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Spin- and charge-fluctuation contribution to mass enhancement

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We study the one-loop contribution of the spin and charge fluctuation to the boson hopping factor in the slave-boson representation of the Hubbard model introduced by Kotliar and Ruckenstein. Whether one uses a low-lying cutoff or sums over the whole bosonic spectrum, the noninteracting limit for the fluctuation correction of the mass enhancement is not recovered for vanishing Coulomb interaction. We argue that one should be cautious when attempting to extend the loop-expansion calculation, in the functional-integral scheme of Kotliar and Ruckenstein, to the observables in which the high-energy excitations may play an important role.

I. INTRODUCTION

The Gutzwiller approach[1] to the Hubbard model is an appealing method for studying strongly correlated Fermi systems. It has been extensively studied for years,[2,3] especially since the discovery of high-T_c superconductors[4] and Anderson's seminal paper.[5] Recently, significant progress was made by Kotliar and Ruckenstein (KR).[6] Their functional-integral slave-boson formulation of the Hubbard model has the Gutzwiller approximation (GA) (Refs. 1 and 3) as a static paramagnetic saddle point.[6]

In principle KR's approach can be pursued beyond the mean-field level. Within KR's scheme, several extensions of the GA can be considered. One may transform the variational scheme into a standard perturbative treatment through a loop expansion. Also one may extend to finite temperature the GA, and approximate variational approach which by itself is valid only for the ground state, thus zero temperature. One may even consider the effects coming from rather high-energy excitations. This is in contrast to the restriction to low-lying excitations around the Fermi level, a crucial assumption of Landau's Fermi-liquid theory (LFLT). Finally, one may apply KR's approach to study more complicated magnetic phases of the Hubbard model, for example, the antiferromagnetic phase, the incommensurate phase, as well as the spiral phase, etc., which may all appear in strongly correlated two-dimensional (2D) fermion systems. There then follows immediate questions: Can any of these extensions be successfully realized, and if so, how far can those extensions be pursued?

Within the paramagnetic metallic phase that will be dealt with in this paper, the hope is that the loop-expansion corrections to the saddle-point solution may improve the GA and may be capable of accounting for new effects which have not been included in the mean-field theory. The effects of thermal fluctuations have been studied recently in the KR slave-boson (SB) approach to one-loop order. Among a few recent[7] investigations let us mention the $T^3 \ln T$ contribution to the low-temperature specific heat and the superfluid transition temperature of ^{3}He in addition to the conductivity of transition metals. Also, all of the two-point dynamical correlation functions have been derived[8] and calculated,[9,10] and then their by-products, the structure factors, have been compared with the Monte Carlo results[11–14] for the 1D and 2D Hubbard lattices and reasonable agreement has been obtained. However, in these calculations of fluctuations, the contribution of the correction to the mass enhancement, beyond the mean-field level, has not been involved. Also it is worthwhile to note that in those successfully calculated observables, only the low-lying excitations or sum rules are involved. The calculation of the dynamical correlation functions[9] is an exception, but in which the high-frequency aspect has not been seriously tested yet, given the lack of either the exact solution or reliable numerical work as a standard for comparison. We[9] have proved that the noninteracting limit is recovered for all those dynamical correlation functions which are beyond the mean-field level.

From those calculations[7] one could see that it is nontrivial to keep track of the contributions from spin and charge fluctuations and put them on an equal footing,[7,15] especially when the repulsive Hubbard interaction U is close to U_c, the critical interaction for the Brinkman-Rice[2] (BR) transition. This transition occurs only at half-filling according to the GA, but when U is larger than U_c, then a strong spin (charge) fluctuation is expected for the repulsive (attractive) U both at half-filling and at light doping. In these cases the fluctuation contribution to the mass enhancement may be important even for the ground state due to the strong zero-point fluctuation.

The GA, an approximation used for evaluating the expectation value in the Gutzwiller wave function (GWF),[1,3] has indicated an instability at half-filling at a finite value of U, which was later interpreted as BR's metal-insulator,[2] or localization,[2,3] transition. This is a remarkable success for the GA. It has been shown recently that the solution to the GWF without the GA can be obtained in two extreme cases, the 1D and the infinite-dimension Hubbard lattice.[16] Also, it was shown that the GA becomes asymptotically exact in the limit of infinite spatial dimension $d=\infty$.[16] However, these results show the absence[16] of an instability, or transition, at finite U. Furthermore, there are reasons to argue that there is no transition at finite U for any finite dimension[16] in an exact evaluation of the expectation value for the GWF. Thus the GA faces a difficult challenge: Its success in explaining the BR, or metal-insulator transition, comes from the approximation itself. However, one may argue, by adopting KR's functional-integral scheme, that the BR transition is retained at the mean-field level only. Then follows the question of the effect of fluctuations within this scheme. On the one hand, as expected, the zero-point fluctuations in the ground state are very strong when U is close to U_c at half-filling, or U even beyond U_c at light doping. On the other hand, the enormously enhanced mass in these cases will suppress the zero-point fluctuations. The final state should stay in some balance between these two opposite effects and one expects that the BR transition should be retained even at some finite doping.

Very recently, the ambiguity in KR's approach was finally clarified by Jolicoeur and Le Guillou (JG):[17] the correct gauge symmetry in KR formalism is $U(1)^{\otimes 3}$ instead of $U(1)^{\otimes 4}$. Also they presented an interesting study of the mass enhancement within the KR approach using the $U(1)^{\otimes 3}$ gauge symmetry, instead of the previously used $U(1)^{\otimes 4}$ symmetry.[7,18] A similar approach has also been used by Frésard and Wölfle.[19] The reason for that replacement is that there are only three constraints. Since there are four slave bosons one of them remains a complex number.[20] Thus one may consider the $U(1)^{\otimes 4}$ approach as an additional approximation, in which one of the integration variables, the extra phase, has been dropped. However, previous experiences have shown that the $U(1)^{\otimes 4}$ approach has worked quite well when compared with the experiments.[7] Also some interesting and transparent analytical results have been obtained via $U(1)^{\otimes 4}$ (Refs. 7 and 9) due to its simplicity. The main merit of the $U(1)^{\otimes 4}$ is its simplicity in contrast to the complexity[17] of $U(1)^{\otimes 3}$. A clear exposition of the true nature of the $U(1)^{\otimes 4}$ approximation would be very interesting. For the time being we know little about it. We will return to this question subsequently.

In the work of JG, the mass enhancement is directly extracted from the calculated low-temperature specific heat at half-filling. JG have shown that the noninteracting limit is not recovered for vanishing on-site repulsive interaction. Also an unphysical result of $m^*/m=-\frac{1}{3}$ is obtained. Hence JG claim that the bosonic Hamiltonian must be adjusted order by order in the loop expansion. We think that this problem is not necessarily related to whether one uses a $U(1)^{\otimes 3}$ or $U(1)^{\otimes 4}$ formalism. The problem may directly come from the expression for the bosonic hopping factor, proposed by KR on the mean-field level. As JG mentioned, in the low-frequency limit one can drop the kinetic term coming from the bosonic phase left after the $U(1)^{\otimes 3}$ gauge transformation, and thus the $T^3 \ln T$ part of the specific heat is recovered. However, both the $T^3 \ln T$ and the linear T behaviors are, strictly speaking, restricted to low temperature and thus both of them come from the low-energy excitation contribution around the Fermi level. Thus for both terms, the frequency dependence mainly comes from the Fermi bubbles. In fact, both behaviors of the low-temperature specific heat have been successfully predicted by LFLT. From the beginning the domain of the validity of the Landau theory has been clearly restricted to phenomena which involve excitations very close to the Fermi surface. If there is a difference between these two terms, it is that the former one comes purely from low-frequency fluctuations while the contribution to the mass enhancement may come from high-energy excitations also. Since the effective mass is directly related to derivatives of the self-energy, a rigorous formula, there is no reason, in principle, to exclude the contribution coming from high-energy excitations. So one should be cautious whenever the contribution from high-energy excitations becomes important for the observables. A possibly more profound reason for the success of the $T^3 \ln T$ calculation and the failure of the m^*/m calculation will be described subsequently. Also the $U(1)^{\otimes 3}$ calculation [JG's Eqs. (13)–(15)] is too complex to show transparently this drawback in the loop expansion. One hopes to find out a simple and clear method to explore this possible drawback in KR's scheme.

However, as we have discussed above, it is nontrivial to examine the low-lying excitation contribution to the mass enhancement even under the $U(1)^{\otimes 4}$ formulation where the $\omega/kv_f \ll 1$ limit is consistent with the fact that one needs to include the frequency dependence of the fluctuation matrix of the fermionic bubbles only. JG have shown the failure of the procedure which extracts the mass enhancement from the formula $C_v = C_{v0} m^*/m$. Instead of using $C_v = C_{v0} m^*/m$, we calculate directly the fluctuation contribution to the bosonic factor which is responsible for the mass enhancement in the KR scheme. Our result explicitly shows that the contributions to the mass enhancement may be disentangled into three terms: a quasiparticle excitation term, and a spin- and a charge-fluctuation term. The quasiparticle term leads to the correct noninteracting limit for vanishing on-site Coulomb interaction U, whereas the spin- and the charge-fluctuation terms do not lead to the correct noninteracting limit. This problem is interesting for the 2D Hubbard model especially since the discovery[4] of the high-T_c superconductors. It is believed that the correct renormalized hopping factor may be closely related to either the quasiparticle weight of the Luttinger liquid[21] or that of the "marginal" Fermi liquid.[22] In fact, some numerical work has been done in the calculation of the dynamic properties of the renormalization factor.[23]

This paper is organized as follows. In Sec. II we first calculate the modified bosonic hopping factor by using, with the $U(1)^{\otimes 4}$ formalism, a low-lying cutoff procedure which has been often used in the one-loop expansion for quantum liquid ^{3}He. As mentioned in the above paragraph, the $\omega/kv_f \ll 1$ limit is consistent with the fact that one needs to include the frequency dependence of the fluctuation matrix of the fermionic bubbles only, thus the $U(1)^{\otimes 4}$ approximation is valued in this calculation. Then, instead of the cutoff procedure, we use a sum rule covering the whole bosonic spectrum to calculate the mass enhancement. The latter is a clear-cut calculation since only the properties of the projection operators are needed. A brief summary and discussions are given in Sec. III.

II. FLUCTUATIONS CONTRIBUTION TO THE BOSONIC FACTOR

In this paper we directly expand the mass enhancement renormalization factor, the bosonic hopping factor, to second order and calculate the Gaussian fluctuation contribution. We avoid the use of the $C_v = C_{v0} m^*/m$ formula. In the KR bosonization, the Hubbard model can be expressed in terms of fermion operators $f_{i\sigma}$ and four SB operators $e_i, p_{i_\uparrow}, p_{i_\downarrow}, d_i$, keeping track of empty, singly occupied and doubly occupied sites:

$$H = \sum_{\substack{\langle i,j \rangle \\ \sigma}} t_{ij} f_{i\sigma}^\dagger z_{i\sigma}^\dagger z_{j\sigma} f_{j\sigma} + U \sum_i d_i^\dagger d_i \ , \tag{1}$$

where the bosonic hopping factor $z_{i\sigma}$ is defined by

$$z_{i\sigma} = [1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma}]^{-1/2} (e_i^\dagger p_{i\sigma} + p_{i-\sigma}^\dagger d_i) \times [1 - e_i^\dagger e_i - p_{i-\sigma}^\dagger p_{i-\sigma}]^{-1/2} \ . \tag{2}$$

The boson operators are subject to the following constraints:

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma p_{i\sigma}^\dagger p_{i\sigma} = 1 \tag{3}$$

and

$$f_{i\sigma}^\dagger f_{i\sigma} = d_i^\dagger d_i + p_{i\sigma}^\dagger p_{i\sigma} \ . \tag{4}$$

The partition function can be written within the functional-integral formalism as follows:

$$Z = Z_{\rm MF} Z_{fl} = Z_{\rm MF} \int D\varphi^T(k) D\varphi(k) \times \exp\{-\Sigma \varphi^T(k) \hat{S}(k) \varphi(k)\} \tag{5}$$

in which $Z_{\rm MF}$ is the mean-field partition function, while the fluctuation vector of Bose fields away from their mean-field values is defined as

$$\varphi^T(k) = \{\delta e, \delta d, \delta p_\uparrow, \delta p_\downarrow, \delta\beta_\uparrow, \delta\beta_\downarrow, \delta\alpha\}(k) \ . \tag{6}$$

$\hat{S}(k)$ is the fluctuation matrix with elements $S_{\alpha\beta}(k) = S_{\beta\alpha}(-k)$. The constraints (3) and (4) are enforced through the introduction of three Lagrangian multiplies $\delta\beta_\uparrow$, $\delta\beta_\downarrow$, and $\delta\alpha$, in addition to the original four bosons describing the fermion states. We have introduced a 4D kinetic momentum notation $k = (\mathbf{k}, \omega_n)$, where $\omega_n = 2\pi n T$ are the bosonic Matsubara frequencies, and thus $\sum_k = (\beta L)^{-1} \sum_{\mathbf{k}} \sum_\omega$, with L the number of the lattice sites and $\beta = 1/k_B T$. The elements of the fluctuation matrix are obtained[7,8] by expanding the effective action,

$$\int d\tau L_{\rm eff} = \int d\tau (L_{\rm eff}^F + L_{\rm eff}^B) \tag{7}$$

in which $L_{\rm eff}^F$ and $L_{\rm eff}^B$ are, respectively, the effective Fermi and Bose part of the Lagrangian $L_{\rm eff}$. By performing a gauge transformation, thus changing the variables, and invoking the periodicity of the Bose fields as well as integrating out the Grassman variables, one obtains a 7×7 fluctuation matrix $\hat{S}(k)$. In this paper, for the purpose of our concern only the one-loop order Bose propagators are considered in the half-filled case. There is no difficulty in extending the calculation to the doped case. We consider first the low-lying excitation limit.

We directly expand the hopping factor z, Eq. (2), to second order,

$$\begin{aligned} z(i,\tau) &= z_0 + \sum_\sigma \sum_\alpha^4 z_{\sigma,\varphi_\alpha} \delta\varphi_\alpha(i,\tau) \\ &\quad + \tfrac{1}{2} \sum_\sigma^4 \sum_{\alpha,\beta=1} z_{\sigma,\varphi_\alpha\varphi_\beta} \delta\varphi_\alpha(i,\tau) \delta\varphi_\beta(i,\tau) \\ &\equiv z_0 + z_1 + z_2 \ , \end{aligned} \tag{8}$$

where

$$z_{\sigma,\varphi_\alpha} = \partial z_\sigma / \partial\varphi_\alpha |_{\rm SPV} \ , \quad z_{\sigma,\varphi_\alpha\varphi_\beta} = \partial^2 z_\sigma / \partial\varphi_\alpha \partial\varphi_\beta |_{\rm SPV}$$

with σ denoting spin and SPV denoting the saddle-point value. z_0 is the mean-field value. According to (6) the values of the four boson fields are

$$\delta\varphi_1(i,\tau) = \delta e(i,\tau) \ , \ \delta\varphi_2(i,\tau) = \delta d(i,\tau) \ ,$$
$$\delta\varphi_3(i,\tau) = \delta p_\uparrow(i,\tau), \quad \delta\varphi_4(i,\tau) = \delta p_\downarrow(i,\tau) \ ,$$

with the notations i for local site and τ for imaginary time. The mass enhancement is

$$m^*/m = \langle z^2 \rangle^{-1} \ . \tag{9}$$

To second order, one has

$$\begin{aligned} \langle z^2 \rangle &= z_0^2 + \sum_\sigma \sum_{\alpha,\beta=1}^4 (z_{\sigma,\varphi_\alpha} z_{\sigma,\varphi_\beta} + z_0 z_{\sigma,\varphi_\alpha\varphi_\beta}) \\ &\qquad \times \sum_k \langle \delta\varphi_\alpha(-k) \delta\varphi_\beta(k) \rangle \\ &\equiv z_0^2 + \langle z_1^2 \rangle + z_0 \langle z_2 \rangle \ . \end{aligned} \tag{10}$$

The correlation functions of the fluctuation fields are obtained by using

$$\langle \delta\varphi_\alpha(-k) \delta\varphi_\beta(k) \rangle = S_{\alpha\beta}^{-1}(k)/2 \ . \tag{11}$$

For the half-filled case, one has the saddle-point values

$$e=d=(1-U/U_c)/4\ ,\quad p_\sigma^2\equiv q^2=\tfrac{1}{2}-e^2\ ,\qquad \alpha=U_c q^2(1+4e^2)\ ,\quad \beta_0=U_c(1-4e^2)/2\ , \tag{12}$$

where $U_c=16|\sum_{\mathbf{k}}t_{\mathbf{k}}|$, with $t_{\mathbf{k}}$ the fermion band energy. Hence, at half-filling one has

$$\begin{aligned}
&z_{\sigma 0}=4eq\ ,\\
&\partial z_\sigma/\partial e=\partial z_\sigma/\partial d=2q(1+4e^2)\ ,\\
&\partial z_\sigma/\partial p_\sigma=\partial z_\sigma/\partial p_{-\sigma}=2e(3-4e^2)\ ,\\
&\partial^2 z_\sigma/\partial e^2=\partial^2 z_\sigma/\partial d^2=16eq(1+3e^2)\ ,\\
&\partial^2 z_\sigma/\partial e\partial p_\sigma=\partial^2 z_\sigma/\partial d\partial p_{-\sigma}=4(1+2e^2-4e^4)\ ,\\
&\partial^2 z_\sigma/\partial e\partial p_\sigma=\partial^2 z_\sigma/\partial d\partial p_{-\sigma}=2(1+12e^2-24e^4)\ ,\\
&\partial^2 z_\sigma/\partial e\partial p_\sigma=\partial^2 z_\sigma/\partial d\partial p_{-\sigma}=8eq(5-6e^2)\ ,\\
&\partial^2 z_\sigma/\partial p_\sigma\partial p_\sigma=8eq(5-6e^2)\ ,\\
&\partial^2 z_\sigma/\partial p_\sigma\partial p_{-\sigma}=16eq(1-e^2)\ ,\\
&\partial^2 z_\sigma/\partial e\partial d=16eq(1/2+e^2)\ ,
\end{aligned} \tag{13}$$

in which the SB saddle-point-value expressions (12) have been used.

Considering the particle-hole symmetry and the spin-up and -down symmetry, only five components of the inverse fluctuation matrix $S_{\alpha\beta}^{-1}(k)$ are needed. They are

$$\begin{aligned}
&S_{dd}^{-1}(k)=\frac{1+S_{vv}(\Delta S/e^2-N)}{2N(e^2+S_{vv}\Delta S)}\ ,\\
&S_{de}^{-1}(k)=\frac{1+S_{vv}(\Delta S/e^2+N)}{2N(e^2+S_{vv}\Delta S)}\ ,\\
&S_{ep_\sigma}^{-1}(k)=1/(2Neq)\ ,\\
&S_{p_\sigma p_{-\sigma}}^{-1}(k)=\frac{1+S_{vv}(\Delta T/q+N)}{2N(q^2+S_{vv}\Delta T)}\ ,\\
&S_{p_\sigma p_\sigma}^{-1}(k)=\frac{1+S_{vv}(\Delta T/q^2-N)}{2N(q^2+S_{vv}\Delta T)}\ ,
\end{aligned} \tag{14}$$

where

$$N=(S_{p_\sigma p_\sigma}+S_{p_\sigma p_{-\sigma}})/q^2+(S_{de}+S_{dd})/e^2-4S_{ep_\sigma}/eq\ ,$$

$$\Delta_S=S_{de}-S_{dd}\ ,\quad \Delta T=S_{p_\sigma p_\sigma}-S_{p_\sigma p_{-\sigma}}\ ,$$

$$S_{vv}=\chi_0^*(k)/2\ ,$$

and

$$\chi_0^*(\mathbf{k},\omega)=2\sum_{\mathbf{p}}\frac{f(E^*(\mathbf{p}))-f(E^*(\mathbf{p}+\mathbf{k}))}{i\omega+E^*(\mathbf{p})-E^*(\mathbf{p}+\mathbf{k})} \tag{15}$$

is the renormalized Lindhard function, in which f is the Fermi distribution

$$f(E)=1/(1+\exp-\beta E)\ . \tag{16}$$

The fermion spectrum is

$$E_{\mathbf{k}}^*=z^2t_{\mathbf{k}}-\mu+\beta_0\ , \tag{17}$$

with β_0 defined as $\beta_0=(\delta\beta_\uparrow+\delta\beta_\downarrow)/\sqrt{2}$, a Bose field coming from the Lagrangian multiplier enforcing the constraint (4). At half-filling one has $\mu=\beta_0=U/2$, hence, for a liquid, $E^*(\mathbf{k})=(1/2m^*)(k^2-k_F^2)$ with m simply replaced by m^*. In the static case χ_0^* reduces to the effective density of states at the Fermi level, $N^*(0)=N(0)/z^2$. Henceforth, we omit for simplicity the superscript for the renormalized Lindhard function. The single f-particle Green function, at the mean-field level, is expressed as

$$G(p)=1/(i\omega_n-E_{\mathbf{k}}) \tag{18}$$

with $\omega_n=(2n+1)\pi T$.

Considering the low-lying excitations, we obtain the mass enhancement for the half-filled case,

$$\begin{aligned}
\langle z^2\rangle=z_0^2+\frac{1}{\beta_T}\sum_{\mathbf{k}}(&(1-4e^2)/2U_ce^2q^2\\
&+32\{e^2F_0^a\chi_0(k)/[1+F_0^a\chi_0(k)]\\
&-q^2F_0^s\chi_0(k)/[1+F_0^s\chi_0(k)]\}/U_c\\
&\times(1-4e^2))
\end{aligned} \tag{19}$$

where the Landau parameters are

$$F_0^a=-p(1-4e^2)(3-4e^2)/4(1-2e^2)$$

and

$$F_0^s=p(1-4e^2)(1+4e^2)/e^4\ . \tag{20}$$

The dimensionless parameter $p=N(0)\sum_{k<k_F}t_{\mathbf{k}}$ is band-structure dependent and is always close to unity. For the spherical Fermi surface, in the long-wavelength and low-momentum-transfer limit as well as $v\equiv\omega/kv_F^*\ll 1$, with v_F^* the effective Fermi velocity, one has the well-known asymptotic expression

$$\chi(\mathbf{k},\omega)=\frac{N^*(0)}{4}\left\{1-\frac{\pi}{2}v+v^2+O(v^3)\right\}\ . \tag{21}$$

Combining Eqs. (19)–(21), we finally obtain the low-lying excitation contribution to the mass enhancement:

$$\begin{aligned}
\langle z^2\rangle=z_0^2+\frac{15}{4\pi}(1-4e^2)\frac{\omega_c}{k_cv_F^*}&+80x^4q^2\left\{\frac{\omega_c}{k_cv_F^*}A_0^a+9A_0^a\left[\frac{\omega_c}{k_cv_F^*}\right]^3[1-(1+\pi^2/4)A_0^a+\pi^2A_0^{a\,2}/4]\right\}\Big/(1-4e^2)\\
&-80e^4q^2\left\{\frac{\omega_c}{k_cv_F^*}A_0^s+9A_0^s\left[\frac{\omega_c}{k_cv_F^*}\right]^3[1-(1+\pi^2/4)A_0^s+\pi^2A_0^{s2}/4]\right\}\Big/(1-4e^2)
\end{aligned} \tag{22}$$

where A_0^s and A_0^a are the main symmetric and antisymmetric isotropic components of the quasiparticle scattering amplitude defined by

$$A_0^{s,a}=F_0^{s,a}/(1+F_0^{s,a}) ,$$

and ω_c and k_c are the cutoff values of the transfer frequency and kinetic momentum, respectively. This cutoff procedure has often been used, e.g., for ^{3}He, in the literature. The mass enhancement includes four terms in Eq. (22). The first term is the mean-field result. The second term, the quasiparticle and quasihole excitation contribution term, vanishes in the free-particle limit, but remains finite as U approaches U_c. The third and the fourth terms are related to spin and charge fluctuations. These two terms do not vanish in the free-particle limit. Thus, by using a direct expansion, the low-lying excitation contribution to the mass enhancement does not reproduce the noninteracting limit for vanishing U.

It is also worthwhile to note that, at half-filling when $U \Longrightarrow U_c$, one has

$$d=e=0 , \quad A_0^s \Longrightarrow 1 , \quad A_0^a \Longrightarrow -3 , \quad z_0 \Longrightarrow 0 ,$$

and thus

$$\langle z^2 \rangle \Longrightarrow \frac{15}{4\pi}\frac{\omega_c}{k_c v_F^*} , \tag{23}$$

so that the mass enhancement will not diverge, implying the disappearance of the BR transition when the one-loop contribution is taken into account. This is in accordance with the conclusion from an exact GWF calculation.[16] It should be noted that this result stands for any dimension. However, it is not a well-established fact even for the one-loop calculation, since Eq. (23) is incorrect at $U=0$. It is worthwhile to note that $d=0$ and the BR transition need not be coincident. The coincidence happens only at the mean-field GA (Ref. 2) level. The coincidence between $d=0$ and BR transitions is lifted here, in the one-loop expansion. This should be considered an interesting result which goes in the right direction.

The following question then arises: Why does the $T^3\ln T$ calculation succeed whereas the mass enhancement one seems to fail even though both problems are treated similarly? One is working in the same KR's SB framework and using the same low-lying excitation cutoff technique. This is not completely understood so far by the author. One possible explanation for the difference is that when making the correction to the mass enhancement of the GA, the contribution coming from the high-energy excitations also has to be taken into account. In fact, in the $U(1)^{\otimes 3}$ scheme, used by JG, the high-frequency part is included. However, in that calculation not only is the noninteracting limit not recovered at $U=0$, but also an unphysical result $m^*/m=-\frac{1}{3}$ is obtained. They have treated the fermion bubbles and the kinetic-energy terms in a different way due to the complexity of the mathematics. For the former one, a $q_0=1-(U/U_c)$ expansion has been used while for the latter one a standard SB procedure is used. Also their result, their Eqs. (13)–(15), is too complex to explore the origin of the drawback of the KR's scheme. We present here a simpler and more transparent way to obtain the one-loop fluctuation correction to the GA's mass enhancement.

Starting from the expansion (8), for notational simplicity, we define the double bracket as

$$\langle\langle \hat{O} \rangle\rangle \equiv (\beta L)^{-1}\sum_i \int d\tau \langle \hat{O}(i,\tau)\rangle , \tag{24}$$

with $\langle\ \rangle$ the quantum-mechanical expectation value. To second order, one has

$$\langle\langle z_\sigma^2 \rangle\rangle = z_0^2 + \sum_\sigma \sum_{\alpha,\beta=1}^{4} a_{\alpha\beta}\langle\langle \delta\varphi_\alpha \delta\varphi_\beta \rangle\rangle , \tag{25}$$

where

$$a_{\alpha\beta}=(\partial z_\sigma/\partial\varphi_\alpha \partial z_\sigma/\partial\varphi_\beta + z_0\partial^2 z_\sigma/\partial\varphi_\alpha\partial\varphi_\beta)=a_{\beta\alpha} . \tag{26}$$

We calculate these coefficients $a_{\alpha\beta}$ first, then the correlation functions between the φs's. Inserting (13) and substituting the free-particle ($U=0$) values for those boson fields,

$$z_0=1 , \quad e=d=q=\tfrac{1}{2} ,$$

one has

$$\begin{aligned} &a_{11}=a_{22}=a_{33}=a_{44}=11 , \\ &a_{12}=a_{34}=7 , \\ &a_{13}=a_{14}=a_{23}=a_{24}=9 . \end{aligned} \tag{27}$$

Considering the exchange symmetry and the spin-up and spin-down symmetry in the paramagnetic phase,

$$\begin{aligned} &\langle\langle \delta\varphi_\alpha\delta\varphi_\beta \rangle\rangle = \langle\langle \delta\varphi_\beta\delta\varphi_\alpha \rangle\rangle , \quad \langle\langle \delta\varphi_1\delta\varphi_3 \rangle\rangle = \langle\langle \delta\varphi_1\delta\varphi_4 \rangle\rangle , \\ &\langle\langle \delta\varphi_2\delta\varphi_3 \rangle\rangle = \langle\langle \delta\varphi_2\delta\varphi_4 \rangle\rangle , \quad \langle\langle \delta\varphi_3\delta\varphi_3 \rangle\rangle = \langle\langle \delta\varphi_4\delta\varphi_4 \rangle\rangle , \end{aligned} \tag{28}$$

one obtains

$$\begin{aligned} \langle\langle z^2 \rangle\rangle = 1 &+ 11(\langle\langle \delta\varphi_1\delta\varphi_1 \rangle\rangle + \langle\langle \delta\varphi_2\delta\varphi_2 \rangle\rangle + 2\langle\langle \delta\varphi_3\delta\varphi_3 \rangle\rangle) \\ &+ 14(\langle\langle \delta\varphi_1\delta\varphi_2 \rangle\rangle + \langle\langle \delta\varphi_3\delta\varphi_4 \rangle\rangle) \\ &+ 36(\langle\langle \delta\varphi_1\delta\varphi_3 \rangle\rangle + \langle\langle \delta\varphi_2\delta\varphi_3 \rangle\rangle) . \end{aligned} \tag{29}$$

We[8] have shown that the original correlation functions defined via Fermi operators may be expressed as the correlation functions of slave-boson fields, if the following replacement are used:

$$\begin{aligned} &\hat{E}(i,\tau)\equiv[1-\hat{n}_\uparrow(i,\tau)][1-\hat{n}_\downarrow(i,\tau)] \Longrightarrow e^\dagger(i,\tau)e(i,\tau) , \\ &\hat{D}(i,\tau)=[\hat{n}_\uparrow(i,\tau)\hat{n}_\downarrow(i,\tau)] \Longrightarrow d^\dagger(i,\tau)d(i,\tau) , \\ &\hat{P}_\sigma(i,\tau)=\hat{n}_\sigma(i,\tau)[1-\hat{n}_{-\sigma}(i,\tau)] \Longrightarrow p_\sigma^\dagger(i,\tau)p_\sigma(i,\tau) . \end{aligned} \tag{30}$$

Considering that the above Fermi operators are projectors, one has

$$\begin{aligned} &\langle\langle \delta\varphi_1\delta\varphi_2 \rangle\rangle = \langle\langle \delta\hat{E}\delta\hat{D} \rangle\rangle /4ed , \\ &\langle\langle \delta\varphi_3\delta\varphi_4 \rangle\rangle = \langle\langle \delta\hat{P}_\uparrow\delta\hat{P}_\downarrow \rangle\rangle /4q^2 , \\ &\langle\langle \delta\varphi_1\delta\varphi_3 \rangle\rangle = \langle\langle \delta\hat{E}\delta\hat{P}_\uparrow \rangle /4eq , \end{aligned} \tag{31}$$

where $\delta\hat{O}\equiv\hat{O}(i,\tau)-\langle\langle \hat{O} \rangle\rangle$. Therefore, one has

$$\langle\langle z^2 \rangle\rangle = 1 + 11(\langle\langle \delta\hat{E}\delta\hat{E} \rangle\rangle + \langle\langle \delta\hat{D}\delta\hat{D} \rangle\rangle + \sum_\sigma \langle\langle \delta\hat{P}_\sigma \delta\hat{P}_\sigma \rangle\rangle) + 7(\langle\langle \delta\hat{P}_\uparrow \delta\hat{P}_\downarrow \rangle\rangle + \langle\langle \hat{\delta}E\hat{\delta}D \rangle\rangle) + 18(\langle\langle \hat{\delta}E\hat{\delta}P_\sigma \rangle\rangle + \langle\langle \hat{\delta}D\hat{\delta}P_\sigma \rangle\rangle) . \tag{32}$$

By using the projector properties,

$$\hat{E}^2 = \hat{E} , \quad \hat{D}^2 = \hat{D} , \quad \hat{P}_\sigma^2 = \hat{P}_\sigma \tag{33a}$$

as well as the completeness,

$$\hat{E} + \hat{D} + \sum \hat{P}_\sigma = 1 \tag{33b}$$

and the fact that all cross products are zero, one finally obtains

$$\langle\langle z^2 \rangle\rangle = 1 + 11[\langle\langle 1 \rangle\rangle - 2(e^4+q^4)] + 14(-\langle\langle 1 \rangle\rangle/4 + e^4 + q^4) + 36(-\langle\langle 1 \rangle\rangle/4 + 2e^2q^2) = 3 \neq 1 . \tag{34}$$

Thus

$$m^*/m(U \Longrightarrow 0) = \langle\langle z^2 \rangle\rangle^{-1} = \tfrac{1}{3} , \tag{35}$$

which improves JG's unphysical result, but still does not reproduce the noninteracting limit at $U=0$. Note that in the above calculation the whole **k** and ω-dependent bosonic spectrum has been involved due to the summation over sites and the integration over imaginary time.

III. DISCUSSION

Since the high-energy excitations have been included in a complete one-loop expansion using $U(1)^{\otimes 3}$ gauge symmetry and the noninteracting limit is not recovered, JG have the reasons to claim that the renormalization factor proposed by KR, a key step in KR's scheme, must be adjusted order by order in the loop-expansion calculation to guarantee the correct vanishing U limit. For this purpose JG even proposed a scheme, which is intractable so far. In the author's opinion, the problem is not only technical. There exists, probably, a more profound difficulty. Indeed, the saddle-point results of GA have the inherent nature of the Landau Fermi liquid, as has been pointed out by Vollhardt.[3] Then the problem arises: How far can the KR scheme be pushed with the loop expansion? The GA, as a starting point in the loop-expansion theory, is confined to describe the ground state and the low-lying excitation behavior, an essential requirement in the LFLT. Hence one has to be cautious when attempting to pursue KR's formulation to depict properties in which the high-energy excitations are involved, such as is the case with the loop expansion for the mass enhancement. Even if one had a tractable technique to handle the loop expansion for KR's scheme, e.g., to adjust the renormalization hopping factor to the $U=0$ limit, its validity would still not be clear-cut. In fact, a test against Monte Carlo (MC) calculations, of the correlation functions[9] obtained through the KR SB scheme, has explicitly shown that the temperature can only be raised above zero in a limited regime. In others words, KR's theory is basically a low-temperature theory.[9] Also, it has been shown that the classical limit of the temperature dependence of the specific heat cannot be recovered in the high-temperature limit.[24] Taking into account previous successful calculations[7,18] one may conclude that KR's scheme works well when it is applied to describe properties in which the low-lying excitations are dominant. This is not in conflict with the point raised by JG that the bosonic hopping factor proposed by KR has the correct noninteracting limit only at the global level, the GA level. However, KR's formulation has been extended for either the temperature and the kinetic momentum[9,10] to some reasonably high values, since structure factors have been obtained from sums over frequencies of the dynamical correlation functions and tested in the 1D (Ref. 9) and 2D (Refs. 14 and 10) Hubbard model in detail. Unfortunately, to date, reliable results for the high-frequency aspects of the correlation functions, which can be used in order to compare with the SB results,[9,10] are lacking. The MC calculations are restricted so far to the equal-time correlation functions, the structure factor, and the zero-frequency susceptibilities.

In summary, we have directly calculated the Gaussian fluctuations of the bosonic hopping factor of KR's SB representation of the Hubbard model. Both the low-lying excitation cutoff procedure and the sum rule, covering the whole bosonic spectrum, have been used. However, the fluctuation contribution to the renormalized mass enhancement m^*/m does not reduce to the correct limit, either for free fermions or in the case of fully polarized spins in the one-loop expansion. We point out that KR's functional-integral scheme is basically a low-temperature (including zero-temperature) as well as low-lying excitation theory. The temperature and frequency dependences have been studied away from their strict asymptotic limit, but a serious test and assessment of the high-frequency aspects of the KR SB theory is still an open problem which has been only partially addressed by the present paper.

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[20]Considering that the KR theory is not a conservative one, some extra constraint(s) may be needed and, thus, the $U(1)^{\otimes 4}$ symmetry may still be recovered. Also, we have mentioned in the text that KR's functional-integral scheme is basically a low-temperature (including zero-temperature) as well as low-lying excitation theory. Hence the high-energy contribution due to the $U(1)^{\otimes 3}$ symmetry may be omitted when one applies KR's theory to reality, such as quantum liquid ^{3}He, etc.

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