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Correct formulation of the $1/N$ expansion for the slave-boson approach within the functional integral

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We consider the slave-boson method within the coherent-state functional integral representation of the partition function, and show how to deal with the continuum imaginary-time limit required by the very definition of the functional integral. We find that a correct treatment of the continuum limit modifies the free energy when fluctuation $(1/N)$ corrections beyond the mean-field solution are considered. Numerical results are presented for a two-level single-site model system (with an infinite Hubbard repulsion), for which the additional terms in the free energy introduced by the correct continuum limit act to validate the $1/N$ expansion. Our analysis calls for a revision of several outcomes of the slave-boson method with the inclusion of fluctuation corrections.

The slave-boson method[1] has been extensively applied in recent years to a variety of problems involving strong electronic correlations, like the Kondo impurity and lattice,[2] the Anderson Hamiltonian,[3] and the Hubbard model(s).[4] The method maps the physical electron (hole) destruction operator c_σ with spin σ into products of (pseudo)fermions d_σ and (slave) bosons b. In particular, when the local repulsion U is infinite the mapping $c_\sigma \to d_\sigma b^\dagger$ requires only one boson, which keeps track of the number of empty sites in the lattice. In terms of the operators d_σ and b, the requirement that there cannot be double occupancy when $U \approx \infty$ at any given site is expressed by the local constraint

$$\sum_\sigma d_\sigma^\dagger d_\sigma + b^\dagger b = 1. \tag{1}$$

The slave-boson method has been usually treated within a functional integral representation of the partition function since this representation suitably enforces the constraint (1) and allows for a large-N expansion, which is free from infrared divergences in the so-called radial gauge.[5,6] In this gauge the complex boson field $b = re^{i\theta}$ is represented via its amplitude and phase at each site, with the real variables r and θ being integrated independently in the functional integral. (The gauge where one keeps the integration over the real and imaginary parts of the complex field b is instead referred to as the Cartesian gauge.)

Notwithstanding the large literature in the field, it appears that the importance of representing properly the boson commutation rules in the functional integral formulation has been so far overlooked, as it has always been assumed that the continuum imaginary time limit (which is implicit in any path integral definition) can be safely taken *at the outset* in the effective action.

In this paper we show that a correct treatment of the continuum limit is actually required in both gauges to implement the boson commutation rules, and that this in turn modifies the free energy when fluctuation $(1/N)$ corrections beyond mean field are considered. For the sake of clarity, we carry out our analysis for a multiband (d-p) model with infinite Hubbard repulsion at d sites since this model involves one boson field only. However, our results apply quite generally to other cases with additional bosons like to the finite-U single-band Hubbard model.[7]

To illustrate the relevance of the additional contributions generated by the proper continuum limit, we shall eventually specify our treatment to a two-level single-site model for which the slave-boson approach was critically examined in Ref. 8. In that reference it was pointed out that (i) there exists a spurious phase transition and (ii) the large-N expansion is inaccurate even far from this spurious transition. We shall find that our correct treatment of the continuum time limit completely solves point (ii) while point (i) remains an open problem to be kept in mind. Additional work will thus be needed to assess fully the validity and limitations of the slave-boson approach.

The functional integral representation of the partition function for the model at hand is formally given by

$$\mathscr{Z} = \int \mathscr{D}p \mathscr{D}\bar{p} \mathscr{D}d \mathscr{D}\bar{d} \mathscr{D}b \mathscr{D}b^* d\lambda \, \exp\{-S\}. \tag{2}$$

Here, p ($\bar{p}$) and d ($\bar{d}$) are Grassmann variables, b (b^*) complex numbers, and the action is given by

$$S = \int_0^\beta d\tau \left\{ \sum_{i,\sigma} \bar{d}_{i\sigma}(\partial/\partial\tau) d_{i\sigma} + \sum_{j,\sigma} \bar{p}_{j\sigma}(\partial/\partial\tau + \Delta) p_{j\sigma} \right.$$

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$$+\sum_i b_i^* \partial/\partial\tau b_i + \sqrt{2/N}\sum_{i,j,\sigma} t_{ij}(\bar{p}_{j\sigma}d_{i\sigma}b_i^* + \text{c.c.})$$
$$+\sum_{j,j'\sigma}(\epsilon_{jj'}\bar{p}_{j\sigma}p_{j'\sigma}+\text{c.c.})$$
$$+i\sum_i \lambda_i\left(\sum_\sigma \bar{d}_{i\sigma}d_{i\sigma}+b_i^*b_i - N/2\right)\Bigg\}, \qquad (3)$$

where an N-spin generalization of the physical model with $N=2$ has been considered and the field λ has been introduced to enforce locally the generalized constraint $\Sigma_{\sigma=1}^N d_\sigma^\dagger d_\sigma + b^\dagger b = N/2$.

With a suitable choice of t_{ij} and $\epsilon_{jj'}$, (2) and (3) represent the three-band model which has been widely used to describe the CuO_2 planes characteristic of the high-temperature superconductors. The case $i \equiv i_0$ describes a single impurity localized at site i_0, while the choice $t_{ij}=t$ and $\epsilon_{jj'}=0$ with i and j restricted to a single site reproduces the two-level single-site model considered in Ref. 8. Since the details of the model are immaterial for most of the following analysis, we shall specify them only whenever necessary.

It should be realized at this point that, although the action (3) is apparently written in terms of a continuum imaginary time τ (with $0 \leqslant \tau \leqslant \beta = 1/T$, T being the temperature), the functional approach is based on a coherent-state representation of normal-ordered products on a *discrete imaginary time mesh*. It should be then understood that the action S is defined on such a mesh, with the continuum limit safely taken *only at the end* of the calculation.[9] However, this point has been overlooked in previous literature and the action (3) has been extensively studied by taking the continuum limit at the outset. We outline briefly the main outcomes of taking the standard continuum limit.

In the saddle-point solution (which is exact for $N=\infty$) $b_i(\tau)$and λ_i equal their time- and site-independent values b_0 and $-i\lambda_0$ (λ_0 being real) determined by the stationary condition for the mean-field free energy at fixed total density $\rho = 2/N\Sigma_{\sigma=1}^N(d_\sigma^\dagger d_\sigma + p_\sigma^\dagger p_\sigma)$. In the zero-temperature limit, the boson field b condenses, irrespective of the parameters appearing in S when $\rho \neq 1$: $b_0=\sqrt{N/2}r_0 \neq 0$. The case $\rho=1$, for which the model presents at the mean-field level a "Brinkman-Rice" transition corresponding to $r_0=0$, is then recovered as the limit $\rho \to 1^\pm$.

To carry out the $1/N$ fluctuations, one expands S about the saddle-point solution by setting $b_i(\tau)=r_i(\tau)\times\exp\{i\theta_i(\tau)\}=b_0+\tilde{b}_i(\tau)$ in the Cartesian gauge and $r_i(\tau)=b_0+\tilde{r}_i(\tau)$ in the radial gauge, respectively. Once the fermionic degrees of freedom are integrated out, one obtains, to the leading order, the following quadratic actions in the bosons fields:

$$S_c^{(C)} = \tfrac{1}{2}\sum_\nu (\tilde{b}_\nu^* \quad \tilde{b}_{-\nu}) \times \begin{pmatrix} -i\omega_\nu+\lambda_0+\Pi_{11}(\omega_\nu) & \Pi_{12}(\omega_\nu) \\ \Pi_{21}(\omega_\nu) & i\omega_\nu+\lambda_0+\Pi_{22}(\omega_\nu)\end{pmatrix} \times \begin{pmatrix}\tilde{b}_\nu \\ \tilde{b}_{-\nu}^*\end{pmatrix} \qquad (4)$$

and

$$S_c^{(R)} = \sum_\nu (\tilde{r}_\nu \quad \tilde{\lambda}_\nu)\begin{pmatrix}\lambda_0+\Pi_{rr}(\omega_\nu) & b_0+\Pi_{r\lambda}(\omega_\nu) \\ b_0+\Pi_{\lambda r}(\omega_\nu) & \Pi_{\lambda\lambda}(\omega_\nu)\end{pmatrix} \times \begin{pmatrix}\tilde{r}_{-\nu} \\ \tilde{\lambda}_{-\nu}\end{pmatrix}, \qquad (5)$$

where the subscript c stands for the continuum limit and the superscripts C and R refer to the Cartesian and radial gauge, respectively. For brevity, we have not indicated explicitly the sum over the wave vector which appears for the lattice models. The polarization bubbles Π in (4) and (5) decay at least as ω_ν^{-1} for large ω_ν. By carrying out the Gaussian integration over the boson fields, the fluctuation corrections to the free energy are then given by

$$\Delta F_c^{(C,R)} = (1/2\beta)\sum_\nu \ln \mathrm{Det}\boldsymbol{\Gamma}_c^{(C,R)}(\omega_\nu), \qquad (6)$$

where $\boldsymbol{\Gamma}_c^{(C,R)}$ are the fluctuation matrices in (4) and (5).[10]

Although the continuum time assumption for S does not pose any problem at the mean-field level, this may be no longer the case when fluctuations are included. This point emerges clearly when considering how the discontinuity of the equal-time bosonic correlator $\langle b(\tau)b^*(\tau^\pm)\rangle$ needs to be handled in the radial gauge. Here, $\tau^\pm=\tau\pm\delta$ with $\delta=\beta/M$ [M being the number of steps considered in the interval $(0,\beta)$], and the bosonic operators are understood to correspond to a given site. A naive transformation to the radial gauge would yield $\langle b(\tau)b^*(\tau^\pm)\rangle = \langle r^2(\tau)\rangle$ *provided* the continuum ($M\to\infty$ and $\delta\to 0^+$) limit is taken at the outset. It is evident that this result is not consistent with the bosonic commutation relation since it would imply $\langle[b,b^\dagger]\rangle=0$ instead of unity. This warns us that, within the functional integral approach, it may not be correct to identify simply $b^*b\to r^2$ in the radial gauge.[11] More generally, proper care should be taken of the fact that the functional integral itself is defined through the limit of a sequence of mesh points in the imaginary time interval.

Following an analogous argument we can show that (6) cannot be correct even in the Cartesian gauge because an additional term is missing. Owing to the presence of the slave-boson condensate, the Cartesian Gaussian fluctuations are described by the matrix in (4), where the boson fields with Matsubara frequencies ω_ν and $-\omega_\nu$ are coupled by the off-diagonal polarization bubbles Π_{12} and Π_{21} (which are in fact proportional to the condensate r_0). The logarithm of the Cartesian determinant in (6) is thus an even function of ω_ν and no regularization factor $e^{\pm i\omega_\nu\delta}$ is required. This contrasts with the fact that, in the absence of condensate (when $\Pi_{12}=\Pi_{21}=0$), the upper and lower diagonal terms of $\boldsymbol{\Gamma}_c^{(C)}$ would independently give the same contribution to the free energy with regularization factors $e^{i\omega_\nu\delta}$ and $e^{-i\omega_\nu\delta}$, respectively. To avoid this doubtful procedure and settle unambiguously the correct expression for the free energy, it is necessary to carry out a careful analysis of S over the discrete imaginary time mesh (see below). However, we can try to guess the correct answer by observing that the equal-time upper and lower bare diagonal elements of $\boldsymbol{\Gamma}_c^{(C)}$ represent

$\frac{1}{2}\lambda_0 b^\dagger b$ and $\frac{1}{2}\lambda_0 b b^\dagger$, respectively, when a common regularization factor $e^{i\omega_\nu\delta}$ is assumed. In analogy with Nambu spinor formalism for superconductivity, we should then subtract $\frac{1}{2}\lambda_0$ from $(\lambda_0/2)(b^\dagger b + bb^\dagger) = \lambda_0(b^\dagger b + \frac{1}{2})$ to represent correctly the term $\lambda_0 b^\dagger b$ in the Hamiltonian.

The term $-1/2\lambda_0$ (for each boson degree of freedom) is what is missing in (6) for the Cartesian gauge. We then obtain for the fluctuation contribution to the free energy

$$\Delta F^{(C)} = \Delta F_c^{(C)} - \tfrac{1}{2}\lambda_0. \tag{7}$$

One may wonder whether the above arguments, which hold for a "pure" bosonic system, might be irrelevant for the slave-boson approach because of the gauge-invariant coupling with the fermionic degrees of freedom. To solve this problem and get the correct additional terms for the free energy, we have explicitly carried out the evaluation of the free energy in both gauges for the two-level single-site problem, keeping the discretized action throughout the calculation. That is to say, in evaluating the $1/N$ corrections we have kept the finite mesh both for bosons and fermions and taken the limit $\delta = \beta/M \to 0$ only at the end of the calculation for the free energy.[12] In the Cartesian gauge we have confirmed the result (7), while in the radial gauge we have obtained

$$\Delta F^{(R)} = \Delta F_c^{(R)} - \tfrac{1}{2}\lambda_0 - \tfrac{1}{4}\partial F_0/\partial b_0^2, \tag{8}$$

where F_0 is the mean-field free energy. Because of the stationary condition, $-\frac{1}{4}\partial F_0/\partial b_0^2$ vanishes when evaluated at the saddle point; this term is, however, relevant in determining the $1/N$ shifts to the mean-field values b_0^2 and λ_0.

Equations (7) and (8) are the main results of this paper. They evidence the additional terms which are introduced by the proper treatment of the regularization at large frequencies (and which thus represent the "contribution from infinity"). In (8) the term $-\frac{1}{2}\lambda_0$ reflects the discontinuity of $\langle r(\tau)\theta(\tau^\pm)\rangle$, which is in turn related to the bosonic commutation rules. The origin of the second term [which vanishes in evaluating (8) at self-consistency] is more subtle since it is related to the discontinuity of $\langle \theta(\tau)\theta(\tau')\rangle$ at $\tau = \tau'$ (which is absent in the continuum limit) and involves both bosons and fermions. For this reason, $-\frac{1}{2}\lambda_0$ represents a "real" contribution to the free energy, independent of the alternative ways of regularizing the continuum limit on a discrete mesh. The term $-\frac{1}{4}\partial F_0/\partial b_0^2$ in (8) is instead related to our regularization procedure. The essential point is that a regularization procedure is required to get consistent results, implying that the continuum limit cannot be naively taken at the outset in the functional integral.

To show in detail the quantitative relevance of the additional terms resulting from the correct handling of the continuum time limit, we perform numerical calculations for the two-level single-site model system. This calculation will enable us to compare the results of the $1/N$ expansion with the exact solution readily available for this simple system for $N=2$, or even for larger values of N as discussed in Ref. 8. Our numerical results will solve some apparent contradictions found by the authors of Ref. 8 for the very same model when considering the $1/N$ expansion without including the additional terms in (7) and (8). We will demonstrate that these additional terms are, in fact, necessary to validate the $1/N$ expansion.

The mean-field total energy (at $T=0$ and $0<\rho<2$) is given by

$$E_{\rm MF}/(N/2) = \rho E_- + \lambda_0(r_0^2 - 1), \tag{9}$$

where $E_- = \frac{1}{2}(\Delta + \lambda_0 - \epsilon)$ and $\epsilon = \sqrt{(\Delta - \lambda_0)^2 + 4t^2 r_0^2}$. r_0^2 and λ_0 are obtained numerically from the mean-field equations by requiring $E_{\rm MF}$ to be stationary. In the special case $\rho = 1$ (i.e., at "half-filling") the mean-field equations can be solved analytically.[8,12] In particular, when $\Delta > 2t$ one gets $r_0^2 = 0$, $E_- = \lambda_0$, and two solutions for λ_0 which correspond to the limits $\rho \to 1^+$ and $\rho \to 1^-$.[12] For both solutions one gets $E_{\rm MF} = 0$ independent of Δ. The special value $\Delta = 2t$ represents the "critical" value for the "Brinkman-Rice" transition for this problem. However, as pointed out in Ref. 8, the presence of this transition is an artifact of the large-N expansion and caution should be exerted in trusting the large-N results just near this point.

To evaluate the $1/N$ corrections, we limit ourselves to consider the radial gauge. According to (8), the fluctuation corrections to the free energy are given by the sum of the "contribution from infinity" plus the standard contribution where the continuum ($\delta \to 0^+$) limit is taken before evaluating the frequency sum. For the present case, the zero-temperature limit of (6) reduces to

$$\Delta F_c^{(R)} \underset{\beta\to\infty}{\longrightarrow} \tfrac{1}{2}(a - \epsilon) \tag{10}$$

with $a = \sqrt{(\Delta - 2\lambda_0)^2 + 4t^2 r_0^2}$.[12,13] Adding the "contribution from infinity" to the result (10) we obtain for the total fluctuation contribution to the free energy

$$\Delta F(R) \underset{\beta\to\infty}{\longrightarrow} \tfrac{1}{2}(a - \epsilon - \lambda_0) \tag{11}$$

with the parameters r_0^2 and λ_0 taken at the mean-field level. Finally, the total energy is obtained by adding (11) to the mean-field value (9):

$$E_{\rm TOT}^{(N)}/(N/2) = \rho E_- + \lambda_0(r_0^2 - 1) + (2/N)(a - \epsilon - \lambda_0)/2, \tag{12}$$

where no $1/N$ correction is required for r_0^2 and λ_0 also in the mean-field contribution.

Expression (12) for the total energy is a single-valued function of the parameters ρ and Δ. In particular, at "half-filling" the two solutions for λ_0 when $\Delta > 2t$ correspond to the same value of the fluctuation contribution (11). Notice that to obtain this result it is *essential* to include in (11) the "contribution from infinity" $-\lambda_0/2$. Otherwise, the fluctuation contribution (10) in the continuum limit would yield two solution-dependent values for the free energy. This shortcoming has been pointed out in Ref. 8, where it was signaled as a failure of the $1/N$ expansion for the slave-boson approach. We have proved that this is not the case, provided the continuum limit is taken appropriately in the functional integral.

Our results can be used to check the validity of the $1/N$ expansion for the slave-boson approach. To this end, we borrow from Ref. 8 the exact results obtained up to $N=16$ by diagonalizing the two-level single-site slave-boson Hamiltonian for the generalized N-component spin system. In Fig. 1 we compare the exact results reported in Ref. 8 for $N=2,4,\ldots,16$ when $\rho=1$ and $\Delta/t = 0.4, 1.3$, with our expression (12) versus $1/N$ for the same values of ρ and Δ/t.

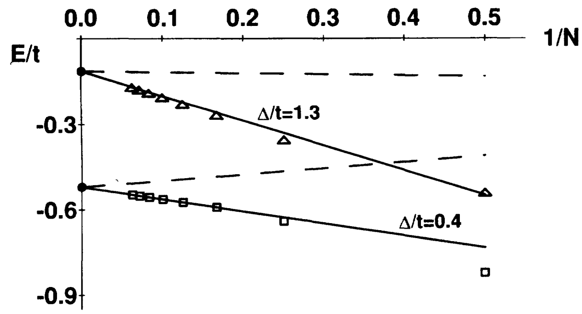

FIG. 1. $E^{(N)}_{\mathrm{TOT}}/(N/2)$ vs $1/N$ for two values of Δ/t with (full line) and without (broken line) the contribution from infinity. Full circles stand for the mean-field results; empty squares and triangles are the exact results borrowed from Ref. 8 for $\Delta/t=0.4$ and 1.3, respectively.

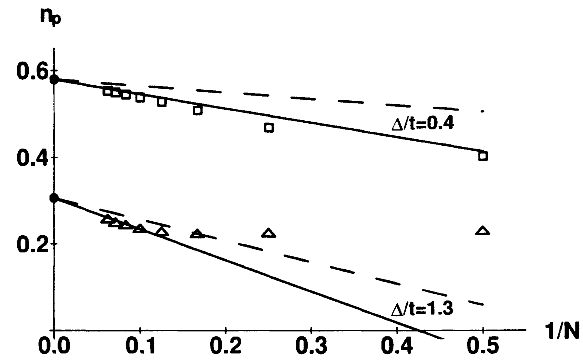

FIG. 2. $n^{(N)}_p$ vs $1/N$. Conventions are as in Fig. 1.

For comparison, we plot also the corresponding expression omitting the "contribution from infinity" $(2/N)(-\lambda_0/2)$.

It is evident from this figure that $1/N$ expression (12) fits rather accurately the exact results up to the lowest N values, at least for the chosen values of Δ/t. Specifically, expression (12) appears to have the correct slope to reproduce the exact results at large N, thereby establishing the validity of the large-N expansion. Omitting the "contribution from infinity" from (12) leads instead to a sizable deviation with respect to the exact result and apparently does not reproduce the leading $1/N$ corrections. This implies that the contribution from infinity, which has so far been omitted in the slave-boson literature, is indeed essential to carry out a correct large-N expansion and make the slave-boson method working in practical cases.

It is also worth verifying to what extent the spurious "transition" at $\Delta/t=2$ affects the total energy (12) as a function of Δ, by comparing with the available exact solution for $N=2$ (i.e., for the case of physical interest where the agreement with the exact solutions is expected to be the worst). We have found that for $\rho\simeq1.0$ it is possible to isolate a "critical" nonconfidence window of width t about $\Delta=2t$, where our $1/N$ expression does not match the exact solution and higher-order fluctuations become important. By contrast, for $\rho\simeq1.5$ the agreement between the exact solution and the $1/N$ expression appears to be really quite good.

As final check for the validity of the $1/N$ expansion, we calculate the fraction of particles n_p in the p level. For any given N, $n^{(N)}_p$ can be obtained by differentiating the expression (12) with respect to Δ. Exact results for $n^{(N)}_p$ are available from Ref. 8 for $N=2,4,\ldots,16$ and $\rho=1$. Comparison of these exact results with our $1/N$ results (with and without the inclusion of the contribution from infinity to $E^{(N)}_{\mathrm{TOT}}$) is reported in Fig. 2. Once more, this picture shows that the contribution from infinity in the functional integral must not be missed.

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[1] The slave-boson method has been introduced by S. E. Barnes [J. Phys. F **6**, 1375 (1976)] and P. Coleman [Phys. Rev. B **29**, 3035 (1984)].

[2] See P. Coleman (Ref. 1); N. Read and D. M. Newns, J. Phys. C **16**, 3273 (1983); A. Auerbach and K. Levin, Phys. Rev. Lett. **57**, 877 (1986).

[3] See S. E. Barnes (Ref. 1); J. Phys. F **7**, 2637 (1977); A. J. Millis and P. A. Lee, Phys. Rev. B **35**, 3394 (1987).

[4] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).

[5] N. Read, J. Phys. C **18**, 2651 (1985).

[6] For an exhaustive list of references, see N. E. Bickers, Rev. Mod. Phys. **59**, 845 (1987).

[7] E. Arrigoni and G. C. Strinati, Phys. Rev. Lett. **71**, 3178 (1993).

[8] L. Zhang, J. K. Jain, and V. J. Emery, Phys. Rev. B **46**, 5599 (1992).

[9] Compare, e.g., L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

[10] The contribution originating from the measure in the radial gauge is implicit in (6).

[11] In a similar fashion, it has been found that the continuum limiting process for path integrals in polar coordinates requires special care even for the simplest case of a free particle: S. F. Edwards and Y. V. Gulyaev, Proc. R. Soc. London Ser. A **279**, 229 (1964).

[12] The extended calculations will be reported elsewhere.

[13] We have found it troublesome to compare our results for the Gaussian fluctuations *in the continuum limit* with the results given in Ref. 8, because of several apparent inconsistencies found in the expressions of Ref. 8 (corrected yet of evident misprints). Nonetheless, we were able to compare numerically our results with Fig. 2 of Ref. 8 for the case $\Delta/t=4.0$ (where $r_0^2\rightarrow0$), provided we assign a missing factor $\frac{1}{2}$ to the fluctuation contribution in Eq. (38) of Ref. 8.