Spin- and charge-rotation invariant approach to the Hubbard model

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We present a slave-boson formulation for the Hubbard model that preserves the spin-rotation and particle-hole symmetries of the paramagnetic phase at half filling. Fermion and boson fields are treated on an equal footing in a functional integral formulation. We show that, while in two and three dimensions there is a metal-insulator transition as the interaction U increases, in one dimension our approach always gives an insulating state. Short-range spin-spin correlations are included at the saddle-point level for all values of U, giving a good description of the insulating state. We show that the energy gap in the one-particle spectrum increases from zero as $(U-U_c)^\alpha$, where U_c is the critical value of the on-site interaction and the exponent α is 1 and 1/2 for 2 and 3 dimensions, respectively. [S0163-1829(96)04839-4]

I. INTRODUCTION

The Hubbard model, which has been studied for almost thirty years, is considered one of the simplest models that contains the essential ingredients for understanding the physics of correlated metals.[1] Despite its simple form, it provides a physical scenario to describe the metal-insulator transition, the formation of localized magnetic moments, and the occurrence of long-range magnetic order. The discovery of high-T_c superconductivity[2] renewed the interest in this model, since it provides a natural framework for describing many properties of the cuprates. Moreover, it has been argued that superconductivity itself could be a consequence of the local repulsion U.[3]

The big effort to obtain solutions to this model—both the ground state[4,5] and the thermodynamic properties—led to only a few controlled results. Probably the best results in the regime of interest, near half filling and intermediate coupling, correspond to those obtained by numerical simulation.[6] However, the slave-boson approach[7]—applied to the Hubbard model by Kotliar and Ruckenstein (KR) (Ref. 8) seems to be an attractive starting point for a systematic study of the model. The KR approach is a functional integral method that reproduces the Gutzwiller solution[4] at the saddle-point level. The advantage of this method over the Gutzwiller variational wave function is that it provides a systematic way to improve the solution. As pointed out by Li, Wölfle, and Hirschfeld,[9] the KR theory does not preserve the spin-rotation invariance of the original Hamiltonian. They generalized the theory and provided a way of formulating a functional integral method which naturally preserves this invariance. In any case, the results at the saddle-point level are equivalent to Gutzwiller's solution, and in the Mott insulating state spin-spin correlations are not included.

In the present work, we introduce slave bosons in the Zou and Anderson[10] scheme to describe the paramagnetic phase of the Hubbard model. We devise a functional integral method which presents the following advantages over previous theories:

(i) It explicitly preserves the full spin-rotation invariance and particle-hole symmetry (charge-rotation invariance) of the original half-filled Hubbard Hamiltonian.

(ii) The insulating state includes short-range spin-spin correlations already at the saddle-point level.

One disadvantage of our approach is that the $U=0$ limit is not exactly reproduced, since we do not renormalize the hopping matrix elements as in the KR formulation. However, this renormalization is inconvenient when fluctuations are incorporated above the saddle-point results.[11]

The rest of the paper is organized as follows: In Sec. II we give a detailed description of the formalism, in Sec. III we present the results for one, two, and three dimensions (3D), and in Sec. IV we summarize our conclusions.

II. SLAVE-BOSON APPROACH

In this section we present the method starting from a functional integral theory that makes apparent the spin-rotation and particle-hole symmetries of the original model. We consider the Hubbard Hamiltonian written in the usual notation:

$$H=-t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}\ (n_{i\uparrow}n_{i\downarrow}-\tfrac{1}{2}\,n_i)-\mu\sum_{i}\ n_i. \quad (1)$$

Here $c_{i\sigma}^{\dagger}$ creates an electron at site i with spin σ, $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ and $n_i=n_{i\uparrow}+n_{i\downarrow}$. Note that we have included an on-site energy $U/2$. In this notation the chemical potential μ is zero for the half-filled case. In the following, we will measure the energy in units of $t=1$.

In order to make apparent the global symmetries of the model, we introduce the following operators:

$$\Psi_i=\begin{pmatrix} c_{i\uparrow} & -c_{i\downarrow}^{\dagger} \\ c_{i\downarrow} & c_{i\uparrow}^{\dagger} \end{pmatrix}, \quad \Psi_i^{\dagger}=\begin{pmatrix} c_{i\uparrow}^{\dagger} & c_{i\downarrow}^{\dagger} \\ -c_{i\downarrow} & c_{i\uparrow} \end{pmatrix}. \quad (2)$$

In this representation the Hamiltonian reads

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} \mathrm{Tr}[\Psi_i^\dagger \Psi_j \sigma_z] + \frac{U}{12} \sum_i \{\mathrm{Tr}[(\Psi_i^\dagger \Psi_i)^2] - 8\}$$

$$-\mu \sum_i \{\tfrac{1}{2}\mathrm{Tr}[\Psi_i^\dagger \Psi_i \sigma_z] + 1\}. \quad (3)$$

Global spin rotations are equivalent to the following transformations: $\widetilde{\Psi}_i = g^s \Psi_i$, where g^s is a SU(2) matrix. Rotations in the charge sector (particle-hole transformations) correspond to $\widetilde{\Psi}_i = \Psi_i g_i^c$, where $g_i^c = (\sigma_z)^i g (\sigma_z)^i$ with σ_z a Pauli matrix and g a SU(2) matrix. Then, it is straightforward to show that the Hamiltonian (3) is invariant under these transformations for $\mu = 0$, i.e., one particle *per site*.

We introduce slave bosons in the Zou and Anderson[10] scheme, where the fermion operators are written in the following way:

$$c_{i\sigma} = s_{i\sigma} e_i^\dagger + \sigma s_{i-\sigma}^\dagger d_i. \quad (4)$$

Here $s_{i\sigma}^\dagger$ is the single-occupancy fermionic operator, and $e_i^\dagger$ and $d_i^\dagger$ are the empty and double-occupancy slave-boson creation operators, respectively. The electron operator Ψ_i is then given by

$$\Psi_i = \Psi_i^s \Psi_i^{c\dagger}, \quad (5)$$

where the spin and charge fields are

$$\Psi_i^s = \begin{pmatrix} s_{i\uparrow} & -s_{i\downarrow}^\dagger \\ s_{i\downarrow} & s_{i\uparrow}^\dagger \end{pmatrix}, \quad \Psi_i^{c\dagger} = \begin{pmatrix} e_i^\dagger & d_i^\dagger \\ -d_i & e_i \end{pmatrix}. \quad (6)$$

Under spin rotations and particle-hole transformations these operators change as $\widetilde{\Psi}_i^s = g^s \Psi_i^s$ and $\widetilde{\Psi}_i^{c\dagger} = \Psi_i^{c\dagger} g_i^c$, respectively, with g^s and g_i^c as above.

The Hamiltonian written in terms of these field operators takes the form

$$H_{cs} = -\frac{1}{2} \sum_{\langle ij \rangle} \mathrm{Tr}[(\Psi_i^{s\dagger} \Psi_j^s \sigma_z)(\sigma_z \Psi_j^{c\dagger} \sigma_z \Psi_i^c)]$$

$$-\left(\mu + \frac{U}{2}\right) \sum_i (\tfrac{1}{2}\mathrm{Tr}[\Psi_i^{s\dagger} \Psi_i^s \sigma_z] + 1) - 2\mu \sum_i d_i^\dagger d_i, \quad (7)$$

and becomes equivalent to (1) provided the following constraint is satisfied:

$$\tfrac{1}{2}\mathrm{Tr}[\Psi_i^{s\dagger} \Psi_i^s \sigma_z] + \tfrac{1}{2}\mathrm{Tr}[\Psi_i^{c\dagger} \Psi_i^c] = 1. \quad (8)$$

The partition function Z is given as a coherent-state functional integral of a Lagrangean $L(\tau)$:

$$Z = \int [Ds][De][Dd][D\lambda] \exp\left[-\int_0^\beta d\tau\, L(\tau)\right], \quad (9)$$

with

$$L(\tau) = \frac{1}{2} \sum_i \mathrm{Tr}[(\Psi_i^{s\dagger} \partial_\tau \Psi_i^s) + (\Psi_i^{c\dagger} \partial_\tau \Psi_i^c \sigma_z)] + H_{cs}$$

$$+ i \sum_i \lambda_i \{\tfrac{1}{2}\mathrm{Tr}[\Psi_i^{s\dagger} \Psi_i^s \sigma_z] + (\Psi_i^{c\dagger} \Psi_i^c)] - 1\}. \quad (10)$$

Here λ_i is a Lagrange multiplier introduced to enforce the constraint (8).

In order to go beyond the standard saddle-point approximation we introduce Hubbard-Stratonovich fields $\chi_{ij}(\tau)$, in terms of which the partition function reads

$$Z = \int [D\chi][Ds][De][Dd][D\lambda]$$

$$\times \exp\left[-\int_0^\beta d\tau\left(\sum_{\langle ij \rangle} \chi_{ij}^\dagger \chi_{ij} + L_s(\tau) + L_c(\tau)\right)\right]. \quad (11)$$

The charge and spin Lagrangeans are given by

$$L_s(\tau) = \frac{1}{2} \sum_i \mathrm{Tr}[\Psi_i^{s\dagger} \partial_\tau \Psi_i^s] - \frac{1}{2} \sum_{\langle ij \rangle} \mathrm{Tr}[(\Psi_i^{s\dagger} \Psi_j^s \sigma_z) \chi_{ji}]$$

$$+ \sum_i \left(i\lambda_i - \mu - \frac{U}{2}\right)(\tfrac{1}{2}\mathrm{Tr}[\Psi_i^{s\dagger} \Psi_i^s \sigma_z] + 1), \quad (12)$$

and

$$L_c(\tau) = \frac{1}{2} \sum_i \mathrm{Tr}[\Psi_i^{c\dagger} \partial_\tau \Psi_i^c \sigma_z]$$

$$- \frac{1}{2} \sum_{\langle ij \rangle} \mathrm{Tr}[\chi_{ij}^\dagger (\sigma_z \Psi_j^{c\dagger} \sigma_z \Psi_i^c)]$$

$$+ \sum_i i\lambda_i (\tfrac{1}{2}\mathrm{Tr}[\Psi_i^{c\dagger} \Psi_i^c] - 2) - 2\mu \sum_i d_i^\dagger d_i. \quad (13)$$

In (9) fermions and bosons can be exactly integrated out, leaving an effective partition function in terms of the Hubbard-Stratonovich fields χ_{ij} and Lagrange multipliers λ_i. Up to this point everything is exact. To proceed further, we perform a saddle-point approximation for the fields χ_{ij} and λ_i. This procedure presents the following advantages over the standard one: (i) fermions and bosons are treated on equal footing; (ii) the saddle-point approximation preserves both the global spin-rotation invariance and particle-hole symmetries of the paramagnetic phase at half filling, regardless of the χ_{ij} values; and (iii) the saddle point includes short-range antiferromagnetic correlations (through the integrated boson dynamics) even in the large-U insulating state. The disadvantage is that the $U=0$ limit is not as well reproduced as in KR's approach, where the hopping term includes normalization operators introduced precisely to reproduce the noninteracting case.

The saddle-point approximation corresponds to replacing the Hubbard-Stratonovich fields and Lagrange multipliers by c numbers and minimizing the effective action $S_{\mathrm{eff}}(\chi_{ji}^{\mathrm{sp}*}, \chi_{ji}^{\mathrm{sp}}, \lambda_i^{\mathrm{sp}})$. The saddle-point equations for the χ numbers are
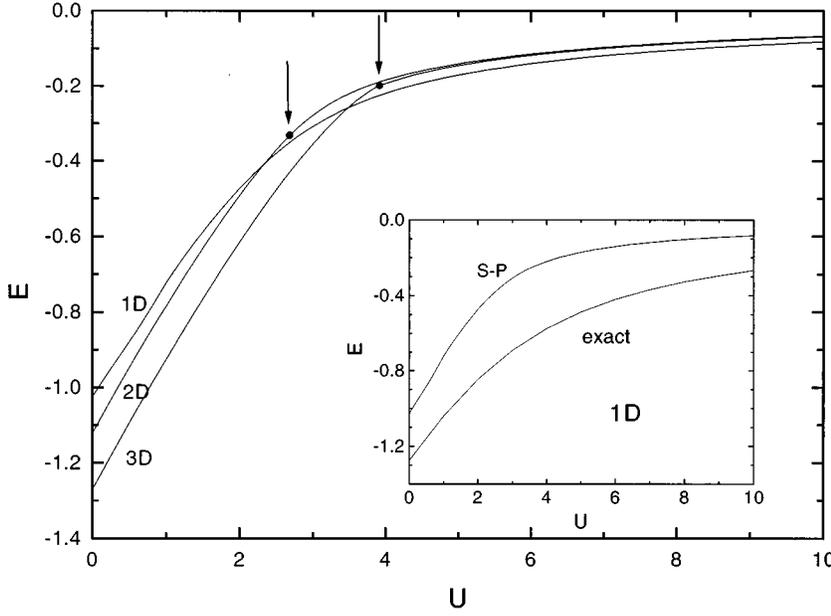
FIG. 1. Energy *per site* as a function of the on-site interaction U, for 1D, 2D, and 3D. The arrows indicate the point where the metal-insulator transition occurs in 2D and 3D. In the inset the energy of the 1D case obtained with the saddle-point approximation (S-P) is compared to the exact result.

$$\chi_{ij}^{\mathrm{sp}}=\langle \sigma_z \Psi_i^{c\dagger} \sigma_z \Psi_j^c \rangle_{\mathrm{sp}}$$

and

$$\chi_{ij}^{\mathrm{sp}*}=\langle \Psi_i^{s\dagger} \Psi_j^s \sigma_z \rangle_{\mathrm{sp}}.$$

The value of the Lagrange multiplier λ_i^{sp} is obtained by satisfying the constraint (8) (details will be discussed in the next section).

Note that in the homogeneous state, where both the χ numbers and the Lagrange multiplier λ are site independent, the formalism is equivalent to a self-consistent diagonalization of the following spin and charge Hamiltonians:

$$H_s=\sum_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}}^s+\lambda^{\mathrm{sp}})s_{\mathbf{k}\sigma}^\dagger s_{\mathbf{k}\sigma}-\sum_{\mathbf{k}}g_{\mathbf{k}}^s[s_{\mathbf{k}\uparrow}^\dagger s_{-\mathbf{k}\downarrow}^\dagger+s_{-\mathbf{k}\downarrow}s_{\mathbf{k}\uparrow}],$$
(14)

and

$$H_c=\sum_{\mathbf{k}}[(\epsilon_{\mathbf{k}}^e+\lambda^{\mathrm{sp}})e_{\mathbf{k}}^\dagger e_{\mathbf{k}}+(\epsilon_{\mathbf{k}}^d+\lambda^{\mathrm{sp}})d_{\mathbf{k}}^\dagger d_{\mathbf{k}}]$$

$$-\sum_{\mathbf{k}}g_{\mathbf{k}}^c[e_{\mathbf{k}}d_{\mathbf{k}}+e_{\mathbf{k}}^\dagger d_{\mathbf{k}}^\dagger].$$
(15)

Here the operators with subindex $\mathbf{k}$ are the Fourier transform of site operators, $\epsilon_{\mathbf{k}}^s=-2A\gamma_{\mathbf{k}}-U/2-\mu$, $g_{\mathbf{k}}^s=2B\gamma_{\mathbf{k}}$ for fermions, $\epsilon_{\mathbf{k}}^e=-2C\gamma_{\mathbf{k}}$, $\epsilon_{\mathbf{k}}^d=2C\gamma_{\mathbf{k}}-2\mu$, $g_{\mathbf{k}}^c=2D\gamma_{\mathbf{k}}$ for bosons, and $\gamma_{\mathbf{k}}=\sum_\alpha \cos k_\alpha$, with k_α the α component of the wave vector $\mathbf{k}$. The parameters A, B, C, and D are obtained from the self-consistency equations $A=\langle e_i^\dagger e_j \rangle-\langle d_i^\dagger d_j \rangle$, $B=\langle e_i d_j \rangle+\langle e_j d_i \rangle$, $C=\sum_\sigma \langle s_{i\sigma}^\dagger s_{j\sigma} \rangle$, and $D=\langle s_{i\downarrow}s_{j\uparrow} \rangle+\langle s_{j\downarrow}s_{i\uparrow} \rangle$.

The energy is given by

$$E=-\frac{1}{2}\sum_{\langle ij \rangle}\mathrm{Tr}[\chi_{ij}^{\mathrm{sp}*}\chi_{ij}^{\mathrm{sp}}]+U\sum_i \langle d_i^\dagger d_i \rangle,$$

while the nearest-neighbor isotropic spin-spin correlation function can be calculated as

$$\langle \mathbf{S}_i . \mathbf{S}_j \rangle=-\tfrac{3}{8}D^2.$$

In the next section we present the results for 1D, 2D, and 3D.

III. RESULTS

We first discuss the results for the half-filling case, which corresponds to $\mu=0$. For this case, in 2D and 3D two different phases—corresponding to the metallic phase for weak coupling and the insulating phase for strong coupling—are obtained. The metallic phase is characterized by a condensation of the charge bosons.[12] As U increases the density of condensed bosons decreases, and at a critical value of the interaction U_c it goes to zero. The insulating phase is characterized by the absence of a boson condensate, i.e., the Mott transition occurs when the effective chemical potential for the bosons $(-\lambda^{\mathrm{sp}})$ is depinned from the bottom of the bosonic excitation band. In 1D only the insulating phase occurs since there is no Bose condensation.

In the metallic phase the number of empty and double-occupancy bosons—which are equal due to the electron-hole symmetry for $\mu=0$—can be separated into two contributions: the condensed and the uncondensed ones. In this way the constraint takes the form

$$\langle e \rangle^2+\langle d \rangle^2+\sum_{\mathbf{k}\neq 0}(\langle e_{\mathbf{k}}^\dagger e_{\mathbf{k}} \rangle+\langle d_{\mathbf{k}}^\dagger d_{\mathbf{k}} \rangle)+\sum_{\mathbf{k}\sigma}\langle s_{\mathbf{k}\sigma}^\dagger s_{\mathbf{k}\sigma} \rangle=1.$$
(16)

The Lagrange multiple is pinned at the bottom of the boson bands. The self-consistent solution of (14) and (15) gives for this case $A=C=0$ and $\lambda^{\mathrm{sp}}=zD$, where z is the lattice coordination number. The density of the condensed bosons is then given by the constraint (16). For $U>U_c$, $\langle e \rangle^2=\langle d \rangle^2=0$, and $\lambda^{\mathrm{sp}}>zD$, and its value is obtained by satisfying the constraint. With this parameter and the self-
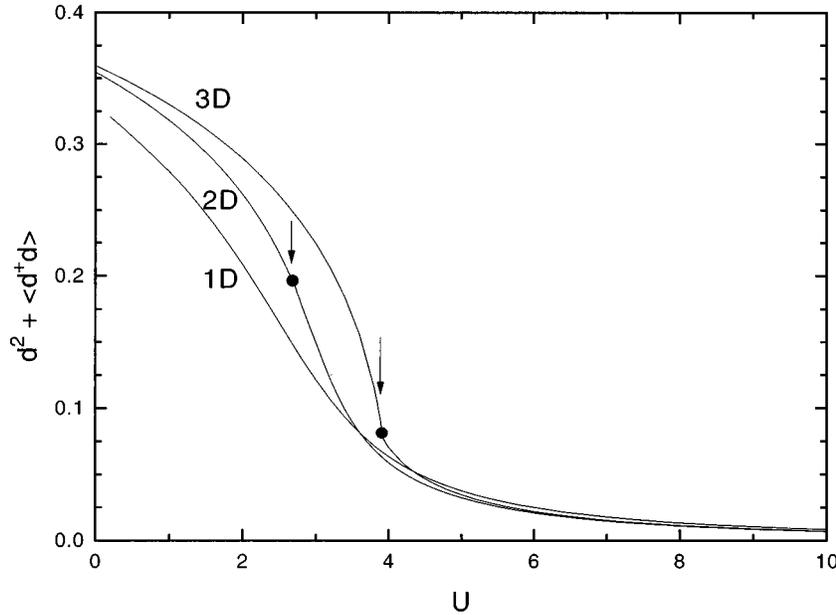
FIG. 2. Double occupation as a function of U for 1D, 2D, and 3D. Arrows indicate the points where metal-insulator transitions occur.

consistent solutions for B and D, the energy and different expectation values can be calculated.

In Fig. 1 we plot the energy as a function of U for 1D, 2D, and 3D. The inset shows the 1D result and the exact energy obtained by the Bethe *ansatz* for comparison. The following points deserve a comment:

(i) For $U=0$ the exact results are not reproduced as anticipated above.

(ii) In the large-U limit the energy is lower than zero due to the antiferromagnetic correlations present for any finite value of the on-site interaction.

(iii) While for 2D and 3D there is a critical value U_c at which the Mott transition occurs, in 1D the present approach gives an insulating state for all values of U.

(iv) The energy and its U derivative are continuous at the Mott transition. As we will show below, the same occurs for the spin-spin, double occupation, and other correlation functions.

In our approximation the double occupation is always different from zero, as shown in Fig. 2. In particular, for $U > U_c$ the double occupation is due to the fluctuations of the vacuum, which are present because we have introduced the boson dynamic effects already at saddle-point order. These fluctuations are responsible for the antiferromagnetic correlations of the insulating state. For $U < U_c$, the condensate contributes with a macroscopic number of empty and double-occupancy bosons.

The nearest-neighbor isotropic spin-spin correlation functions are shown in Fig. 3. For small U they decrease as the dimension increases, as expected for uncorrelated electrons in a lattice. This tendency is maintained for all values of U. For large U the correlations saturate and become U independent, like in the true antiferromagnetic ground state. Notice, however, that we are describing a paramagnetic (Mott) insulating phase, so that in 2D and 3D these correlations do not correspond to the standard Heisenberg correlations. In
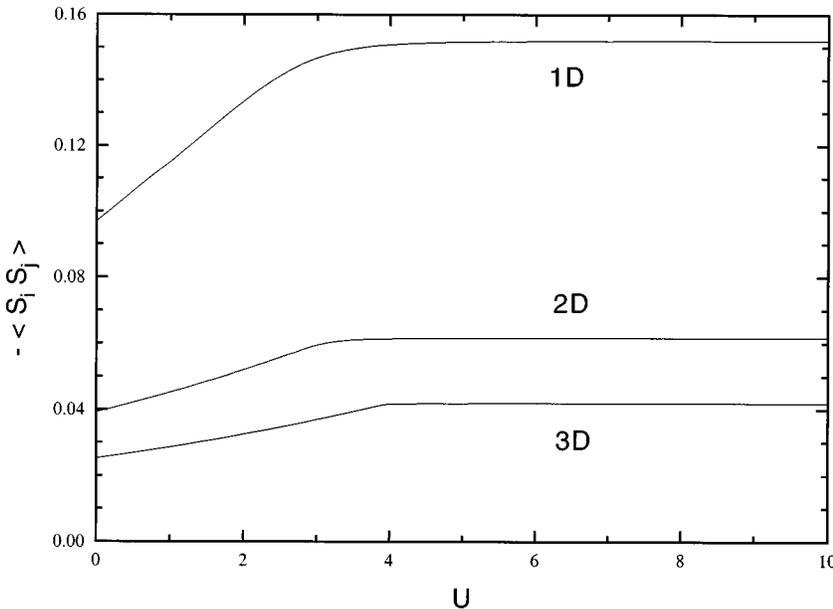

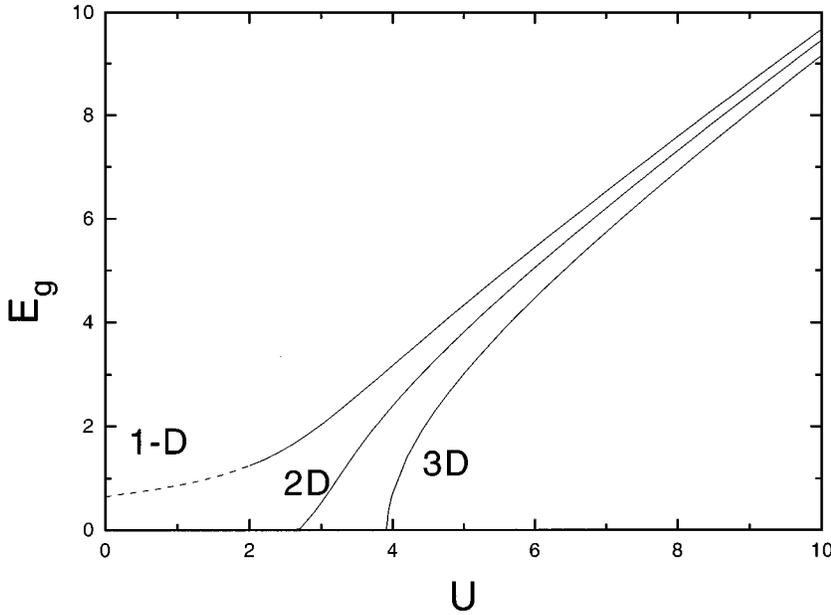FIG. 3. Nearest-neighbor isotropic spin-spin correlation for 1D, 2D, and 3D as indicated.

FIG. 4. Gap E_g as a function of U. In the 1D case the gap obtained for small values of U is plotted with a dashed line.

1D our result is sensibly smaller than the Bethe *ansatz* result, since at saddle-point order our approach introduces the short-range spin-spin correlations only partially. This quantitative aspect can be corrected by the inclusion of Gaussian fluctuations.

Away from half-filling the electron-hole symmetry must be broken. Since according to (15) the zero-point excitations of the e and d fields are paired, the number of empty and double-occupancy condensed bosons must be different. The saddle-point equations force their densities to be related by

$$\frac{\langle e \rangle}{\langle d \rangle} = \frac{zD}{zC - \mu + \sqrt{(zC - \mu)^2 + (zD)^2}}.$$

Using this relation and adjusting the chemical potential to fix the number of electrons, we can calculate all the self-consistent parameters A, B, C, and D.

The one-particle gap E_g of the Mott insulating phase is calculated as the jump in the chemical potential when the total number of particles changes from $1 - \epsilon$ to $1 + \epsilon$, and is given by

$$E_g = 2\sqrt{(\lambda^{\rm sp})^2 - (zD)^2}.$$

This expression has to be evaluated numerically. The results are shown in Fig. 4, where the gap is plotted as a function of U for 1D, 2D, and 3D. In the 2D and 3D cases we found $E_g \sim (U - U_c)^\alpha$ for $U \to U_c$, the exponent α being 1 and 1/2 for 2D and 3D, respectively. In 3D it is easy to obtain an analytical expression for the gap when $U \to U_c$, and the KR dependence is reproduced, i.e., $E_g \propto \sqrt{(U - U_c)}$. For the 2D case the expansion is cumbersome; however, the exponent α can be obtained numerically from Fig. 5, where $\ln E_g$ vs $\ln(U - U_c)$ is shown with the best numerical fit giving $\alpha = 1.0$ within our numerical accuracy. In 1D our approach
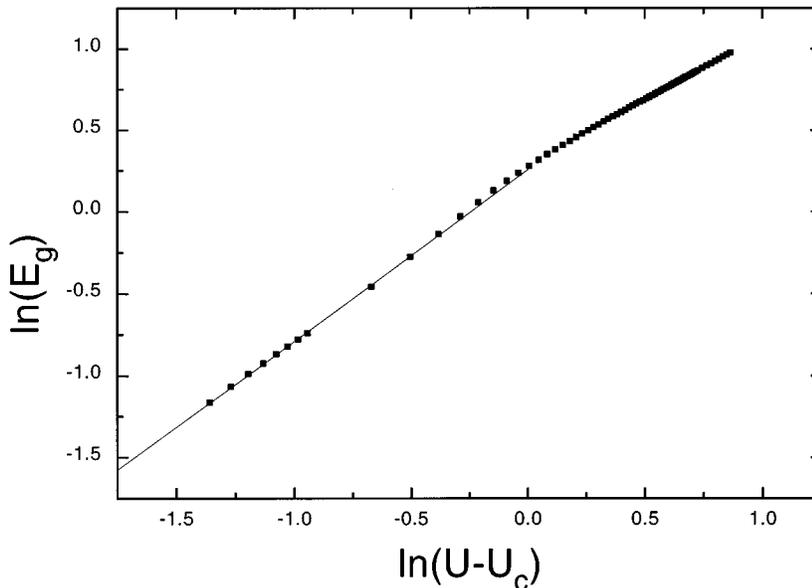

FIG. 5. $\ln(E_g)$ vs $\ln(U - U_c)$ for the 2D case. The line is the best fit of the points with U close to U_c giving an exponent $\alpha = 1.0$.
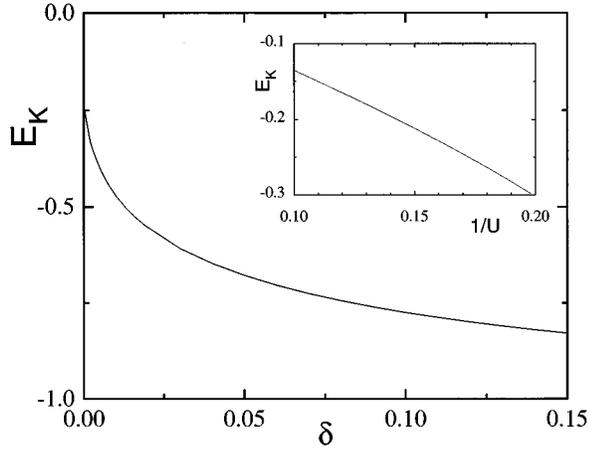
FIG. 6. Kinetic energy E_K as a function of the hole doping δ in 2D for $U=6$. Inset: Kinetic energy at half filling as a function of $1/U$.

gives a nonzero gap for all values of U, including $U=0$. This is a consequence of the fact that our approximation does not reproduce the uncorrelated case. In order to overcome this difficulty fluctuations should be included. However, an interesting point is that, contrary to what happens in the KR treatment, our approach makes apparent the differences between 1D, 2D, and 3D due to the dynamics of the boson fields. Clearly, our results are better than KR's for large U since spin-spin correlations are present even for $U \to \infty$, and are less accurate for small U (notice, however, that we do not include *ad hoc* renormalization factors in this limit).

We have also evaluated the kinetic energy in 2D as a function of doping for $U=6$, that is, above the critical value for the Mott transition at half filling (Fig. 6). There is a cusp at $\delta=1-n=0$ and a steep drop as soon as we dope the system. In particular, the behavior near half filling is given by $E_K(0)-E_K(\delta) \sim \delta^{\alpha(U)}$, with $\alpha(U) \simeq 0.6$ for $U=6$. In the inset to Fig. 6, we show the expected linear behavior of $E_K(0)$ as a function of $1/U$.

IV. CONCLUSIONS

We presented a functional integral formulation for the Hubbard model in terms of boson and fermion fields. Bosons are associated with empty and double-occupancy configurations, while fermions describe single-occupancy states. The formalism preserves the spin-rotation invariance for all occupations and the particle-hole symmetry for one electron *per site*. Furthermore, bosons and fermions are treated on equal footing. In this work we studied the saddle-point approximation of the corresponding functional integral theory.

We found that in 2D and 3D for one electron *per site* there is a metal-insulator transition at a critical value U_c of the on-site interaction. The gap in the one-particle spectrum behaves as $E_g \propto (U-U_c)^\alpha$ for $U \to U_c$, with an exponent $\alpha=1$ and $1/2$ for 2D and 3D, respectively. In our approximation, for the half-filling case the double occupation is always different from zero. For $U<U_c$ there is a condensation of bosons with a macroscopic $\mathbf{k}=\mathbf{0}$ contribution to the number of empty and double occupancy. For $U>U_c$ the double occupancy occurs due to the fluctuations of the vacuum, which are responsible for the antiferromagnetic correlations of the insulating state. These short-range magnetic correlations give a correction to the ground state energy which is always lower than zero. For large U the spin-spin correlation saturates and becomes U independent; in this limit the energy goes as $1/U$ in agreement with the canonical transformation that maps the Hubbard Hamiltonian onto the Heisenberg model.

In order to treat fermions and bosons in an equivalent way, we did not introduce a renormalization of the hopping matrix elements with an operator z as in the KR formalism. The price we paid is that the noninteracting case is not reproduced exactly. However, our results give a better description in the intermediate and large U limit.

We expect the introduction of Gaussian fluctuations above the saddle-point values should bring our results more in line with the exact ones. In particular, preliminary calculations in 1D give a remarkable good agreement with the exact energy shown in the inset of Fig. 1, especially for large U. These results will be presented in a forthcoming publication.

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[12] Notice that by using the constraint (8) the total charge can be written $Q=q_e \Sigma_i(e_i^\dagger e_i - d_i^\dagger d_i)$, that is, it can be assigned entirely to the bosons. Since the Hamiltonian (15) pairs e and d particles with opposite charges in its ground state, only the charged condensate can respond to an static electric field. Consequently, the existence of a boson condensate is a necessary condition to have a metallic phase.