Landau–Gutzwiller quasi-particles

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We define Landau quasi-particles within the Gutzwiller variational theory, and derive their dispersion relation for general multi-band Hubbard models in the limit of large spatial dimensions D. Thereby we reproduce our previous calculations which were based on a phenomenological effective single-particle Hamiltonian. For the one-band Hubbard model we calculate the first-order corrections in $1/D$ and find that the corrections to the quasi-particle dispersions are small in three dimensions. They may be largely absorbed in a rescaling of the total band width, unless the system is close to half band filling. Therefore, the Gutzwiller theory in the limit of large dimensions provides quasi-particle bands which are suitable for a comparison with real, three-dimensional Fermi liquids.

I. INTRODUCTION

The calculation of the band structure of metals and insulators is a central task in solid-state theory. A commonly accepted method for this purpose is the density-functional theory (DFT) which provides surprisingly accurate results for the band structure of many materials[1]. Furthermore, the DFT is an 'ab-initio' theory, i.e., it starts from the full Hamiltonian of a real system and does not require the introduction of any simplified models. The only competing 'ab-initio' theory was Hartree-Fock theory, which has shown very many shortcomings as compared to DFT, such as gross overestimation of band widths and band gaps.

However, from a theoretical point of view, the success of the DFT for band structures is rather astonishing because this theory is a generic approach to ground-state properties only. All results on energy bands are extracted from auxiliary one-particle dispersions which have no physical meaning at the outset. Indeed, some shortcomings of the DFT energy bands have become evident very early, in particular the underestimation of the fundamental gap in semiconductors. In semiconductors and insulators, the so-called GW approximation to the one-particle Green function has been put forward[2]. There, the single-particle self energy is calculated using a Green function based on the DFT wave functions and the screened Coulomb interaction. It turns out that the GW quasi-particle bands are more or less rigidly shifted against the DFT bands so that the band gap results of GW calculations for semiconductors and insulators agree much better with experiment.

For materials with strong electron-electron interactions, the DFT results have not been too convincing, in particular for magnetic insulators and other strongly correlated electron systems. For the iron group metals the discrepancies of DFT results to experimental data, e.g., angle-resolved photo-emission spectroscopy (ARPES), increase towards the end of the series, i.e., towards nickel; for a detailed discussion on the discrepancies between DFT results and experimental data on nickel, see Refs. 3,4. For the iron group metals, GW calculations did not yield significant improvements over the DFT results; for nickel, see Ref. 5.

A proper description of solids with strong Coulomb interactions requires true many-particle approaches. In the past, the notorious difficulties of many-particle systems have restricted such theories to the study of rather simplified model systems, e.g., the one-band Hubbard model. Therefore, a comparison with experiments on real materials could hardly be performed. Only recently, new non-perturbative many-particle methods have become available which have made possible the investigation of more realistic many-particle models; see, for example, Refs. 3,4,6–8. In Ref. 8 we introduced a class of Gutzwiller variational wave functions which allow us to study general multi-band Hubbard models. Expectation values with these correlated electron states are evaluated exactly in the limit of large spatial dimensions, $D \to \infty$. When applied to nickel, the remaining minimization problem is numerically non-trivial because of the large number of variational parameters; first results are reported in Refs. 3,4.

The Gutzwiller variational theory provides an approximate picture of the ground state but, in principle, it lacks any information about excited states. This drawback can be overcome in two ways. First, if we take for granted that the variational ground state is at least qualitatively close to the true ground state, we may use the variational state as a starting point for the variational calculation of excited states. In Ref. 9 we have used this idea

to determine the spin-wave dispersion in ferromagnetic multi-band Hubbard models. We have successfully reproduced the experimental observation that the low-energy spin excitations in itinerant ferromagnets are very similar to those of a system with localized spins. Second, the calculation of the variational ground-state energy in the limit of infinite dimensions[8] naturally leads to the definition of an effective single-particle Hamiltonian which, in some limits, can also be derived in Slave-Boson mean-field theory[10]. Very much in the spirit of the DFT we used the band structure of this effective Hamiltonian for a successful comparison with ARPES data for nickel. We have been able to resolve basically all of the LDA shortcomings.

Despite its success, the second approach still lacks a sound theoretical basis. In this work we derive the (variational) quasi-particle dispersion referring back to Landau's original ideas on Fermi liquids. The Gutzwiller variational state is an illustrative example for a Fermi-liquid ground state: the Gutzwiller many-body correlator acts on the Fermi-gas ground state whereby energetically unfavorable configurations are gradually reduced. In the spirit of Fermi-liquid theory, a quasi-particle excitation is readily viewed as a Gutzwiller-correlated single-particle excitation of the Fermi-gas ground state. The energy of this excitation is identical to the quasi-particle dispersion in our original work[8]. Therefore, no revision of our previous numerical results on nickel[3,4] is necessary.

The evaluation of the variational energy in our method is exact only in the limit of infinite spatial dimensions. Our application to realistic three-dimensional systems requires that $1/D$ corrections are well controlled. As is known from the one-band model, these corrections are small for ground-state properties such as the (variational) energy or the effective mass of the quasi-particles at the Fermi surface. In this work we will present additional results on $1/D$ corrections of the quasi-particle dispersion for the one-band Hubbard model.

Our work is organized as follows. In Sec. II we summarize the basic ideas of Landau-Gutzwiller theory. In Sect. III we discuss the variational ground state for multi-band Hubbard models. In Sec. IV we define Landau-Gutzwiller quasi-particles and derive their energy dispersion. In Sect. V we calculate $1/D$ corrections for the quasi-particle dispersion of the one-band model. Our presentation closes with short conclusions. Some technical details are deferred to the appendix.

II. LANDAU-GUTZWILLER THEORY

In second quantization the Hamilton operator for non-interacting electrons reads

$$\widehat{H}_1 = \sum_{i \neq j; \sigma, \sigma'} t_{i,j}^{\sigma, \sigma'} \widehat{c}_{i;\sigma}^+ \widehat{c}_{j;\sigma'} + \sum_{i;\sigma} \widetilde{\epsilon}_\sigma \widehat{c}_{i;\sigma}^+ \widehat{c}_{i;\sigma} . \quad (1)$$

Here, $\widehat{c}_{i;\sigma}^+$ creates an electron with combined spin-orbit index $\sigma = 1, \ldots, 2N$ ($N = 5$ for $3d$ electrons) at the lattice site i of a solid with L lattice sites. The electron density, $n = N/L$, is finite in the thermodynamic limit $N \to \infty, L \to \infty$.

For a translationally invariant system, as considered throughout this work, this single-particle Hamiltonian is readily diagonalized in momentum space. Its eigenstates are one-particle product states $|\Psi\rangle$. In particular, the ground state $|\Psi_0\rangle$ is the filled Fermi sea where all single-particle states below the Fermi energy are occupied. All other eigenstates can be understood as particle-hole excitations of $|\Psi_0\rangle$.

One essential idea behind Landau's Fermi liquid theory is the assumption that the Fermi-gas picture remains valid qualitatively when electron-electron interactions are switched on; for an introduction, see, e.g., Ref. 11. The Fermi-gas eigenstates transform adiabatically into those of the Fermi liquid while keeping their physical properties. For example, the momentum distribution displays a discontinuity at the Fermi energy both in the Fermi gas and in the Fermi liquid. Naturally, the properties of the ground state and of the particle-hole excitations change quantitatively. Therefore, the excitations are called quasi-particles and quasi-holes in the Fermi liquid.

Gutzwiller's variational theory closely follows the idea of an adiabatic continuity from the Fermi gas to the Fermi liquid. Let us introduce a general class of Gutzwiller-correlated wave functions via

$$|\Psi_G\rangle = \widehat{P}_G |\Phi\rangle . \quad (2)$$

Here, $|\Phi\rangle$ is any normalized one-particle product state. The Gutzwiller correlator

$$\widehat{P}_G = \prod_i \widehat{P}_{i;G} \quad (3)$$

is a many-body operator which suppresses those configurations which are energetically unfavorable with respect to the electron-electron interaction. Therefore, the (approximate) Fermi-liquid ground state

$$|\Psi_G^0\rangle = \widehat{P}_G |\Phi_0\rangle \quad (4)$$

evolves smoothly from a Fermi-gas ground state $|\Phi_0\rangle$ when the electron-electron interaction is switched on. In fact, this concept has been used by Vollhardt[12] to develop a microscopic theory for the ground-state properties of liquid ^{3}He on the basis of Gutzwiller's approach.

In this work, we use Landau's idea to extend Gutzwiller's variational approach to quasi-particle excitations. In principle, this does not pose a big problem. Instead of a Fermi-liquid ground state $|\Phi_0\rangle$, we use single-particle excitations $|\Phi\rangle$ of the Fermi gas in (2) to define quasi-particle states. In Sect. IV we will give a proper mathematical definition of a quasi-particle excitation. Here we point out that all restrictions of Fermi-liquid theory apply. For example, only the low-energy properties of metals, close to the Fermi energy, ought to be described in this way. Nevertheless, experiments on metals show

that well-defined but life-time broadened quasi-particle excitations can be found even for energies of about 10 eV below the Fermi energy. Therefore, the concept of quasi-particles and quasi-holes remains meaningful for those parts of the valence and conduction bands which are relevant in solid-state physics.

III. VARIATIONAL ENERGY

A. Multi-band Hubbard Hamiltonian and Gutzwiller variational states

In the following we study multi-band Hubbard models where the electron-electron interaction is purely local,

$$\widehat{H} = \widehat{H}_1 + \sum_i \widehat{H}_{i;\text{at}} \ . \tag{5}$$

Here, the atomic Hamiltonian $\widehat{H}_{i;\text{at}}$ contains all possible Coulomb-interaction terms between electrons on site i,

$$\widehat{H}_{i;\text{at}} = \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \mathcal{U}^{\sigma_1,\sigma_2;\sigma_3,\sigma_4} \widehat{c}^+_{i;\sigma_1} \widehat{c}^+_{i;\sigma_2} \widehat{c}_{i;\sigma_3} \widehat{c}_{i;\sigma_4} \ . \tag{6}$$

We assume that the eigenstates $|\Gamma\rangle_i$ of the atomic Hamiltonian have been determined

$$\widehat{H}_{i;\text{at}} = \sum_\Gamma E_{i;\Gamma} \widehat{m}_{i;\Gamma} \quad , \quad \widehat{m}_{i;\Gamma} = |\Gamma\rangle_{i\ i}\langle\Gamma| \ . \tag{7}$$

This is possible in all cases of interest, at least numerically. In the following, the site index will often be suppressed as we are primarily interested in translationally invariant systems.

The Gutzwiller theory allows us to study the Hamiltonian (5) with an arbitrary number of orbitals[8]. In this work, however, we will restrict ourselves to the special case where non-degenerate orbitals belong to different representations of the respective point-symmetry group. For example, in cubic symmetry we allow for only one set of s, p, $d(e_g)$ and $d(t_{2g})$ orbitals.

The Gutzwiller correlator

$$\widehat{P}_{\text{G}} = \prod_i \widehat{P}_{i;\text{G}} = \prod_{i;\Gamma} \lambda^{\widehat{m}_{i;\Gamma}}_{i;\Gamma} \tag{8}$$

is parameterized by 2^{2N} real numbers $\lambda_{i;\Gamma}$. For an energetically unfavorable atomic configuration $|\Gamma_i\rangle$ the minimization will result in $\lambda_{i;\Gamma} < 1$ whereby its weight in $|\Phi\rangle$ is reduced.

B. Extrema of the variational energy

In the limit of large spatial dimensions, the expectation value of the Hamiltonian (5) in the wave function (2) can be expressed in terms of the one-particle product wave function $|\Phi\rangle$ and the expectation values

$$m_\Gamma = \langle\widehat{m}_\Gamma\rangle_{\Psi_{\text{G}}} = \frac{\langle\Psi_{\text{G}}|\widehat{m}_\Gamma|\Psi_{\text{G}}\rangle}{\langle\Psi_{\text{G}}|\Psi_{\text{G}}\rangle} \ ; \tag{9}$$

for all details, see Ref. 8. After a lengthy calculation one obtains the following variational energy

$$E^{\text{var}} = \langle\widehat{H}\rangle_{\Psi_{\text{G}}} = \sum_{\sigma,\sigma'} \sum_{\mathbf{k}} S_{\sigma,\sigma'}(\mathbf{k})\langle\widehat{c}^+_{\mathbf{k};\sigma}\widehat{c}_{\mathbf{k};\sigma'}\rangle_\Phi$$

$$+ L\sum_\Gamma E_\Gamma m_\Gamma \ , \tag{10a}$$

$$S_{\sigma,\sigma'}(\mathbf{k}) = \sqrt{q_\sigma}\sqrt{q_{\sigma'}}\epsilon_{\sigma,\sigma'}(\mathbf{k}) + \delta_{\sigma,\sigma'}\widetilde{\epsilon}_\sigma \ , \tag{10b}$$

where

$$\epsilon_{\sigma,\sigma'}(\mathbf{k}) = \frac{1}{L}\sum_{l\neq m} t^{\sigma,\sigma'}_{l,m} \exp\left(-\mathrm{i}\mathbf{k}(\mathbf{R}_l - \mathbf{R}_m)\right) \ . \tag{11}$$

The calculation only requires $|\Phi\rangle$ to be a one-particle product wave state; $|\Phi\rangle$ need not be a filled Fermi sea.

For a given set of Coulomb parameters in (6) the renormalization factors

$$q_\sigma = q_\sigma(n^0_\sigma, m_\Gamma) \tag{12}$$

only depend on the local spin-orbital densities

$$n^0_\sigma = \langle\widehat{n}_\sigma\rangle_\Phi \tag{13}$$

and the variational parameters m_Γ for states $|\Gamma\rangle$ with more than one electron. An explicit expression for (12) has been given in Ref. 8, but it is not needed for our further considerations. Note that for our symmetry-restricted orbital basis

$$n^0_\sigma = n_\sigma = \langle\widehat{n}_\sigma\rangle_{\Psi_{\text{G}}} \tag{14}$$

holds.

E^{var} in (10) depends on the variational parameters m_Γ, the local densities n_σ, and the wave function $|\Phi\rangle$. However, the constraints

$$n_\sigma = \langle\Phi|\widehat{n}_\sigma|\Phi\rangle \quad ; \quad n = \sum_\sigma n_\sigma \tag{15}$$

have to be respected during the minimization as we work for fixed n_σ and n in the sub-space of normalized one-particle product states, $\langle\Phi|\Phi\rangle = 1$. We introduce Lagrange parameters E_{SP}, λ_σ, and Λ for these constraints which leads to the energy functional

$$\begin{aligned} E_{\text{c}}[\Phi, m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda] = \ & E^{\text{var}}[|\Phi\rangle, m_\Gamma, n_\sigma] \\ & - L\sum_\sigma \lambda_\sigma\left[n_\sigma - \langle\Phi|\widehat{n}_\sigma|\Phi\rangle\right] \\ & - L\Lambda(n - \sum_\sigma n_\sigma) \\ & + E_{\text{SP}}(1 - \langle\Phi|\Phi\rangle) \ . \end{aligned} \tag{16}$$

E_{c} has now to be minimized with respect to all quantities $|\Phi\rangle$, E_{SP}, m_Γ, n_σ, λ_σ, and Λ independently.

First, we use the condition that (16) is extremal with respect to $|\Phi\rangle$ and E_{SP}. This gives us the following effective Schrödinger equation which has to be solved in the sub-space of normalized states $|\Phi\rangle$

$$\widehat{H}^{\text{eff}} |\Phi\rangle = E_{\text{SP}} |\Phi\rangle \tag{17}$$

with

$$\widehat{H}^{\text{eff}} = \sum_{\sigma,\sigma'}\sum_{\mathbf{k}}(S_{\sigma,\sigma'}(\mathbf{k}) + \delta_{\sigma,\sigma'}\lambda_\sigma)\widehat{c}^+_{\mathbf{k};\sigma}\widehat{c}_{\mathbf{k};\sigma'} . \quad (18)$$

The effective one-particle Hamiltonian $\widehat{H}^{\text{eff}}$ can be diagonalized,

$$\widehat{H}^{\text{eff}} = \sum_{\mathbf{k},\mathrm{r}} E(\mathbf{k},\mathrm{r})\widehat{h}^+_{\mathbf{k},\mathrm{r}}\widehat{h}_{\mathbf{k},\mathrm{r}} \quad (19)$$

by introducing proper creation and annihilation operators

$$\widehat{h}^+_{\mathbf{k},\mathrm{r}} := \sum_\sigma F_{\mathbf{k},\sigma,\mathrm{r}}\widehat{c}^+_{\mathbf{k},\sigma} \quad ; \quad \widehat{h}_{\mathbf{k},\mathrm{r}} := \sum_\sigma F^*_{\mathbf{k},\sigma,\mathrm{r}}\widehat{c}_{\mathbf{k},\sigma} . \quad (20)$$

Note that the amplitudes $F_{\mathbf{k},\sigma,\mathrm{r}}$, the energies $E(\mathbf{k},\mathrm{r})$, and the operators $\widehat{h}^+_{\mathbf{k},\mathrm{r}}$, $\widehat{h}_{\mathbf{k},\mathrm{r}}$ still depend on the parameters m_Γ, n_σ, and λ_σ.

Solving the eigenvalue equation (17) is only a necessary but not a sufficient condition for a state $|\Phi\rangle$ to minimize the original energy expression (10). In Sect. III we will use this ambiguity to define quasi-particles excitations of the variational Fermi-liquid ground state.

C. Variational Fermi-liquid ground state

In order to obtain our variational Fermi-liquid ground state, it appears to be the most natural choice to proceed with the filled Fermi sea for the effective Hamiltonian $\widehat{H}^{\text{eff}}$,

$$|\Phi_0\rangle = \prod_{\mathbf{k},\mathrm{r};E(\mathbf{k},\mathrm{r})<E_{\mathrm{F}}} \widehat{h}^+_{\mathbf{k},\mathrm{r}}|\text{vacuum}\rangle . \quad (21)$$

Here, the Fermi energy E_{F} is determined by the condition

$$\frac{1}{L}\sum_{\mathbf{k},\mathrm{r}}\Theta(E_{\mathrm{F}} - E(\mathbf{k},\mathrm{r})) = n . \quad (22)$$

The corresponding eigenvalue E_{SP} becomes

$$E_{\mathrm{SP}} = \sum_{\mathbf{k},\mathrm{r}} E(\mathbf{k},\mathrm{r})\Theta(E_{\mathrm{F}} - E(\mathbf{k},\mathrm{r})) . \quad (23)$$

It is difficult to prove rigorously that the state (21) leads to the global minimum of (10). However, $|\Phi_0\rangle$ is at least stable with respect to single-particle excitations and it is difficult to conceive any other state which is consistent with our underlying Fermi-liquid picture.

When we insert $|\Phi_0\rangle$ into (16) we are led to the energy function

$$\widetilde{E}_{\mathrm{c}}[m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda] = E_{\mathrm{SP}} + L\sum_\Gamma E_\Gamma m_\Gamma - L\sum_\sigma \lambda_\sigma n_\sigma$$
$$- L\Lambda(n - \sum_\sigma n_\sigma) . \quad (24)$$

In the variational ground state this expression is extremal with respect to m_Γ, n_σ, λ_σ, and Λ,

$$\left.\frac{\partial}{\partial x_i}\widetilde{E}_{\mathrm{c}}\right|_{\{x_j\}=\{\overline{x}_j\}} = 0 \quad \text{with} \quad x_i \in \{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda\} .$$
$$(25)$$

The optimum values $\overline{m}_\Gamma$, $\overline{n}_\sigma$, $\overline{\lambda}_\sigma$, and $\overline{\Lambda}$ define the optimum values for the energies $\overline{E}(\mathbf{k},\mathrm{r})$, the amplitudes $\overline{F}_{\mathbf{k},\sigma,\mathrm{r}}$, and the operators $\overline{\widehat{h}}^+_{\mathbf{k},\mathrm{r}}$, $\overline{\widehat{h}}_{\mathbf{k},\mathrm{r}}$. Furthermore, we can write the variational ground-state energy as

$$E_0^{\text{var}} = \widetilde{E}_{\mathrm{c}}[\overline{m}_\Gamma, \overline{n}_\sigma, \overline{\lambda}_\sigma, \overline{\Lambda}] . \quad (26)$$

The energy (26) depends on the particle density n both implicitly, mediated by the optimum values $\overline{m}_\Gamma(n)$, $\overline{n}_\sigma(n)$, $\overline{\lambda}_\sigma(n)$, and $\overline{\Lambda}(n)$, and explicitly, due to the term $-L\overline{\Lambda}(n)n$ and the Fermi energy $E_{\mathrm{F}} \equiv E_{\mathrm{F}}(n)$ in E_{SP} of (24). Therefore, the (variational) chemical potential

$$\mu = \frac{1}{L}\frac{dE_0^{\text{var}}}{dn} \quad (27)$$

can be written as

$$\mu = \frac{1}{L}\frac{\partial E_{\mathrm{SP}}}{\partial n} - \overline{\Lambda} \quad (28)$$
$$+ \frac{1}{L}\sum_{x_i \in \{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda\}} \left.\frac{\partial}{\partial x_i}\widetilde{E}_{\mathrm{c}}\right|_{\{x_j\}=\{\overline{x}_j\}} \frac{\partial\overline{x}_i}{\partial n} .$$

The sum in (28) vanishes due to (25) whereas the derivative of E_{SP} just gives the Fermi energy E_{F},

$$\frac{1}{L}\frac{\partial E_{\mathrm{SP}}}{\partial n} = E_{\mathrm{F}} . \quad (29)$$

Therefore, the variational chemical potential reads

$$\mu = E_{\mathrm{F}} - \overline{\Lambda} . \quad (30)$$

The strategy for the numerical minimization is not important for our analysis of Landau-Gutzwiller quasi-particles in the rest of our work. For further reference we give a short summary of our most efficient procedure.

First, we note that the conditions $(\partial\widetilde{E}_{\mathrm{c}})/(\partial\lambda_\sigma) = 0$ and $(\partial\widetilde{E}_{\mathrm{c}})/(\partial\Lambda) = 0$ take us back to the original constraints (15),

$$n_\sigma = \frac{\partial}{\partial\lambda_\sigma}E_{\mathrm{SP}} = \langle\widehat{n}_\sigma\rangle_{\Phi_0}$$
$$= \sum_{\mathbf{k},\mathrm{r}}|F_{\mathbf{k},\sigma,\mathrm{r}}|^2\Theta(E_{\mathrm{F}} - E(\mathbf{k},\mathrm{r})) , \quad (31\mathrm{a})$$
$$n = \sum_\sigma n_\sigma . \quad (31\mathrm{b})$$

Therefore, we are left with two different sets of variational parameters, the 'internal' parameters m_Γ and the 'external' parameters λ_σ. Optimizing the energy with respect to both of these sets is time-costly, for different reasons. The problem with the internal parameters is their large

number which is of the order 2^{2N} (≈ 500 for d orbitals). Compared to this there are only a few, $2N$, external parameters λ_σ. However, each modification of one of these external parameters demands for momentum-space integrations according to the sums in (31a) and (23). We found these integrations to be the most time-consuming part of our numerical minimization. In principle, such integrals must also be calculated whenever we change the parameters m_Γ, because they determine the amplitudes $F_{\mathbf{k},\sigma,\mathrm{r}}$ and the energies $E(\mathbf{k},\mathrm{r})$. In order to avoid this large number of integrations we write E_{SP} in (24) as

$$
\begin{aligned}
E_{\mathrm{SP}} &= \sum_{\sigma,\sigma'} \sqrt{q_\sigma}\sqrt{q_{\sigma'}} {\sum_{\mathbf{k},\mathrm{r}}}' \epsilon_{\sigma,\sigma'}(\mathbf{k}) F^*_{\mathbf{k},\sigma,\mathrm{r}} F_{\mathbf{k},\sigma',\mathrm{r}} \\
&\quad + \sum_\sigma (\widetilde{\epsilon}_\sigma + \lambda_\sigma) {\sum_{\mathbf{k},\mathrm{r}}}' |F_{\mathbf{k},\sigma,\mathrm{r}}|^2 \,,
\end{aligned}
\tag{32}
$$

where the prime on the sums implies $E(\mathbf{k},\mathrm{r})) < E_{\mathrm{F}}$. Eqs. (24) and (32) show that the parameters m_Γ enter the energy $\widetilde{E}_{\mathrm{c}}$ in two different ways: (i), indirectly, via the amplitudes $F_{\mathbf{k},\sigma,\mathrm{r}}$ or the energies $E(\mathbf{k},\mathrm{r})$ and, (ii), directly, via q_σ in (32) and the second term in (24). This separation suggests the following numerical iteration scheme:

1. Start with an initial guess for the parameters m_Γ, e.g., their statistical values in the uncorrelated limit.

2. Minimize the energy with respect to the parameters λ_σ while all m_Γ are fixed. During this minimization the constraint (31b) must be respected.

3. Minimize the energy with respect to the parameters m_Γ, while the parameters λ_σ, the amplitudes $F_{\mathbf{k},\sigma,\mathrm{r}}$, the energies $E(\mathbf{k},\mathrm{r})$ and the wave function $|\Phi_0\rangle$ remain fixed during step 3.

4. Go back to step 2 unless the reduction of E^{var} becomes sufficiently small.

The above procedure represents only a rough picture of our numerical minimization. For example, in practice one finds that some of the parameters λ_σ play only a minor role and, therefore, are fixed during the whole minimization. However, we are not going to discuss these numerical details in this work because they depend on the specific material under investigation.

IV. LANDAU-GUTZWILLER QUASI-PARTICLES

A. Definition

The Gutzwiller theory provides $|\Psi_{\mathrm{G}}^0\rangle$, an approximate description of the true many-body ground state. In order to extend the variational description to quasi-particle excitations, we closely follow Landau's ideas. We seek

creation and annihilation operators $\widehat{e}^+_{\mathbf{p},t}$ and $\widehat{v}_{\mathbf{p},t}$ which must obey the same Fermi-Dirac distribution around the Fermi surface as uncorrelated electrons, i.e., we postulate

$$
\frac{\langle \Psi_{\mathrm{G}}^0 | \widehat{e}^+_{\mathbf{p},t} \widehat{v}_{\mathbf{p},t} | \Psi_{\mathrm{G}}^0 \rangle}{\langle \Psi_{\mathrm{G}}^0 | \Psi_{\mathrm{G}}^0 \rangle} = \Theta(E_{\mathrm{F}} - \overline{E}(\mathbf{p},t)) \,,
\tag{33}
$$

at zero temperature. We will see below that it is actually possible to define operators $\widehat{e}^+_{\mathbf{p},t}$ and $\widehat{v}_{\mathbf{p},t}$ which obey (33) in the whole Brillouin zone and not only around the Fermi surface. This implies that our variational approach does not capture the damping of quasi-particles.

1. Quasi-particles for a rigid Fermi-sea background

First, we adopt the viewpoint of a fixed Fermi-sea background, i.e., we assume that a quasi-particle is added to the N-particle system whose variational parameters have been fixed by the minimization of the energy expression (10), or equivalently, by the conditions (25). This leads to the optimum one-particle product state for the N-particle system

$$
|\overline{\Phi}_0\rangle = \prod_{\mathbf{k},\mathrm{r};\overline{E}(\mathbf{k},\mathrm{r})<E_{\mathrm{F}}} \widehat{\overline{h}}^+_{\mathbf{p},\mathrm{r}} |\mathrm{vacuum}\rangle \,,
\tag{34}
$$

which actually is the ground state of the effective one-particle Hamiltonian

$$
\widehat{\overline{H}}^{\mathrm{eff}} = \sum_{\mathbf{k},\mathrm{r}} \overline{E}(\mathbf{k},\mathrm{r}) \widehat{\overline{h}}^+_{\mathbf{k},\mathrm{r}} \widehat{\overline{h}}_{\mathbf{k},\mathrm{r}} \,.
\tag{35}
$$

The conditions (25) furthermore lead to optimum parameters $\overline{m}_\Gamma$ and by these means define an optimum correlation operator $\widehat{\overline{P}}_{\mathrm{G}}$. Using the one-particle operators $\widehat{\overline{h}}^+_{\mathbf{p},t}$ and $\widehat{\overline{h}}_{\mathbf{p},t}$ we can now identify

$$
\widehat{e}^+_{\mathbf{p},t} := \widehat{\overline{P}}_{\mathrm{G}} \widehat{\overline{h}}^+_{\mathbf{p},t} (\widehat{\overline{P}}_{\mathrm{G}})^{-1} \,,
\tag{36a}
$$

$$
\widehat{v}_{\mathbf{p},t} := \widehat{\overline{P}}_{\mathrm{G}} \widehat{\overline{h}}_{\mathbf{p},t} (\widehat{\overline{P}}_{\mathrm{G}})^{-1}
\tag{36b}
$$

as those operators which obey the quasi-particle condition (33). Note that the inverse operator $(\widehat{\overline{P}}_{\mathrm{G}})^{-1}$ in (36) is well defined since we expect all parameters $\overline{m}_\Gamma$ to be finite in Fermi-liquid systems.

Adding/removing a quasi-particle to/from the ground state generates the excited states

$$
|\overline{\Psi}_{\mathrm{G}}^{(\mathbf{p},t)}\rangle_{\mathrm{qp}} = \widehat{e}^+_{\mathbf{p},t} |\overline{\Psi}_{\mathrm{G}}^0\rangle = \widehat{\overline{P}}_{\mathrm{G}} \widehat{\overline{h}}^+_{\mathbf{p},t} |\overline{\Phi}_0\rangle \,,
\tag{37a}
$$

$$
|\overline{\Psi}_{\mathrm{G}}^{(\mathbf{p},t)}\rangle_{\mathrm{qh}} = \widehat{v}_{\mathbf{p},t} |\overline{\Psi}_{\mathrm{G}}^0\rangle = \widehat{\overline{P}}_{\mathrm{G}} \widehat{\overline{h}}_{\mathbf{p},t} |\overline{\Phi}_0\rangle
\tag{37b}
$$

with fixed Fermi-liquid background. As described in Sect. II, these equations constitute an explicit example for Landau's ideas. The Gutzwiller correlator $\widehat{\overline{P}}_{\mathrm{G}}$ in (2) adiabatically transforms Fermi-gas eigenstates $|\Phi\rangle$ into (approximate) eigenstates of the Fermi liquid.

The energy of quasi-particles or quasi-holes is defined as

$$\overline{E}_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) = \pm(\overline{E}_0^{\mathrm{var}}(\mathbf{p},\mathrm{t}) - E_0^{\mathrm{var}}) - \mu \qquad (38)$$

where

$$E_0^{\mathrm{var}} = \langle \widehat{H} \rangle_{\overline{\Psi}_{\mathrm{G}}} = (26) , \qquad (39\mathrm{a})$$

$$\overline{E}_0^{\mathrm{var}}(\mathbf{p},\mathrm{t}) = \langle \widehat{H} \rangle_{\overline{\Psi}_{\mathrm{G}}^{(\mathbf{p},\mathrm{t})}} . \qquad (39\mathrm{b})$$

The $\pm$-sign refers to quasi-particle or quasi-hole states, respectively. We define the quasi-particle energy (38) in reference to the (variational) chemical potential of the system, see (27). Note that the energy in (38) is of order unity whereas those in (39) are of $\mathcal{O}(L)$.

2. Quasi-particles with background relaxation

When we add a particle to the N-particle system we may expect that the variational parameters will adjust to the presence of the additional particle. Therefore, we may want to work with

$$|\Psi_{\mathrm{G}}^{(\mathbf{p},\mathrm{t})}\rangle_{\mathrm{qp}} = \widehat{P}_{\mathrm{G}}\widehat{h}_{\mathbf{p},\mathrm{t}}^+|\Phi_0\rangle \quad , \quad |\Psi_{\mathrm{G}}^{(\mathbf{p},\mathrm{t})}\rangle_{\mathrm{qh}} = \widehat{P}_{\mathrm{G}}\widehat{h}_{\mathbf{p},\mathrm{t}}|\Phi_0\rangle ,$$
$$(40)$$

where the N-particle Fermi sea $|\Phi_0\rangle$ is defined according to (21). Note that the operators $\widehat{h}_{\mathbf{p},\mathrm{t}}^+, \widehat{h}_{\mathbf{p},\mathrm{t}}$ still depend on the parameters m_Γ, n_σ, and λ_σ for a system with $N \pm 1$ particles. Then,

$$E_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) = \pm(E_0^{\mathrm{var}}(\mathbf{p},\mathrm{t}) - E_0^{\mathrm{var}}) - \mu \qquad (41)$$

with

$$E_0^{\mathrm{var}}(\mathbf{p},\mathrm{t}) = \underset{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda}{\mathrm{Min}} \left[\langle \widehat{H} \rangle_{\Psi_{\mathrm{G}}^{(\mathbf{p},\mathrm{t})}} - L\Lambda(n \pm \frac{1}{L} - \sum_\sigma n_\sigma) \right]$$
$$(42)$$

is the definition of the quasi-particle and quasi-hole energy with background relaxation.

One may wonder whether the two definitions (38) and (41) will lead to different results for the energies of quasi-particles and quasi-holes. Fortunately, this is not the case in the thermodynamic limit, i.e.,

$$\overline{E}_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) = E_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) + \mathcal{O}(1/L) , \qquad (43)$$

as we will show explicitly in appendix A. The addition/subtraction of one particle leads to a change in the optimized variational parameters to order $(1/L)$, and, in principle, this could result in a change of the variational energy E_0^{var} to order unity. However, this quantity is extremal with respect to the variational parameters, so that it changes only to order $(1/L)$ for parameter variations around their optimal values. Therefore, the change of the quasi-particle energies due to the background relaxation vanishes in the thermodynamic limit.

B. Quasi-particle dispersion

In the following we focus on $E_{\mathrm{qp}}(\mathbf{p},\mathrm{t})$ because the evaluation of (38) is more involved. The energy (42) is given by

$$E_0^{\mathrm{var}}(\mathbf{p},\mathrm{t}) = \underset{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda}{\mathrm{Min}} \left[\widetilde{E}_{\mathrm{c}}^{(\mathbf{p},\mathrm{t})}[m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda] \right] \qquad (44)$$

where

$$\widetilde{E}_{\mathrm{c}}^{(\mathbf{p},\mathrm{t})}[m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda] = E_{\mathrm{SP}}^{(\mathbf{p},\mathrm{t})} + \sum_\Gamma E_\Gamma m_\Gamma - L \sum_\sigma \lambda_\sigma n_\sigma$$
$$- L\Lambda(n \pm \frac{1}{L} - \sum_\sigma n_\sigma) \qquad (45)$$

and

$$E_{\mathrm{SP}}^{(\mathbf{p},\mathrm{t})} = \pm E(\mathbf{p},\mathrm{t}) + \sum_{\mathbf{k},\mathrm{r}} E(\mathbf{k},\mathrm{r})\Theta(E_{\mathrm{F}} - E(\mathbf{k},\mathrm{r})) . \quad (46)$$

The $(\pm)$ sign in (45) and (46) correspond to a quasi-particle and quasi-hole state, respectively.

Adding or removing a particle changes the parameters m_Γ, n_σ, λ_σ, and Λ and the energies $E(\mathbf{k},\mathrm{t})$ only by terms of the order $(1/L)$ compared to their values in the N-particle ground state,

$$x_i = \overline{x}_i + \frac{\delta x_i}{L} \quad \text{with} \quad x_i \in \{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda\} ,$$
$$(47\mathrm{a})$$

$$E(\mathbf{k},\mathrm{t}) = \overline{E}(\mathbf{k},\mathrm{t}) + \frac{\delta E(\mathbf{k},\mathrm{t})}{L} . \qquad (47\mathrm{b})$$

Thus we may expand (45) in terms of $(1/L)$ up to order unity,

$$\widetilde{E}_{\mathrm{c}}^{(\mathbf{p},\mathrm{t})}[m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda] = \widetilde{E}_{\mathrm{c}}[\overline{m}_\Gamma, \overline{n}_\sigma, \overline{\lambda}_\sigma, \overline{\Lambda}]$$
$$\pm (\overline{E}(\mathbf{p},\mathrm{t}) - \overline{\Lambda}) + \delta\widetilde{E}_{\mathrm{c}} \qquad (48)$$

$$\delta\widetilde{E}_{\mathrm{c}} = \sum_{x_i \in \{m_\Gamma, n_\sigma, \lambda_\sigma, \Lambda\}} \left. \frac{\partial}{\partial x_i} \widetilde{E}_{\mathrm{c}} \right|_{x_i = \overline{x}_i} \frac{\delta x_i}{L} .$$
$$(49)$$

The sum in (49) vanishes according to (25). Using (29) the quasi-particle dispersion (41) becomes

$$E_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) = \overline{E}(\mathbf{p},\mathrm{t}) - E_{\mathrm{F}} . \qquad (50)$$

This result does not come as a surprise since the Fermi surfaces, as defined by the conditions $\overline{E}(\mathbf{p},\mathrm{t}) = E_{\mathrm{F}}$ and $E_{\mathrm{qp}}(\mathbf{p},\mathrm{t}) = 0$, must coincide. In addition, eq. (50) shows that the quasi-particle dispersion is given by the eigenvalues $\overline{E}(\mathbf{p},\mathrm{t})$ of the effective Hamiltonian (35) not only around the Fermi surface but in the whole Brillouin zone.

Note that there are two important differences between the effective Hamiltonian (35), or, equivalently, (18), and the bare one-particle Hamiltonian $\widehat{H}_1$ in (5). First, the

bands are narrowed in $\widehat{\overline{H}}^{\text{eff}}$ because the Coulomb interaction reduces the mobility of the electrons. Second, the fields λ_σ which were originally introduced as auxiliary Lagrange parameters act as observable shifts of the energy bands, e.g., in terms of a magnetic exchange splitting. Our detailed numerical investigations on Nickel[3,4] showed that both effects, i.e., band-narrowing and band-shifts, are relevant for a proper description of quasi-particles in real materials.

V. 1/D CORRECTIONS FOR THE ONE-BAND HUBBARD MODEL

The energy expression (10) for the wave function (2) is exact in the limit of infinite spatial dimensions D. Therefore, its evaluation for real, finite-dimensional systems constitutes an additional approximation. For the one-band model it has been shown[13] that $1/D$ corrections of ground-state properties are actually small in most cases of interest. An exception is the half-filled Hubbard model where, in infinite dimensions, the Gutzwiller theory predicts the so-called Brinkman-Rice transition where all electrons become localized at some finite critical interaction strength U_{BR}. This metal-insulator is known to be an artifact of the limit $D \to \infty$ because it is absent in all finite dimensions[14]. Consequently, $1/D$ corrections must become important in this special case.

A. First order corrections: analytical results

In the case of only one orbital per lattice site, the general Hamiltonian (5) reduces to

$$\hat{H} = \sum_{\mathbf{k}} \sum_{\sigma=\uparrow,\downarrow} \varepsilon(\mathbf{k}) \hat{c}_{\mathbf{k},\sigma}^+ \hat{c}_{\mathbf{k},\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} . \tag{51}$$

We consider a hyper-cubic lattice with only nearest-neighbor hopping-terms where the bare dispersion in (51) is given by

$$\varepsilon(\mathbf{k}) = -\sqrt{\frac{2}{D}} \sum_{l=1}^D \cos(k_l) . \tag{52}$$

The Gutzwiller wave function will be evaluated in its original form[13], i.e., the variational parameter $\lambda_{(\uparrow\downarrow)}$ for the doubly occupied state $|\Gamma\rangle = |\uparrow\downarrow\rangle$ is replaced by the parameter g. For the one-band model both definitions are equivalent.

The variational ground-state energy of the Hamiltonian (51) in infinite dimension reads

$$E^\infty(g,n) = L \left[q(g,n)\bar{\varepsilon}_0 + U\bar{d}(g,n) \right] , \tag{53}$$

where

$$\bar{\varepsilon}_0 := \frac{1}{L} \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}^0 \varepsilon(\mathbf{k}) \tag{54}$$

is the mean kinetic energy of the non-interacting system. Here, the renormalization factors $q(g,n)$ and the average double occupancy per lattice site $\bar{d}(g,n)$ are given by

$$q(g,n) = \frac{4}{n(2-n)} \left(\frac{n}{2} - \bar{d}(g,n) \right)$$
$$\times \left(\sqrt{1-n+\bar{d}(g,n)} + \sqrt{\bar{d}(g,n)} \right)^2 , \tag{55a}$$

$$\bar{d}(g,n) = \frac{n}{2} \frac{G+n-1}{G+1} \tag{55b}$$

with

$$G = \sqrt{1 + n(2-n)(g^2-1)} . \tag{56}$$

The momentum distribution of the non-interacting system,

$$n_{\mathbf{k},\sigma}^0 = \Theta(E_{\text{F}} - \varepsilon(\mathbf{k})) , \tag{57}$$

and the electron density,

$$\frac{1}{L} \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}^0 = n , \tag{58}$$

determine the Fermi energy E_{F}.

We set up the $1/D$ expansion of a function $A(g,n)$ in the form

$$A(g,n) = A^\infty(g,n) + \frac{1}{D} A^{(1)}(g,n) + \dots . \tag{59}$$

Then, the first-order correction of the ground-state energy reads

$$E^{(1)}(g,n) = L \left[t^{(1)}(g,n) + U\bar{d}^{(1)}(g,n) \right] , \tag{60}$$

where the corrections to the average kinetic energy and the double occupancy can be written as

$$t^{(1)}(g,n) = \frac{1}{L} \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}^{(1)} \varepsilon_\sigma(\mathbf{k}) , \tag{61}$$

$$n_{\mathbf{k},\sigma}^{(1)}(g,n) = f(g,n) \left[\frac{(n-1)(G-1)}{n(2-n)G} \bar{\varepsilon}_0 + \varepsilon_\sigma(\mathbf{k}) \right] (\bar{\varepsilon}_0)^3$$
$$\times [n(G+1-n) + 2(1-n)(G-1)n_{\mathbf{k},\sigma}^0] , \tag{62}$$

and

$$\bar{d}^{(1)}(g,n) = h(g,n)(\bar{\varepsilon}_0)^4 . \tag{63}$$

Here, we introduced the factors

$$f(g,n) = -\left(\frac{1}{1+g} \right)^2 \left(\frac{G-1}{G+1} \right)^2 \left(\frac{1}{n(2-n)} \right)^3 , \tag{64a}$$

$$h(g,n) = \frac{(G+1-n)(G+n-1)(G-1)}{2G(G+1)^3 n^2 (2-n)^2} . \tag{64b}$$

The total ground-state energy to first order in $1/D$,

$$E(g,n) = E^\infty(g,n) + \frac{1}{D}E^{(1)}(g,n) , \qquad (65)$$

has to be minimized with respect to g. However, the optimum value $\overline{g}$ of this minimization differs from the respective value $\overline{g}^\infty$ in infinite dimensions only by terms of the order $1/D$,

$$\overline{g} = \overline{g}^\infty + \frac{1}{D}\overline{g}^{(1)} . \qquad (66)$$

Therefore, we can expand the optimum ground-state energy in terms of $1/D$ as

$$
\begin{aligned}
E(\overline{g},n) &= E^\infty\left(\overline{g}^\infty + \frac{1}{D}\overline{g}^{(1)},n\right) \\
&\quad + \frac{1}{D}E^{(1)}\left(\overline{g}^\infty + \frac{1}{D}\overline{g}^{(1)},n\right) \qquad (67\text{a}) \\
&\approx E^\infty(\overline{g}^\infty,n) + \frac{\overline{g}^{(1)}}{D}\left.\frac{\partial E^\infty(g,n)}{\partial g}\right|_{g=\overline{g}^\infty} \\
&\quad + \frac{1}{D}E^{(1)}(\overline{g}^\infty,n) , \qquad (67\text{b})
\end{aligned}
$$

which leads to

$$E(\overline{g},n) \approx E^\infty(\overline{g}^\infty,n) + \frac{1}{D}E^{(1)}(\overline{g}^\infty,n) = E(\overline{g}^\infty,n) \quad (68)$$

because the derivative in (67b) vanishes. From (68) we see that the optimum ground-state energy is determined by the optimum parameter $\overline{g}^\infty$ in infinite dimensions and no minimization of the total energy (65) is required.

In order to determine the quasi-particle dispersion as defined in (38), we evaluate (39a) and (39b) to order $1/D$. The energy (39a) is given by (68). The expression (68) also yields the energy (39b) when we perform the replacements

$$n \rightarrow n \pm \frac{1}{L} \qquad (69\text{a})$$

$$n^0_{\mathbf{k},\sigma} \rightarrow n^0_{\mathbf{k},\sigma} \pm \delta_{\mathbf{k},\mathbf{p}}\delta_{\sigma,\tau} \qquad (69\text{b})$$

for a quasi-particle state ($+$ sign) or quasi-hole state ($-$ sign) with momentum $\mathbf{p}$ and spin τ. A straightforward expansion of (39b) in terms of $1/L$ leads to the quasi-particle energy

$$\overline{E}_{\text{qp}}(\mathbf{p},\tau) = \overline{E}^\infty_{\text{qp}}(\mathbf{p},\tau) + \frac{1}{D}\overline{E}^{(1)}_{\text{qp}}(\mathbf{p},\tau) . \qquad (70)$$

Here, we recover the quasi-particle dispersion in infinite dimensions,

$$\overline{E}^\infty_{\text{qp}}(\mathbf{p},\tau) = \pm q(\overline{g}^\infty,n)(\varepsilon(\mathbf{p}) - E_{\text{F}}) , \qquad (71)$$

as already derived in Sec. IV. The first-order correction reads

$$\overline{E}^{(1)}_{\text{qp}}(\mathbf{p},\tau) = \pm\left[\varepsilon(\mathbf{p}) - E_{\text{F}}\right]\widetilde{E}\left[\varepsilon(\mathbf{p})\right] \qquad (72)$$

with

$$
\begin{aligned}
\widetilde{E}\left[\varepsilon(\mathbf{p})\right] = f(\overline{g}^\infty,n)(\overline{\varepsilon}_0)^2\Big\{ &- 10\frac{(n-1)^2(\overline{G}^\infty - 1)^2}{n(2-n)\overline{G}^\infty}(\overline{\varepsilon}_0)^2 \\
&+ 6n(\overline{G}^\infty + 1 - n) + 6(1-n)(\overline{G}^\infty - 1)\overline{\varepsilon}_0^2 \\
&+ (\varepsilon(\mathbf{p}) + E_{\text{F}})\,2(1-n)(\overline{G}^\infty - 1)\overline{\varepsilon}_0\Big\} \qquad (73) \\
&+ 4Uh(\overline{g}^\infty,n)(\overline{\varepsilon}_0)^3 .
\end{aligned}
$$

The quantity $\overline{G}^\infty$ is given by (56), evaluated at $g = \overline{g}^\infty$, and $\overline{\varepsilon}_0^2$ is defined by

$$\overline{\varepsilon}_0^2 = \frac{1}{L}\sum_{\mathbf{k},\sigma} n^0_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})^2 . \qquad (74)$$

Note that in deriving (73) we have used the relations

$$\sum_{\mathbf{k}} \varepsilon(\mathbf{k}) = 0 \quad , \quad \frac{1}{L}\sum_{\mathbf{k}}[\varepsilon(\mathbf{k})]^2 = 1 , \qquad (75)$$

which hold for the dispersion relation (52).

B. First-order corrections: numerical results

We are interested in the relative size of the $1/D$ corrections compared to the result in $D = \infty$ dimensions. For this purpose we introduce

$$m(\mathbf{p}) = \frac{\overline{E}_{\text{qp}}(\mathbf{p},\tau)}{\overline{E}^\infty_{\text{qp}}(\mathbf{p},\tau)} - 1 \qquad (76)$$

as a measure for the deviations from the result in infinite dimensions.

In the half-filled case, $n = 1$, the ratio $m(\mathbf{p})$ is independent of the wave vector $\mathbf{p}$,

$$m = m(\mathbf{p}) = \frac{1}{2D}\frac{g-1}{g+1}\overline{\varepsilon}_0^2\left[\overline{\varepsilon}_0 U - \frac{3(g-1)}{g+1}\right] . \qquad (77)$$

The inset of Fig. 1 shows $m = m(\mathbf{p})$ as a function of $s = 4\overline{d}/n^2$ for spatial dimensions $D = 1,2,3$. Here, $0 \le s \le 1$ provides a measure for the correlation strength in the system. The value $s = 1$ corresponds to $U = 0$ and $s = 0$ is realized at the Brinkman-Rice transition, $U = U_{\text{BR}} = 8|\overline{\varepsilon}_0|$. As seen from the inset of Fig. 1, $1/D$ corrections are not negligible over a wide range of interactions, especially in one dimension. In three dimensions, these corrections are much smaller but still about 25% close to the Brinkman-Rice transition.

Since this transition is spurious in finite dimensions, $1/D$ corrections have to be large in the half-filled Hubbard model. For an application of our method to real Fermi-liquid systems it is more reasonable to study cases of non-integer band filling. Fig. 1 shows the ratio $m(\mathbf{p}_{\text{F}})$ at the Fermi surface for different band fillings $n = 1, 0.99, 0.95, 0.9, 0.8, 0.5, 0.2$ in three dimensions. The respective results for band-fillings $n' = 2 - n$ follow
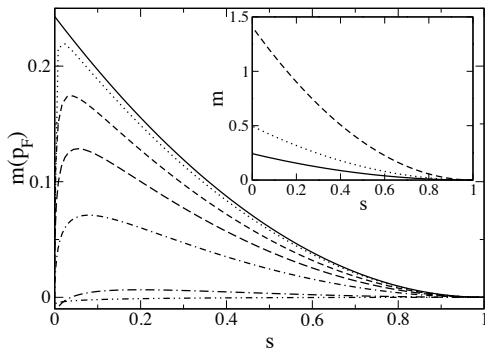
FIG. 1: Renormalization factor $m(\mathbf{p}_F)$ for the quasi-particle dispersion at the Fermi energy as a function of $s = 4\bar{d}/n^2$ for band fillings $n = 1, 0.99, 0.95, 0.9, 0.8, 0.5, 0.2$ (from top to bottom at $s = 0.2$) in three dimensions. Inset: special case of half band-filling for dimensions $D = 1$ (dashed line), $D = 2$ (dotted line), and $D = 3$ (full line).

FIG. 2: Maximal width of the renormalization factor Δm for the quasi-particle dispersion as a function of $s = 4\bar{d}/n^2$ for band fillings $n = 1, 0.99, 0.95, 0.9, 0.8, 0.5, 0.2$ in three dimensions, shown on a logarithmic scale; notation as in Fig. 1.

identically due to particle-hole symmetry. As expected, the corrections in Fig. 1 become much smaller away from integer filling.

The data in Fig. 1 show $m(\mathbf{p}_F)$ at the Fermi energy. However, for $n \neq 1$, there also is a momentum dependence of $m(\mathbf{p})$ which can become significant close to half band filling. In Fig. 2 we show the width of first order contributions,

$$\Delta m = \underset{\mathbf{p}}{\text{Max}} \, |m(\mathbf{p}) - m(\mathbf{p}_F)| \,, \qquad (78)$$

on a logarithmic scale for the same band fillings as in Fig. 1. Although Δm strictly vanishes for $n = 1$ we see from Fig. 2 that Δm can become relatively large for $n \lesssim 1$. This means that around the half-filled case we find $1/D$ corrections which strongly depend on the wave vector.

As long as $\Delta m \ll m(\mathbf{p}_F)$, a finite value of $m(\mathbf{p})$ amounts to a rescaling of the overall band width. When we apply our theory to real materials[3,4] the band width is basically controlled by the Racah-parameter A which we adjust to fit the experimental band width. Therefore, $1/D$ corrections without a significant momentum dependence will not modify the band structure in our variational approach.

As shown in Figs. 1, 2 the results for $D \to \infty$ become questionable only close to integer filling and for very strong correlations. Therefore, we have reasons to believe that the quasi-particle dispersions as calculated in $D = \infty$ in Sect. IV provide a good starting point for a sensible comparison with experimental data. The good agreement between experiments and our theoretical results on nickel[3,4] supports such an optimistic point of view.
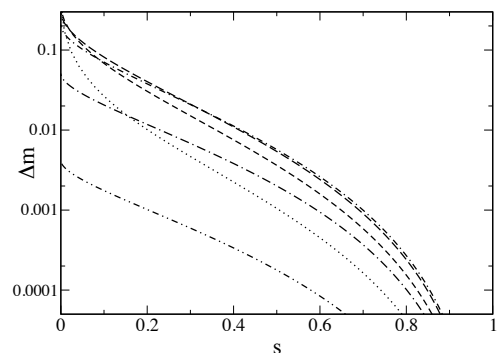
VI. CONCLUSIONS

In this work we used Landau's Fermi-liquid picture to define quasi-particle excitations in terms of Gutzwiller-correlated wave functions. Starting from the optimum variational ground state of a general multi-band Hubbard-model we identified operators which describe the creation and annihilation of quasi-particles in this state. We calculated the quasi-particle dispersion analytically in the limit of infinite dimensions. Our variational states provide an illustrative example for Landau quasi-particles. They are also suitable for numerical investigations, e.g., with variational Monte-Carlo techniques.

We gave two definitions of quasi-particle operators, with and without a relaxation of the Fermi-sea background. It turns out that it is more convenient to allow a (small) change of the variational parameters of the Fermi-sea background in the presence of the quasi-particles. We showed that both cases lead to the same result for the quasi-particle dispersion. This absence of a orthogonality catastrophe is characteristic for Fermi liquids.

Our results confirm our earlier calculations in which the quasi-particle dispersion had been extracted phenomenologically from an effective one-particle Hamiltonian[3,4,8]. In contrast to density-functional theory, our quasi-particle dispersions correspond to mathematically well-defined (variational) states in realistic multi-band Hubbard models. In general, our quasi-particle bands are narrower than the DFT bands because of the hopping-reduction factors q_σ in (10). Moreover, as seen in (18), the Gutzwiller theory has the flexibility for the adjustment of the orbital energies through the parameters λ_σ so that the DFT bands are shifted and mixed into the Landau-Gutzwiller quasi-particle bands.

Our derivation of the Gutzwiller theory uses approximations which become exact in the limit of infinite spatial dimensions, $D \to \infty$. For this reason, we calculated first-order corrections in $1/D$ for the quasi-particle dispersion of the one-band Hubbard model. Apart from

the special case close to half band-filling, these corrections were found to be relatively small. Consequently, the quasi-particle bands as derived in $D = \infty$ for multi-band Hubbard models contain the essential information of the Gutzwiller states in three dimensions, and are thus suitable for a meaningful comparison with real, three-dimensional Fermi liquids.

Acknowledgments

APPENDIX A: QUASI-PARTICLE DISPERSION FOR A RIGID FERMI-SEA BACKGROUND

In this appendix we evaluate the quasi-particle dispersion (38) and thereby prove that it is identical to the energy (50).

The variational ground state $\left|\overline{\Psi}_{\mathrm{G}}^{0}\right\rangle$ in (39a) is given as

$$\left|\overline{\Psi}_{\mathrm{G}}^{0}\right\rangle = \widehat{\overline{P}}_{\mathrm{G}}\left|\overline{\Phi}_{0}\right\rangle , \tag{A1}$$

where $\left|\overline{\Phi}_{0}\right\rangle$ is the state (21) evaluated for the optimum values $\overline{m}_{\Gamma}$, $\overline{n}_{\sigma}$, $\overline{\lambda}_{\sigma}$, and $\overline{\Lambda}$. The variational ground-state energy (39a) therefore reads

$$
\begin{aligned}
E_{0}^{\mathrm{var}} &= \sum_{\sigma,\sigma'}\sum_{\mathbf{k}} S_{\sigma,\sigma'}(\mathbf{k};\overline{n}_{\sigma},\overline{m}_{\Gamma})\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}_{0}} \\
&+ L\sum_{\Gamma} E_{\Gamma}\overline{m}_{\Gamma} .
\end{aligned}
\tag{A2}
$$

Here, we made it explicit that the numbers $S_{\sigma,\sigma'}(\mathbf{k})$ in (10) depend on n_{σ} and m_{Γ}. The state (37), which determines the expectation value (39b) can be written as

$$\left|\overline{\Psi}_{\mathrm{G}}^{(\mathbf{p},\mathrm{t})}\right\rangle = \widehat{\overline{P}}_{\mathrm{G}}\left|\overline{\Phi}^{(\mathbf{p},\mathrm{t})}\right\rangle , \tag{A3}$$

where

$$\left|\overline{\Phi}^{(\mathbf{p},\mathrm{t})}\right\rangle = \widehat{\overline{h}}_{\mathbf{p},\mathrm{t}}^{(+)}\left|\overline{\Phi}_{0}\right\rangle . \tag{A4}$$

The densities n_{σ} and the parameters m_{Γ} for the state $\left|\overline{\Phi}^{(\mathbf{p},\mathrm{t})}\right\rangle$ differ from those of the N-particle ground state only by terms of the order $1/L$,

$$n_{\sigma} = \overline{n}_{\sigma} + \frac{1}{L}\delta n_{\sigma} , \tag{A5a}$$

$$m_{\Gamma} = \overline{m}_{\Gamma} + \frac{1}{L}\delta m_{\Gamma} , \tag{A5b}$$

where, for example,

$$\delta n_{\sigma} = \pm|\overline{F}_{\mathbf{p},\sigma,\mathrm{t}}|^{2} . \tag{A5c}$$

Here, the signs $\pm$ refer to a quasi-particle or quasi-hole state, respectively. Using (A4)–(A5) we can write the energy (39b) as

$$
\begin{aligned}
\overline{E}_{0}^{\mathrm{var}}(\mathbf{p},\mathrm{t}) &= \sum_{\sigma,\sigma'}\sum_{\mathbf{k}} S_{\sigma,\sigma'}(\mathbf{k};\overline{n}_{\sigma}+\frac{1}{L}\delta n_{\sigma},\overline{m}_{\Gamma}+\frac{1}{L}\delta m_{\Gamma}) \\
&\qquad \times \langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}^{(\mathbf{p},\mathrm{t})}} \\
&+ L\sum_{\Gamma} E_{\Gamma}(\overline{m}_{\Gamma}+\frac{1}{L}\delta m_{\Gamma}) .
\end{aligned}
\tag{A6}
$$

For the expectation value in (A6) we find

$$\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}^{(\mathbf{p},\mathrm{t})}} = \langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}_{0}} \pm \delta_{\mathbf{k},\mathbf{p}}\overline{F}_{\mathbf{p},\sigma,\mathrm{t}}^{*}\overline{F}_{\mathbf{p},\sigma',\mathrm{t}} . \tag{A7}$$

An expansion of (A6) in terms of $1/L$ up to and including terms of order unity leads to

$$
\begin{aligned}
\overline{E}_{0}^{\mathrm{var}}(\mathbf{p},\mathrm{t}) &= E_{0}^{\mathrm{var}} \pm \sum_{\sigma,\sigma'} S_{\sigma,\sigma'}(\mathbf{p};\overline{n}_{\sigma},\overline{m}_{\Gamma})\overline{F}_{\mathbf{p},\sigma,\mathrm{t}}^{*}\overline{F}_{\mathbf{p},\sigma',\mathrm{t}} \\
&+ \sum_{\gamma}\delta n_{\gamma}\frac{1}{L}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}}\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}_{0}} \\
&\qquad \times \left.\frac{\partial}{\partial n_{\gamma}}S_{\sigma,\sigma'}(\mathbf{k};n_{\sigma},\overline{m}_{\Gamma})\right|_{n_{\sigma}=\overline{n}_{\sigma}} \\
&+ \sum_{\Gamma'}\delta m_{\Gamma'}\Bigg[E_{\Gamma'} + \frac{1}{L}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}}\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}_{0}} \\
&\qquad \times \left.\frac{\partial}{\partial m_{\Gamma'}}S_{\sigma,\sigma'}(\mathbf{k};\overline{n}_{\sigma},m_{\Gamma})\right|_{m_{\Gamma}=\overline{m}_{\Gamma}} \Bigg] .
\end{aligned}
\tag{A8}
$$

With the help of equations (17) and (18) we find

$$
\begin{aligned}
\frac{\partial}{\partial n_{\gamma}}E^{\mathrm{SP}} &= \left\langle\frac{\partial}{\partial n_{\gamma}}\widehat{H}^{\mathrm{eff}}\right\rangle_{\overline{\Phi}_{0}} \tag{A9a} \\
&= \sum_{\sigma,\sigma'}\sum_{\mathbf{k}}\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}} \\
&\qquad \times \left.\frac{\partial}{\partial n_{\gamma}}S_{\sigma,\sigma'}(\mathbf{k};n_{\sigma},\overline{m}_{\Gamma})\right|_{n_{\sigma}=\overline{n}_{\sigma}} \tag{A9b} \\
&= L(\overline{\lambda}_{\gamma}-\overline{\Lambda}) \tag{A9c}
\end{aligned}
$$

where the third line (A9c) follows from (24) and (25). In the same way we can show that

$$
\begin{aligned}
\sum_{\sigma,\sigma'}\sum_{\mathbf{k}}\langle\widehat{c}_{\mathbf{k};\sigma}^{+}\widehat{c}_{\mathbf{k};\sigma'}\rangle_{\overline{\Phi}_{0}}\left.\frac{\partial}{\partial m_{\Gamma'}}S_{\sigma,\sigma'}(\mathbf{k};\overline{n}_{\sigma},m_{\Gamma})\right|_{m_{\Gamma}=\overline{m}_{\Gamma}} &= \\
-L\cdot E_{\Gamma'} . &
\end{aligned}
\tag{A10}
$$

Therefore, the energy difference in (38) becomes

$$
\begin{aligned}
\overline{E}_{0}^{\mathrm{var}}(\mathbf{p},\mathrm{t}) - E_{0}^{\mathrm{var}} = \pm\sum_{\sigma,\sigma'}\Big(&S_{\sigma,\sigma'}(\mathbf{p};\overline{n}_{\sigma},\overline{m}_{\Gamma})\overline{F}_{\mathbf{p},\sigma,\mathrm{t}}^{*}\overline{F}_{\mathbf{p},\sigma',\mathrm{t}} \\
&+ \delta_{\sigma,\sigma'}(\overline{\lambda}_{\sigma}-\overline{\Lambda})|\overline{F}_{\mathbf{p},\sigma,\mathrm{t}}|^{2}\Big) .
\end{aligned}
\tag{A11}
$$

The first two terms in this expression just give the eigenvalues $\overline{E}(\mathbf{p}, \mathrm{t})$ of the effective Hamiltonian (35), which leads to

$$\overline{E}_0^{\mathrm{var}}(\mathbf{p}, \mathrm{t}) - E_0^{\mathrm{var}} = \pm(\overline{E}(\mathbf{p}, \mathrm{t}) - \overline{\Lambda}) . \qquad (\text{A12})$$

Thus, by use of (30), the quasi-particle dispersion (39b)

finally becomes

$$\overline{E}_{\mathrm{qp}}(\mathbf{p}, \mathrm{t}) = \overline{E}(\mathbf{p}, \mathrm{t}) - E_{\mathrm{F}} , \qquad (\text{A13})$$

in agreement with our result for $E_{\mathrm{qp}}(\mathbf{p}, \mathrm{t})$ as derived in Sec. IV B.

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