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LETTER TO THE EDITOR

On handling the measure in the slave-boson functional integral

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Abstract. We present an approach for dealing with the contribution following from the measure which occurs when going over from the Cartesian to the radial representation in the slave-boson functional integral. The connection with previous calculations is established and we treat as an example the $U = \infty$ one-band Hubbard model in the large-spin-degeneracy limit. The results that we obtain are in total agreement with those of a recent X-operator approach.

The slave-boson (SB) functional integral (FI) approach [1–6] has been repeatedly used for the investigation of models for strongly correlated systems, especially in connection with large-spin-degeneracy (N) treatments. However, some intrinsic fine details which have formerly not been addressed in a proper way have to be taken into account when this approach is used. These are, for example, the change of variables in the FI representation and the correct use of the time discretization in the FI. The latter problem has been investigated in detail by Arrigoni *et al* [7]. These authors find that a correct treatment of the time-discretized formulation of the FI gives additional terms to the free energy as calculated in the commonly applied time-continuum limit, provided that fluctuation ($1/N$-) corrections beyond the saddle-point solution are considered.

Here we apply the commonly used time-continuum limit. This can be justified by the fact that these differences should not occur when such physical quantities as correlation functions are calculated. The latter has been shown in a strict sense [8] for the leading order of the density correlation function by comparing the SB result with that of a totally independent $1/N$-expansion [8, 9] based on Hubbard's X-operator formulation [10] and a Baym–Kadanoff perturbation expansion [11, 12]. Here we want to address the change of variables in the slave-boson FI when the radial representation of the fields is used. Due to this change some additional terms appear in the measure which are not considered in the usual treatments [13]. We deal with them in a proper way and discuss the results as compared with the common approach.

As an example we consider the one-band Hubbard model [14, 15] in the limit of infinite Coulomb repulsion and large spin degeneracy. This limit allows for a controlled expansion in the (artificial) small parameter $1/N$. To make the comparison with the usual approach comprehensible and self-contained we have to review some well known steps of the usual SB treatment in a detailed way.

In this work we investigate electrons on a lattice, subject to an infinitely strong local

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interaction. Allowing for an arbitrary spin degeneracy N, the Hamiltonian is given by

$$H = \sum_{ip} E_{ip} d_{ip}^{\dagger} d_{ip} + \sum_{i,j,p} \frac{t_{ij}}{N} d_{ip}^{\dagger} b_i b_j^{\dagger} d_{jp}. \tag{1}$$

Above, b_i denotes the annihilation operator of a boson and d_{ip} that of a fermion with spin p at site i [1, 2]. The spin indices run from 1 to N. The first term in equation (1) describes isolated atoms, the second one the hopping between atoms with matrix elements t_{ij}. The scaling factor N has been introduced so that the limit $N \to \infty$ is non-trivial. For $N = 2$, the Hamiltonian (1) reduces to the original Hubbard model. The bosonic and fermionic operators act within a restricted Hilbert space defined by the constraint

$$Q_i = b_i^{\dagger} b_i + \sum_{p=1}^{N} d_{ip}^{\dagger} d_{ip} = \frac{N}{2}. \tag{2}$$

Equation (2) implies that, at most, $N/2$ of the N states at each site can be occupied at the same time. Note that this constraint allows for an $1/N$-expansion around the saddle point of the functional integral in which the saddle-point solution itself becomes exact for $N \to \infty$ at *all* temperatures. This would not be the case if the constraint was not enlarged, i.e., if $N/2$ on the r.h.s. of equation (2) was replaced by unity [16]. Now we consider the partition function Z for the Hamiltonian (1). Formulating Z as a functional integral over anticommuting Grassmann (d^*, d) and commuting Bose (b^*, b) fields one obtains [19]

$$Z = \int \mathrm{D}[d^*, d]\ \mathrm{D}[b^*, b]\ \mathrm{D}[\lambda]\ \exp\left(- \int_0^{\beta} \mathrm{d}\tau\ L(\tau) \right) \tag{3}$$

with

$$L(\tau) = \sum_i \left[b_i^* \left(\frac{\partial}{\partial \tau} + \mathrm{i}\lambda_i \right) b_i - \mathrm{i}\lambda_i q_0 N + \sum_p d_{ip}^* \left(\frac{\partial}{\partial \tau} + \mathrm{i}\lambda_i - \mu \right) d_{ip} \right] + \sum_{i,j,p} \frac{t_{ij}}{N} d_{ip}^* b_i b_j^* d_{jp} \tag{4}$$

in which τ is the imaginary-time index and $q_0 = 1/2$. The integration over λ ensures the fulfilment of the constraint. Expressing the bosonic fields in terms of modulus and phase

$$b_i(\tau) = r_i(\tau) \exp(\mathrm{i}\theta_i(\tau)) \tag{5}$$

one can see that the phase of the bosonic field in equation (4) can be eliminated. This is done via the following local transformation [4]:

$$d_{ip} \to d'_{ip} = \exp(-\mathrm{i}\theta_i) d_{ip}$$

and

$$\lambda_i \to \lambda'_i(\tau) = \lambda_i + \dot{\theta}_i(\tau).$$

Expressing (4) in terms of the new variables and leaving out the primes one gets

$$L(\tau) = \sum_i \left\{ r_i \left(\frac{\partial}{\partial \tau} + \mathrm{i}\lambda_i \right) r_i - \mathrm{i}\lambda_i q_0 N + q_0 N i \dot{\theta}_i(\tau) + \sum_p d_{ip}^* \left(\frac{\partial}{\partial \tau} + \mathrm{i}\lambda_i - \mu \right) d_{ip} \right\} + \sum_{i,j,p} \frac{t_{ij}}{N} d_{ip}^* r_i r_j d_{jp}. \tag{6}$$

Now θ decouples and can be integrated out. Note that when using the radial representation Elitzur's theorem [20] is not violated in the saddle-point approximation, which is in contrast

to what is the case for the Cartesian representation. The change from the Cartesian to the radial representation is connected with a change in the measure:

$$\mathrm{D}[b(\tau)]\ \mathrm{D}[b^*(\tau)] = \left(\prod_\tau r(\tau)\right)\ \mathrm{D}[r(\tau)]\ \mathrm{D}[\theta(\tau)].$$

Usually the product term

$$\prod_\tau r(\tau)$$

is neglected in the SB treatments. Let us first continue with this way of reviewing the steps within the usual approach, before dealing with this point in detail. Integrating out the fermionic degrees of freedom one arrives at

$$Z = \int \mathrm{D}[r]\ \mathrm{D}[\lambda]\ \exp\left\{-\int_0^\beta \mathrm{d}\tau\ L(\tau)\right\} \tag{7}$$

in which

$$L(\tau) = \sum_i \left[r_i(\mathrm{i}\lambda_i)r_i - \mathrm{i}\lambda_i q_0 N\right] - \frac{N}{\beta}\,\mathrm{tr}\left[\ln\left\{\left(\frac{\partial}{\partial\tau} + \mathrm{i}\lambda_i - \mu\right)\delta_{ij} + \frac{t_{ij}}{N} r_i r_j\right\}\right]. \tag{8}$$

The trace (tr) runs only over the time and site variables; the summation over the spin degrees of freedom has already been taken into consideration in the prefactor N.

Let us now turn to the saddle-point equations. The action S in equation (7) has a static homogeneous saddle point S_0 at $r_i(\tau) = \sqrt{N} r_0$ and $\mathrm{i}\lambda_i(\tau) = \lambda_0$, determined by the saddle-point equations

$$\delta S/\delta r|_{\lambda_0, r_0} = 0 \qquad \delta S/\delta\lambda|_{r_0,\lambda_0} = 0.$$

Introducing the effective dispersion relation (the atomic energies are set to zero here):

$$\epsilon(\boldsymbol{k}) = \lambda_0 + \frac{t(\boldsymbol{k})}{N} {r_0}^2 N \tag{9}$$

the saddle-point equations are solved via

$$r_0\lambda_0 = -r_0 \frac{1}{N_S}\sum_{\boldsymbol{k}} t(\boldsymbol{k})\, f(\epsilon(\boldsymbol{k})) \tag{10}$$

and

$$r_0^2 - q_0 = -\frac{1}{N_S}\sum_{\boldsymbol{k}} f(\epsilon(\boldsymbol{k})) = -n_p \tag{11}$$

in which N_S denotes the number of sites and n_p the density per spin degree of freedom. The free energy is given by

$$F = -k_B T\left[-\beta N_S(\lambda_0 - \mu) N({r_0}^2 - q_0) + N\sum_{\boldsymbol{k}} \ln\left(1 + \mathrm{e}^{-\beta(\epsilon(\boldsymbol{k})-\mu)}\right)\right]. \tag{12}$$

So far we have dealt with the results for the usual treatment. We have calculated the same quantities as in equations (9)–(11) with an alternative method [8, 9], using Hubbard's X-operator formulation [10] and the Baym–Kadanoff perturbation expansion [11, 12]. The detailed calculation will be given in a longer publication [21]. In leading order of the $1/N$-expansion we get the same results as with the SB method except for equation (10). In addition to the X-operator solution

$$\lambda_0 = -\frac{N}{N_S}\sum_{\boldsymbol{k}} \frac{t(\boldsymbol{k})}{N} f(\epsilon(\boldsymbol{k}))$$

the equations (10)–(11) allow for having the solution $r_0 = 0$ occurring as an independent one. For the latter, equation (10) does not determine an explicit expression for λ_0. However, equation (11) implies that for $r_0 = 0$ it follows that $\lambda_0 = \mu$ (atomic energies set to zero). This means that in the grand canonical ensemble for the $r_0 = 0$ solution, λ_0 should be adjusted for any given μ in such a way that the system is half-filled and the density becomes independent of the chemical potential! In this context this solution appears spurious, and, as such, is discarded. It nevertheless exists and seems to lead to a difference between the results of the SB and X-operator approaches. However, we will show that this difference is an artifact resulting from the unsatisfactory treatment of the measure leading to the independent solution $r_0 = 0$. We present an approach in which this product term is entirely taken into account. Within this approach no additional solution $r_0 = 0$ occurs and we get total agreement with the X-operator results. Let us first continue with describing the usual approach.

We now consider Gaussian fluctuations around the saddle point of the FI. Derivation of the known expressions is necessary to make the changes visible when the measure is treated in a proper way. To deal with the Gaussian fluctuations one expands the tr ln term in the action (8) of the FI as

$$\mathrm{tr}(\ln G^{-1}) = \mathrm{tr}\ln\left(G_0^{-1}(1 - G_0\Sigma)\right) = \mathrm{tr}(\ln G_0^{-1}) - \mathrm{tr}(G_0\Sigma) - \frac{1}{2}\mathrm{tr}(G_0\Sigma G_0\Sigma) - \dots \tag{13}$$

up to the third term. The first term is known from the saddle-point solution. For G_0 the fields have to be replaced by their saddle-point values. The fluctuation fields $\delta r'$, $\delta\lambda'$ are defined as follows:

$$r_i = r_0\sqrt{N}(1 + \delta r_i') \tag{14}$$

$$\mathrm{i}\lambda_i = \lambda_0 + \mathrm{i}\,\delta\lambda_i'. \tag{15}$$

Thus one gets for Σ

$$\Sigma_{ij} = -\frac{t}{N}Nr_0^2(\delta r_i' + \delta r_j' + \delta r_i'\,\delta r_j') - \mathrm{i}\,\delta\lambda_i'\,\delta_{ij}. \tag{16}$$

The following rescaling of the fields by $\sqrt{N}$

$$\delta r' = \delta r/\sqrt{N} \qquad \delta\lambda' = \delta\lambda/\sqrt{N}$$

ensures that for the calculation of the O(1) contributions to the free energy F it is sufficient to retain those terms that are quadratic in the fluctuation fields in equation (13). Thus the quadratic term $\delta r'\,\delta r'$ in equation (16) can occur only linearly in equation (13). One gets

$$Z = \exp(-\beta S_0)\int \mathrm{D}[\delta r]\ \mathrm{D}[\delta\lambda]\ \exp(-\delta S). \tag{17}$$

The action now reads

$$\delta S = \frac{1}{\beta N_S}\sum_{\omega_n,\boldsymbol{q}}(\delta r(-\boldsymbol{q},-\omega_n)\ \delta\lambda(-\boldsymbol{q},-\omega_n))\,\hat{L}(\boldsymbol{q},\omega_n)\begin{pmatrix}\delta r(\boldsymbol{q},\omega_n)\\ \delta\lambda(\boldsymbol{q},\omega_n)\end{pmatrix} \tag{18}$$

with the matrix

$$\hat{L}(\boldsymbol{q},\omega_n) = \begin{pmatrix}L_{rr} & L_{r\lambda}\\ L_{\lambda r} & L_{\lambda\lambda}\end{pmatrix}_{(\boldsymbol{q},\omega_n)} \tag{19}$$

having the matrix elements

$$L_{\lambda\lambda}(\boldsymbol{q},\omega_n) = -\frac{1}{2\ N_S}\sum_{\boldsymbol{k}}[f(\epsilon(\boldsymbol{k}+\boldsymbol{q})) - f(\epsilon(\boldsymbol{k}))]\frac{1}{\epsilon(\boldsymbol{k}+\boldsymbol{q}) - \epsilon(\boldsymbol{k}) - \mathrm{i}\omega_n} \tag{20}$$

$$L_{\lambda r}(\boldsymbol{q},\omega_n) = L_{r\lambda}(\boldsymbol{q},\omega_n)$$
$$= -\mathrm{i}r_0^2 - \mathrm{i}\frac{r_0^2}{2N_S}\sum_{\boldsymbol{k}}[f(\epsilon(\boldsymbol{k}+\boldsymbol{q})) - f(\epsilon(\boldsymbol{k}))]\frac{t(\boldsymbol{k}+\boldsymbol{q})+t(\boldsymbol{k})}{\epsilon(\boldsymbol{k}+\boldsymbol{q})-\epsilon(\boldsymbol{k})-\mathrm{i}\omega_n} \tag{21}$$

$$L_{rr}(\boldsymbol{q},\omega_n) = \frac{r_0^4}{2\ N_S}\sum_{\boldsymbol{k}}[f(\epsilon(\boldsymbol{k}+\boldsymbol{q})) - f(\epsilon(\boldsymbol{k}))]\frac{[t(\boldsymbol{k}+\boldsymbol{q})+t(\boldsymbol{k})]^2}{\epsilon(\boldsymbol{k}+\boldsymbol{q})-\epsilon(\boldsymbol{k})-\mathrm{i}\omega_n}$$
$$+\frac{r_0^2}{N_S}\sum_{\boldsymbol{k}} f(\epsilon(\boldsymbol{k}))t(\boldsymbol{k}+\boldsymbol{q}) + r_0^2\lambda_0. \tag{22}$$

To calculate the FI one has to integrate out the λ-fields first [19], leading to

$$Z = \mathrm{e}^{-\beta S_0}\int \mathrm{D}[\delta r^*, \delta r]\ \mathrm{e}^{-\delta S} \tag{23}$$

with

$$-\delta S = -\frac{1}{\beta N_S}\sum_{(\boldsymbol{q},\omega_n)\geqslant 0}\delta r^*(\boldsymbol{q},\omega_n)\left[\bar{L}_{rr} - \frac{\bar{L}_{r\lambda}^2}{\bar{L}_{\lambda\lambda}}\right]_{(\boldsymbol{q},\omega_n)}\delta r(\boldsymbol{q},\omega_n). \tag{24}$$

Above, we have used the abbreviation

$$L_{\alpha\beta}(\boldsymbol{q},\omega_n) + L_{\alpha\beta}(-\boldsymbol{q},-\omega_n) = \bar{L}_{\alpha\beta}(\boldsymbol{q},\omega_n)$$

for $(\boldsymbol{q},\omega_n) \neq (0,0)$ and $\alpha,\beta = r,\lambda$.

Let us now investigate the role played by the product term in the measure. We give here a novel treatment of the product term $\left(\prod_\tau r(\tau)\right)$ which appears in the measure of the FI when going over from the Cartesian to the radial representation (equation (5)):

$$\mathrm{D}[b(\tau)]\ \mathrm{D}[b^*(\tau)] = \left(\prod_\tau r(\tau)\right)\mathrm{D}[r(\tau)]\ \mathrm{D}[\theta(\tau)]. \tag{25}$$

The term $\prod_\tau r(\tau)$ is usually neglected. Because the consideration of this term in the form of equation (25) is quite difficult, we go over to a formulation in which $\prod_\tau r(\tau)$ vanishes. Following Popov [22] we define

$$r = \sqrt{R} \tag{26}$$

in which the variables have to be understood as fields. Now one has $r\ \mathrm{d}r = \frac{1}{2}\ \mathrm{d}R$ and the factor r in the measure has gone. In this way we avoid having to deal with terms O(1) in the Lagrangian in contrast to the physical ones which are O(ϵ), ϵ being the time discretization. However, one has to pay for this advantage. Now, the expansion around the saddle-point solution

$$r = r_0\sqrt{N}(1+\delta r')$$

(see equation (14)) yields an additional term. One has

$$r = \sqrt{R} = \sqrt{R_0}\sqrt{N}\sqrt{1+\delta R'}$$

with $\sqrt{R_0} = r_0$. Taylor expansion of $\sqrt{1+\delta R'}$ and the rescaling $\delta R'/2 \to \delta R'$ leads to

$$r = \sqrt{R} = \sqrt{R_0}\sqrt{N}\left(1+\delta R' - \frac{(\delta R')^2}{2} + \ldots\right). \tag{27}$$

We now perform the rescaling $\delta R' = \delta R/\sqrt{N}$. For large N, the expansion in equation (27) can be truncated after the third summand. Now, the saddle point is determined by the

variational differentiation of the action $\delta S/\delta R|_{\lambda_0,R_0}$ instead of $\delta S/\delta r|_{\lambda_0,r_0}$ in the common approach. As a result, we do not get the additional independent saddle-point solution $r_0 = 0$. This is in contrast to the usual treatment (compare equation (10)) and in agreement with the results of a recent X-operator approach [8].

In the following we redetermine the propagator matrix equation (19) by employing the expansion (27). Equation (27) has a form analogous to that of the expression for r, equation (14). One simply has to replace $\delta r'$ by $\delta R'$ and add the quadratic term. The latter can give contributions (in leading order of $1/N$ [23]) only within the term which is quadratic in δR, and as a result the last two contributions to L_{rr}, equation (22), are modified. The one stemming from $r_i(\mathrm{i}\lambda_i)r_i$ disappears since this term turns into $2\mathrm{i}\,R_0\,\delta\lambda_i\,\delta R_i$ and gives the first contribution to $L_{r\lambda}$ as before. Due to this there follows a loss of the term $r_0^2\lambda_0$ in L_{rr}, equation (22). For the second summand

$$-\frac{N}{\beta}\mathrm{tr}\left[\ln\left\{\left(\frac{\partial}{\partial\tau}+\mathrm{i}\lambda_i-\mu\right)\delta_{ij}+\frac{t_{ij}}{N}r_ir_j\right\}\right]$$

of the action given by equation (8), there is a local contribution following from the quadratic term in equation (27) leading to

$$r_ir_j \to \left(1+\delta R_i'-\frac{(\delta R_i')^2}{2}\right)\left(1+\delta R_j'-\frac{(\delta R_j')^2}{2}\right).$$

Thus in the expression for Σ_{ij}, equation (16), $\delta r_i' + \delta r_j' + \delta r_i'\,\delta r_j'$ turns into

$$\delta R_i' + \delta R_j' + \delta R_i'\,\delta R_j' - \frac{(\delta R_i')^2}{2} - \frac{(\delta R_j')^2}{2}.$$

The other terms are of higher order in $1/N$ [23]. Note that the new expressions in Σ can contribute only to such terms stemming from the expansion of the logarithm in equation (13), which are linear in Σ. These linear terms give the first term of the second summand in L_{rr}, equation (22),

$$-\frac{1}{N_S}\sum_{\boldsymbol{k}} f(\epsilon(\boldsymbol{k}))t(\boldsymbol{k}+\boldsymbol{q}).$$

The additional terms $((\delta R')^2/2)$ in equation (27) lead to a replacement $t(\boldsymbol{k}+\boldsymbol{q}) \to t(\boldsymbol{k}+\boldsymbol{q}) - t(\boldsymbol{k})$ in equation (22). Altogether, L_{rr} is now given by

$$L_{rr}(\boldsymbol{q},\omega_n) = \frac{r_0^4}{2\,N_S}\sum_{\boldsymbol{k}}[f(\epsilon(\boldsymbol{k}+\boldsymbol{q})) - f(\epsilon(\boldsymbol{k}))]\frac{[t(\boldsymbol{k}+\boldsymbol{q})+t(\boldsymbol{k})]^2}{\epsilon(\boldsymbol{k}+\boldsymbol{q})-\epsilon(\boldsymbol{k})-\mathrm{i}\omega_n}$$
$$+\frac{r_0^2}{N_S}\sum_{\boldsymbol{k}} f(\epsilon(\boldsymbol{k}))[t(\boldsymbol{k}+\boldsymbol{q})-t(\boldsymbol{k})]. \tag{28}$$

However, on employing the saddle-point equation (10) it turns out that the two expressions for L_{rr}, equation (22) and equation (28), are numerically identical. Other changes do not occur. Thus the expression for the FI including Gaussian fluctuations is obtained by replacing in the expressions (17) and (18) all δr by δR and $r_0^2\lambda_0$ by

$$-\frac{r_0^2}{N_S}\sum_{\boldsymbol{k}} t(\boldsymbol{k})f(\epsilon(\boldsymbol{k}))$$

in L_{rr}, equation (22). If just the FI representation of the partition function is considered, the integration variable can be chosen arbitrarily. Consequently we can replace the new variables R formally by the usual r but have to take into account that the independent

solution $r_0 = 0$ no longer occurs. Thus one gets formally the correct solutions if the product term is simply neglected as well as the saddle-point solution $r_0 = 0$. This applies to the calculation of correlation functions as well. We consider the hole–hole correlation function:

$$H(i - j, \tau) = \langle b_i^+(\tau) b_i(\tau) b_j^+(0) b_j(0) \rangle. \tag{29}$$

Using the expansion (15) and leaving out the static contributions and the product term in the measure, this turns into

$$H(i - j, \tau) = 4r_0^4 N \langle \delta r_i(\tau)\, \delta r_j(0) \rangle + \mathrm{O}(1). \tag{30}$$

Now carrying through the same expansion but taking the measure into account leads to the first term in equation (30), without the O(1) corrections, which would follow from higher-order terms in the action. Thus the two sets of results coincide to leading order in $1/N$. Even when calculating the Green's function the two procedures lead to the same result, even though some care has to be taken to deal with the time discretization [7]. However, choosing one procedure or the other will make a difference when performing self-consistent one-loop calculations.

In this letter we have clarified the circumstances under which the product term in the measure, which occurs when going over from the Cartesian to the radial representation in the slave-boson functional integral, can be neglected. To this end we considered the $U = \infty$ one-band Hubbard model in the limit of large spin degeneracy. We derived both expressions for the propagators and found that they differ at the self-consistent one-loop level only. In contrast to what is the case in the usual approach, in which the product term is neglected, we do not get an additional unphysical saddle-point solution becoming important if, for example, next-nearest-neighbour hopping is included [8]. The results that we get for $N \to \infty$ are in total agreement with recent results from an alternative X-operator approach [8, 9].

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