayed in the third panel of Fig. 2. Note that the overall spectral weight $\int d\omega \int d\epsilon \rho(\epsilon) A(\epsilon, \omega)$, where $\rho(\epsilon)$ is the semicircular DOS, is not z as in the ordinary GA theory, but it is $z + h = [\tilde{\mathcal{R}}^\dagger \tilde{\mathcal{R}}]_{11}$, which is almost equal to 1 for all values of U (see the inset of the third panel in Fig. 2). The additional spectral contribution h , which is not present in the ordinary GA approximation, enables the ghost-GA theory to account for the Hubbard bands.

In the Mott phase, an explicit ghost-GA calculation obtained employing one ghost orbital shows that the matrices $\tilde{\mathcal{R}}$ and $\tilde{\lambda}$ are represented as follows:

$$\tilde{\lambda}_{ij} = l \delta_{ij} (\delta_{1i} - \delta_{2i}) \quad (10)$$

$$\tilde{\mathcal{R}}_{ij} = \delta_{j1} \sqrt{h} (\delta_{i1} + \delta_{i2}) / \sqrt{2}, \quad (11)$$

where l and h are real positive numbers determined numerically as in Ref. [19]. Note that $h = [\tilde{\mathcal{R}}^\dagger \tilde{\mathcal{R}}]_{11} \simeq 1$ (see the inset of the third panel in Fig. 2). The corresponding self-energy, see Eq. (6), is [36]:

$$\Sigma(\omega) = -\frac{1-h}{h}\omega + \frac{l^2}{h} \frac{1}{\omega}. \quad (12)$$

The pole of the self energy at $\omega = 0$, which is the source of the Mott gap, is captured by the ghost-GA theory. The analysis above clarifies also why, by construction, within the ghost-GA approximation the self-energy can develop poles, see Eqs. (9) and (12), but can not capture branch-cut singularities on the real axis.

We point out that enlarging the Hilbert space has been essential in order to capture the effect of the electron correlations on the topology of the excitations, such as the change of the number of bands at the Mott transition (between three bands in the metallic phase and two bands in the Mott phase). In fact, without extending the Hilbert space, the ordinary GA theory enables us only to renormalize and shift the band structure with respect to the uncorrelated limit $U = 0$, without affecting its qualitative topological structure. On the other hand, extending the Hilbert space enables us to relax this constraint, as $G(\epsilon, \omega)$, see Eq. (6), is variationally allowed to have any number of distinct poles equal or smaller to the corresponding total (physical and ghost) number of orbitals [11]. It is for this reason that only one ghost (two orbitals) is sufficient to describe the Mott phase of the single-band Hubbard model, while at least two ghosts (three orbitals) are necessary in order to describe its metallic phase, whose spectra includes the QP excitations and the two Hubbard bands. A remarkable aspect of this construction is that, within the ghost-GA theory, the information concerning the spectral function, including the Hubbard bands, is entirely encoded in only three parameters (z, h, l) in the metallic phase, and in two parameters (h, l) in the Mott phase, see Eqs. (7), (8), (10), (11).

V. CONCLUSIONS

We derived a unified theoretical picture for excitations in Mott systems based on a generalization of the GA, which captures not only the low-energy QP excitations, but also the Hubbard bands. The key idea consists in enlarging the Hilbert space of the system by introducing auxiliary “ghost” orbitals. This construction enables us to express analytically many important features of both types of excitations in terms of the bare DOS of the uncorrelated system and a few renormalization parameters, in a similar fashion as for the QP excitations in Landau theory of Fermi liquids. In particular, this provides us with a conceptual picture which assigns naturally a Bloch character to the Hubbard bands even in Mott insulators. In this respect, we note that our theory presents a few suggestive analogies with the interesting idea of “hidden Fermi liquid”, previously introduced by Anderson [37] within the context of the BCS wave function (for superconductors) and the Laughlin’s Jastrow wave function (for the fractional hall effect). In fact, they both propose a descriptions of non-Fermi liquid states related to ordinary Fermi liquids residing in unphysical Hilbert spaces, see, e.g., Ref. [38]. From the computational perspective, the ghost-GA theory constitutes a very promising tool for *ab initio* calculations in combination with density functional theory [16,18,39–41], as it is substantially more accurate with respect to the ordinary GA approximation, without much additional computational cost. In fact, within the numerical scheme described in Refs. [16,19], our theory results in solving iteratively a finite impurity model, where the number of bath sites grows linearly with the total number of ghost orbitals [11]. Since there exist numerous available techniques enabling us to solve efficiently this auxiliary problem, see, e.g., Refs. [42–46], this work opens an exciting avenue for realistic modeling of many challenging materials, including predictions of ARPES spectra for complex orbitally selective Mott insulators and “materials by design” of strongly correlated electron systems. Furthermore, since the ghost-GA theory is based on the multiorbital GA [16,19], it can be straightforwardly generalized to finite temperatures [47–49], to nonequilibrium problems [50,51], and to calculate linear response functions [52]. For the same reason, the ghost-GA theory can be reformulated [14,16,53] in terms of the rotationally invariant slave boson (RISB) theory [11,54,55], whose exact operatorial foundation recently derived in Ref. [19] constitutes a starting point to calculate further corrections [56]. It would be also interesting to apply the ghost-orbital Hilbert space extension in combination with the variational Monte Carlo method [57] or the generalization of the GA to finite dimensions of Ref. [58], which might lead to a more accurate description of strongly correlated electron systems, even beyond the DMFT approximation.

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- [1] L. D. Landau, *Sov. Phys. JETP* **3**, 920 (1957).
- [2] A. Damascelli, *Phys. Scr.* **T109**, 61 (2004).
- [3] G. Binnig, H. Rohrer, C. Gerber, and E. Weibel, *Phys. Rev. Lett.* **49**, 57 (1982).
- [4] D. V. Evtushinsky, M. Aichhorn, Y. Sassa, Z.-H. Liu, J. Maletz, T. Wolf, A. N. Yaresko, S. Biermann, S. V. Borisenko, and B. Buchner, [arXiv:1612.02313](https://arxiv.org/abs/1612.02313).
- [5] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [6] V. Anisimov and Y. Izyumov, *Electronic Structure of Strongly Correlated Materials* (Springer, New York, 2010).
- [7] M. C. Gutzwiller, *Phys. Rev.* **137**, A1726 (1965).
- [8] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, *Phys. Rev. Lett.* **59**, 799 (1987).
- [9] F. Vaesrate, J. Cirac, and V. Murg, *Adv. Phys.* **57**, 143 (2008).
- [10] U. Schollwöck, *Ann. Phys. (N.Y.)* **96**, 326 (2011).
- [11] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.96.195126> for technical details and ghost-GA calculations using more ghost orbitals, which includes Refs. [12,13].
- [12] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1997).
- [13] N. Lanatà, *Phys. Rev. B* **82**, 195326 (2010).
- [14] N. Lanatà, P. Barone, and M. Fabrizio, *Phys. Rev. B* **78**, 155127 (2008).
- [15] J. Büneemann, W. Weber, and F. Gebhard, *Phys. Rev. B* **57**, 6896 (1998).
- [16] N. Lanatà, Y. Yao, C.-Z. Wang, K.-M. Ho, and G. Kotliar, *Phys. Rev. X* **5**, 011008 (2015).
- [17] C. Attaccalite and M. Fabrizio, *Phys. Rev. B* **68**, 155117 (2003).
- [18] X.-Y. Deng, L. Wang, X. Dai, and Z. Fang, *Phys. Rev. B* **79**, 075114 (2009).
- [19] N. Lanatà, Y. Yao, X. Deng, V. Dobrosavljević, and G. Kotliar, *Phys. Rev. Lett.* **118**, 126401 (2017).
- [20] Note also that, as the MPS, the ghost-GA wave function does not break artificially the translational invariance of the system.
- [21] J. Büneemann, F. Gebhard, and R. Thul, *Phys. Rev. B* **67**, 075103 (2003).
- [22] N. Lanatà, Ph.D. thesis, SISSA-Trieste, 2009.
- [23] S. Y. Savrasov, K. Haule, and G. Kotliar, *Phys. Rev. Lett.* **96**, 036404 (2006).
- [24] S. Y. Savrasov, V. Oudovenko, K. Haule, D. Villani, and G. Kotliar, *Phys. Rev. B* **71**, 115117 (2005).
- [25] Our results do not qualitatively depend on the specific choice of DOS.
- [26] R. Zitko, *Comp. Phys. Comm.* **182**, 2259 (2011).
- [27] D. J. García, K. Hallberg, and M. J. Rozenberg, *Phys. Rev. Lett.* **93**, 246403 (2004).
- [28] P. Werner and A. J. Millis, *Phys. Rev. B* **75**, 085108 (2007).
- [29] R. Bulla, *Phys. Rev. Lett.* **83**, 136 (1999).
- [30] N.-H. Tong, S.-Q. Shen, and F.-C. Pu, *Phys. Rev. B* **64**, 235109 (2001).
- [31] M. C. O. Aguiar, V. Dobrosavljević, E. Abrahams, and G. Kotliar, *Phys. Rev. B* **71**, 205115 (2005).
- [32] P. Limelette, P. Wzietek, S. Florens, A. Georges, T. A. Costi, C. Pasquier, D. Jérôme, C. Mézière, and P. Batail, *Phys. Rev. Lett.* **91**, 016401 (2003).
- [33] W. F. Brinkman and T. M. Rice, *Phys. Rev. B* **2**, 4302 (1970).
- [34] M. Karski, C. Raas, and G. S. Uhrig, *Phys. Rev. B* **77**, 075116 (2008).
- [35] Equation (6) is invariant with respect to any gauge transformation $\tilde{\mathcal{R}} \rightarrow u^\dagger \tilde{\mathcal{R}}, \tilde{\lambda} \rightarrow u^\dagger \tilde{\lambda} u$, where u is unitary, see Ref. [19].
- [36] Note that the expression for $\Sigma(\omega)$ is k independent as expected, since we employed the GA.
- [37] P. W. Anderson, *Phys. Rev. B* **78**, 174505 (2008).
- [38] J. K. Jain and P. W. Anderson, *Proc. Nat. Acad. Sci.* **106**, 9131 (2009).
- [39] P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, B864 (1964).
- [40] W. Kohn and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).
- [41] K. M. Ho, J. Schmalian, and C. Z. Wang, *Phys. Rev. B* **77**, 073101 (2008).
- [42] F. A. Wolf, A. Go, I. P. McCulloch, A. J. Millis, and U. Schollwöck, *Phys. Rev. X* **5**, 041032 (2015).
- [43] H. Saberi, A. Weichselbaum, and J. von Delft, *Phys. Rev. B* **78**, 035124 (2008).
- [44] A. Weichselbaum, F. Verstraete, U. Schollwöck, J. I. Cirac, and J. von Delft, *Phys. Rev. B* **80**, 165117 (2009).
- [45] Y. Lu, M. Höppner, O. Gunnarsson, and M. W. Haverkort, *Phys. Rev. B* **90**, 085102 (2014).
- [46] N. Lanatà, Y.-X. Yao, X. Deng, C.-Z. Wang, K.-M. Ho, and G. Kotliar, *Phys. Rev. B* **93**, 045103 (2016).
- [47] N. Lanatà, X.-Y. Deng, and G. Kotliar, *Phys. Rev. B* **92**, 081108 (2015).
- [48] M. Sandri, M. Capone, and M. Fabrizio, *Phys. Rev. B* **87**, 205108 (2013).
- [49] W.-S. Wang, X.-M. He, D. Wang, Q.-H. Wang, Z. D. Wang, and F. C. Zhang, *Phys. Rev. B* **82**, 125105 (2010).
- [50] M. Schirò and M. Fabrizio, *Phys. Rev. Lett.* **105**, 076401 (2010).
- [51] N. Lanatà and H. U. R. Strand, *Phys. Rev. B* **86**, 115310 (2012).
- [52] M. Fabrizio, *Phys. Rev. B* **95**, 075156 (2017).
- [53] J. Büneemann and F. Gebhard, *Phys. Rev. B* **76**, 193104 (2007).
- [54] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, *Phys. Rev. B* **76**, 155102 (2007).
- [55] T. Li, P. Wölfle, and P. J. Hirschfeld, *Phys. Rev. B* **40**, 6817 (1989).
- [56] V. H. Dao and R. Frésard, *Phys. Rev. B* **95**, 165127 (2017).
- [57] D. Ceperley, G. V. Chester, and M. H. Kalos, *Phys. Rev. B* **16**, 3081 (1977).
- [58] K. Münster and J. Büneemann, *Phys. Rev. B* **94**, 045135 (2016).