

On the correct continuum limit of the functional-integral representation for the four-slave-boson approach to the Hubbard model: Paramagnetic phase

E. Arrigoni *

Max-Planck-Institut für Physik Complexer Systeme, D-70569 Stuttgart, Fed. Rep. Germany

G.C. Strinati †

Dipartimento di Fisica, III Università di Roma, I-00146 Roma, Italy

The Hubbard model with finite on-site repulsion U is studied via the functional-integral formulation of the four-slave-boson approach by Kotliar and Ruckenstein. It is shown that a correct treatment of the continuum imaginary time limit (which is required by the very definition of the functional integral) modifies the free energy when fluctuation ($1/N$) corrections beyond mean-field are considered, thus removing the inconsistencies originating from the incorrect handling of this pathologic limit so far performed in the literature. In particular, our treatment correctly restores the decrease of the average number of doubly occupied sites for increasing U . Our analysis requires us to suitably interpret the Kotliar and Ruckenstein choice for the bosonic hopping operator and to abandon the commonly used normal-ordering prescription, in order to obtain meaningful fluctuation corrections. In this way we recover the exact solution at $U = 0$ not only at the mean-field level but *also* at the next order in $1/N$. In addition, we consider alternative choices for the bosonic hopping operator and test them numerically for a simple two-site model for which the exact solution is readily available for any U . We also discuss how the $1/N$ expansion can be formally generalized to the four-slave-boson approach, and provide a simplified prescription to obtain the additional terms in the free energy which result at the order $1/N$ from the correct continuum limit.

PACS numbers : 71.30.+h, 05.30.-d, 71.10.+x

I. INTRODUCTION

The Hubbard model (with its variations) is often adopted to represent the essential correlations among electrons (holes) in a lattice, especially in the intermediate- and strong-coupling regimes (relevant to heavy-fermion and high-Tc materials). In these regimes, the use of conventional many-body techniques (that rely on expansions in terms of the on-site repulsion U) becomes questionable and alternative non-perturbative methods are required.¹ Specifically, in the strong-coupling limit the need for *projecting out* the electronic configurations with double occupancy at any given site acquires the role of a “constraint” which has to be enforced for a correct description of correlations. Special methods have accordingly been developed to satisfy the local constraints in the strong-coupling limit.²

In particular, slave-boson representations have been introduced to allow for field-theoretical treatments of strong correlations with constraints, amounting to a projection method that employs auxiliary (or “slave”) bosonic particles.³ While in the original version slave bosons were referring only to empty and doubly occupied states at any given lattice site, the method was later extended by Kotliar and Ruckenstein⁴ (KR) who assigned slave bosons also to the singly-occupied states. The KR four-slave-boson method maps the physical fermion (destruction) operator $\tilde{f}_{i,\sigma}$ with spin σ at site i onto the product of a (pseudo) fermion $f_{i,\sigma}$ with the same spin and of a bosonic operator $z_{i,\sigma}$ (see below), and is especially suited to deal with the Hubbard model for *any* U . The KR method is also particularly appealing for the treatment of magnetic problems, which can be approached already at the mean-field-level owing to the presence of the single-occupancy bosons. For these reasons the KR method has been adopted to treat several problems, both at its mean-field level⁵ and with the inclusion of fluctuation corrections,⁶ by relying on a functional-integral formulation which is ideally suited to implement the local constraints for slave bosons.⁷ Specifically, it has been found that the KR mean-field solution gives remarkable agreement with more elaborate Monte Carlo results over a wide

*Present address: Institut für Theoretische Physik, Universität Würzburg, D-97074 Würzburg, Germany

†Present address: Dipartimento di Matematica e Fisica, Università di Camerino, I-62032 Camerino, Italy

range of interactions and particle densities.⁸ This success is not entirely surprising since the KR (paramagnetic) mean-field solution has been modeled after the Gutzwiller results and thus is identical to the Gutzwiller approximation⁹ (the latter having been further shown recently to become exact in infinite dimensions¹⁰). The KR finding that the Gutzwiller results can be recovered without explicit wave functions has then prompted the hope to improve the theory systematically by the inclusion of fluctuation corrections, using the KR saddle-point solution as a good starting point.

The use of the KR four-slave-boson method was for us originally motivated by the interest in describing the magnetic properties of CuO₂ layers with an itinerant approach in the limit of large repulsion U_d at Cu sites. Antiferromagnetic calculations at the mean-field level within a three-band Hubbard model with $U_d \approx \infty$ (where the double occupancy boson does not enter) were actually quite promising.¹¹ However, our attempts to include fluctuations along the lines of Refs.⁶ and⁷ met with inconsistencies, leading to an instability of our previous mean-field results. Further consideration of the single-band Hubbard model with *finite* U did not remove the unpleasant features of fluctuation calculations (for instance, the average number of doubly occupied sites away from “half filling” was found to unphysically increase for increasing U with the inclusion of fluctuations). We were thus unavoidably led to conclude that there was something *systematically* wrong in the standard procedure adopted in the literature to include fluctuation corrections within the KR method.

About at the same time Jolicoeur and Le Guillou¹² signaled the occurrence of additional inconsistencies when including fluctuation corrections within the KR method at $U = 0$, and proposed to modify the bosonic hopping operator z mentioned above at each order in the loop expansion (without suggesting, however, any explicit form of z even at the one-loop order).

On the other hand, it was soon clear that the inconsistencies found when including fluctuations were not limited to the KR four-slave-boson method (and thus to the presence of the operator z whose choice is to a large extent arbitrary). In fact, Emery and coworkers¹³ have shown that inconsistencies arise when including fluctuations even in the simpler $U = \infty$ one-slave-boson problem (where only the empty boson appears), which is free from the arbitrariness related to the operator z . This result then suggested that the origin of the problems was in the slave-boson approach itself, irrespective of its particular version.

The solution to these problems was obtained eventually by deeper examination of the functional-integral formulation on which slave-boson methods rely. Specifically, it turned out that the *continuum* imaginary time *limit* of the functional-integral representation of the partition function had been incorrectly implemented beyond the mean-field level in the slave-boson literature, by performing the continuum limit in the action at the outset. By doing so, the bosonic commutators were not properly represented in the functional integral, a shortcoming which turns out to be crucial in the presence of (slave-) boson condensates. The peculiarities of the continuum imaginary time limit within a coherent-state functional-integral approach in the presence of a slave-boson condensate have been originally demonstrated in the context of the simpler $U = \infty$ one-slave-boson problem.¹⁴ In the present paper we concentrate on the implications of taking the correct continuum limit with the four-slave-boson method, which prove to be nontrivial due to the presence of the bosonic operator z . A short preliminary version of the results presented here can be found in Ref.¹⁵

Taking the continuum time limit at the end of the calculation is actually a well-established procedure for Feynman’s path integrals.¹⁶ On the other hand, for the functional integrals based on the coherent-state representation it has been common practice to consider the continuum limit at the outset, although warnings have been given that this procedure might lead to inconsistencies.¹⁷ Taking the continuum limit at the outset considerably simplifies the calculations, by making the expression of the action more manageable and allowing for the use of standard Matsubara techniques developed for the diagrammatic Green’s functions approach.¹⁸ Conversely, keeping a finite imaginary time mesh until the end of the calculation requires one to reconsider the Matsubara techniques for a finite set of (fermionic or/and bosonic) frequencies. Although this task has been avoided in the previous slave-boson literature, our work^{14,15} demonstrates unambiguously that, in the presence of bosonic condensates, it is necessary to preserve the discretized form of the action until the end of the calculation when resorting to a coherent-state functional-integral representation of the partition function. In fact, proper account of the discretized nature of the functional integral yields *additional terms* for the free energy when including fluctuations, which would otherwise be missed by taking the continuum limit at the outset.

Concerning further the KR four-slave-boson method, the presence of several bosons and of the bosonic operator z makes unavoidably the derivation of the above additional terms more involved than for the one-slave-boson method considered in Ref.¹⁴. These additional terms turn out to be essential for both methods to heal the inconsistencies found in the literature when taking the continuum limit at the outset. In the present paper we derive in detail these additional terms for the four-slave-boson method with a *generic* form of z . In particular, we will show that the form of the bosonic operator z proposed by Kotliar and Ruckenstein (which, for the sake of a direct mapping onto a functional-integral formulation, has been invariably interpreted in the literature within a normal-ordering prescription and which will be referred to as z_{KR} in the following) leads to inconsistencies when including fluctuations even by taking carefully the continuum limit at the end of the calculation.¹⁵ Nonetheless, we will also show that

these inconsistencies can be overcome by suitably relaxing the normal-ordering prescription on the KR choice for the bosonic operator z . In this way, the preliminary results presented in Ref.¹⁵ are extended and improved. In particular, this form of z without the normal-ordering prescription (which we shall refer to as z_{SQ}) turns out to reproduce the correct independent-particle solution at $U = 0$ not only at the mean-field level but *also* with the inclusion of the $1/N$ corrections. (Numerical results will be considered in the zero-temperature limit only throughout this paper). In addition, we shall consider for comparison two alternative forms of z (different from z_{KR} and z_{SQ}) which are also free from the inconsistencies occurring for z_{KR} . Specifically, we will consider a “linearized” form z_{LIN} which preserves, by construction, the KR mean-field solution at “half filling” of the paramagnetic band for any value of U and also strongly suppresses the contribution of fluctuations to the free energy at $U = 0$ (although not completely and at “half filling” only). Our finding that the results obtained for the ground-state energy alternatively with z_{SQ} and z_{LIN} do not differ appreciably for large values of U (say, for $U \gtrsim 4t$) even away from “half filling” hints further that the results obtained with the four-slave-boson method might not depend crucially on the choice of the operator z for practical purposes.

Numerical calculations will be mainly carried out for a one-level two-site model, which avoids the complications due to the spatial structure and keeps those due to the imaginary time discretization of the functional integral which we are mostly interested in. Restriction to a two-site model will enable us to compare our numerical results, obtained within alternative approximations to the functional integral, with the exact solution which is readily available for any value of U and band filling.

The plan of the paper is the following. Section II deals with the formal problems related to the correct functional-integral formulation of the four-slave-boson method over a discretized imaginary time mesh, and with the peculiar problems related to the choice of the bosonic factor z . The novel terms for the free energy, resulting at the Gaussian level from taking the continuum limit of the functional integral only at the end of the calculation, are derived in detail for any given form of the bosonic factor z and interpreted by the need of restoring the correct bosonic commutators. Section III presents our numerical calculations with the four-slave-boson method for the ground-state energy of a simple two-site model and compares them with the available exact results for any U and band filling. The results obtained with alternative forms of the bosonic operator z are discussed in this context. Section IV gives our conclusions. Finally, the Appendices contain additional mathematical arguments which are needed for making the material presented in the text self-contained. In particular, Appendix A discusses the $1/N$ expansion for the four-slave-boson method, and Appendix C recovers within the “Cartesian” gauge the additional terms for the free energy (which were derived in the text within the “radial” gauge). The problem of obtaining the additional terms (due to a correct handling of the continuum limit of the functional integral) also for the correlation functions (and not only for the free energy) is briefly discussed in this context.

II. FUNCTIONAL-INTEGRAL FORMULATION OF THE FOUR-SLAVE-BOSON METHOD

In this Section, we discuss the procedure to formulate the four-slave-boson method via the coherent-state functional-integral representation of the partition function, by keeping the discretized imaginary time mesh (which is required by the very definition of the functional integral) until the end of the calculation. Specifically, we will demonstrate at the Gaussian level that this correct procedure yields additional terms for the free energy, which were missed in the previous literature when the continuum limit of the functional integral was taken incorrectly in the effective action at the outset. By doing so, we extend to the four-slave-boson method the results obtained in Ref.¹⁴ for the simpler $U = \infty$ one-slave-boson problem. Mastering the formal apparatus with a discretized time mesh, however, is now unavoidably more involved.

For the sake of definiteness, we consider the single-band Hubbard Hamiltonian

$$H = t \sum_{i, \Delta, \sigma} \tilde{f}_{i, \sigma}^\dagger \tilde{f}_{i+\Delta, \sigma} + U \sum_i \tilde{f}_{i, \uparrow}^\dagger \tilde{f}_{i, \uparrow} \tilde{f}_{i, \downarrow}^\dagger \tilde{f}_{i, \downarrow} \quad (1)$$

with on-site repulsion U , where σ is a spin label and Δ runs over the “star” of nearest neighbors to site i in a two-dimensional square lattice of \mathcal{N} sites. Extension of the following arguments to more complex lattices with multi-band structures and to off-site repulsive terms should, in principle, be straightforward.

As mentioned in the Introduction, an essential requirement on any method for an approximate solution of (1) in the strong-coupling regime ($U \gg t$) is that double occupancy at a given site is properly treated. To this end, suppression of double occupancy in the limit $U/t \rightarrow \infty$ acquires the role of a “constraint” for the many-body problem, whose enforcement poses no problem for systems of small size but is difficult to implement for an infinite system. In this case, the introduction of auxiliary variables in the form of slave bosons, which keep track of the occupancy at any given lattice site, looks particularly convenient for enforcing the “constraint”.

A. THE FOUR-SLAVE-BOSON METHOD

For any given U , Kotliar and Ruckenstein⁴ have mapped the physical fermion operator $\tilde{f}_{i,\sigma}$ in Eq. (1) onto the product $f_{i,\sigma} z_{i,\sigma}$ of a (pseudo) fermion $f_{i,\sigma}$ and of a bosonic operator $z_{i,\sigma}$ (at any given site). In its *simplest* version $z_{i,\sigma}$ has the form

$$z_{i,\sigma} = z_{i,\sigma}^0 = s_{i,-\sigma}^\dagger d_i + e_i^\dagger s_{i,\sigma}, \quad (2)$$

where the bosonic destruction operators e_i , $s_{i,\sigma}$, and d_i refer to empty, singly, and doubly occupied states (in the order) at site i . To establish a one-to-one correspondence between the original Fock space and the enlarged one which contains also the bosonic states, the following constraints must be satisfied:

$$d_i^\dagger d_i + \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma} + e_i^\dagger e_i = 1 \quad (3a)$$

$$f_{i,\sigma}^\dagger f_{i,\sigma} - s_{i,\sigma}^\dagger s_{i,\sigma} - d_i^\dagger d_i = 0. \quad (3b)$$

However, enforcement of the constraints (3) allows for alternative choices of $z_{i,\sigma}$ different from (2). This observation has been exploited by Kotliar and Ruckenstein who have accordingly modified the form (2) as follows

$$z_{i,\sigma} = s_{i,-\sigma}^\dagger R_{i,\sigma} d_i + e_i^\dagger R_{i,\sigma} s_{i,\sigma}, \quad (4)$$

with the requirement that the *subsidiary operator* $R_{i,\sigma}$ acts as the unit operator in the subspace specified by the constraints (3). In particular, Kotliar and Ruckenstein have considered the nonlinear form

$$R_{i,\sigma} = R_{i,\sigma}^{KR} =: R_{i,\sigma}^{SQ} : \quad (5a)$$

$$R_{i,\sigma}^{SQ} = \frac{1}{\sqrt{1 - d_i^\dagger d_i - s_{i,\sigma}^\dagger s_{i,\sigma}} \sqrt{1 - e_i^\dagger e_i - s_{i,-\sigma}^\dagger s_{i,-\sigma}}}, \quad (5b)$$

where $: \mathcal{O} :$ denotes the normal ordering of the operator \mathcal{O} . This expedient has enabled Kotliar and Ruckenstein to recover the Gutzwiller solution for a paramagnetic band in a straightforward way, by considering the mean-field solution whereby each bosonic operator is replaced by its average value. Other forms of $R_{i,\sigma}$ different from the KR choice (5a) are, however, possible in principle. We shall exploit this freedom in the following, and explore also alternative expressions containing the bosonic number operators $e_i^\dagger e_i$, $s_{i,\sigma}^\dagger s_{i,\sigma}$, and $d_i^\dagger d_i$.

B. FUNCTIONAL-INTEGRAL FORMULATION

Functional integrals provide an ideal framework to enforce constraints like (3). This is achieved by introducing a Lagrange multiplier for each constraint (say, λ_i^a and $\lambda_{i,\sigma}^b$ for the constraints (3), in the order). The functional-integral formulation based on coherent states¹⁷ rests on breaking up the (imaginary time) interval $(0, \beta)$ into M steps (where $\beta = 1/(k_B T)$ is the inverse temperature and $M \rightarrow \infty$ eventually),¹⁹ and yields the following expression for the grand-canonical partition function:

$$\begin{aligned} \mathcal{Z} = & \lim_{M \rightarrow \infty} \int \prod_i d\lambda_i^a \left(\prod_{\sigma} d\lambda_{i,\sigma}^b \right) \prod_{m=0}^{M-1} d^2 e_{i,m} d^2 d_{i,m} \\ & \times \left(\prod_{\sigma} d^2 s_{i,\sigma,m} d \bar{f}_{i,\sigma,m} d f_{i,\sigma,m} \right) \exp\{-S_M\}, \end{aligned} \quad (6)$$

where m labels the imaginary time steps, (e, s_{σ}, d) are complex boson fields, f and \bar{f} are Grassmann variables, and S_M is the discretized action given by

$$S_M = \delta \sum_{m=0}^{M-1} \sum_i \left(W_{i,m}^{(F)} + W_{i,m}^{(B)} + W_{i,m}^{(FB)} - \lambda_i^a \right). \quad (7)$$

Here, $\delta = \beta/M$ is the elementary time step,

$$W_{i,m}^{(F)} = \frac{1}{\delta} \sum_{\sigma} \bar{f}_{i,\sigma,m} \left[f_{i,\sigma,m} - \left(1 - \delta \lambda_{i,\sigma}^b + \delta \mu \right) f_{i,\sigma,m-1} \right] \quad (8)$$

(μ being the chemical potential) and²⁰

$$\begin{aligned} W_{i,m}^{(B)} = & \frac{1}{\delta} e_{i,m}^* [e_{i,m} - (1 - \delta \lambda_i^a) e_{i,m-1}] \\ & + \frac{1}{\delta} \sum_{\sigma} s_{i,\sigma,m}^* \left[s_{i,\sigma,m} - \left(1 - \delta \lambda_i^a + \delta \lambda_{i,\sigma}^b \right) s_{i,\sigma,m-1} \right] \\ & + \frac{1}{\delta} d_{i,m}^* \left[d_{i,m} - \left(1 - \delta \lambda_i^a + \delta \sum_{\sigma} \lambda_{i,\sigma}^b - \delta U \right) d_{i,m-1} \right], \end{aligned} \quad (9)$$

are functions of the Grassmann variables and of the boson fields, respectively, while

$$W_{i,m}^{(FB)} = t \sum_{\Delta,\sigma} \bar{f}_{i+\Delta,\sigma,m} z_{i+\Delta,\sigma}^* (m-1, m) z_{i,\sigma}(m, m-1) f_{i,\sigma,m-1} \quad (10)$$

is the mixed fermion-boson term which derives from the kinetic term in the Hamiltonian (1) and thus depends explicitly on the form of the bosonic operator $z_{i,\sigma}$. [In the above expressions, the label σ takes the two values ± 1 corresponding to spin $\frac{1}{2}$. A generalized label S which can take $2N$ values (with N positive integer) will be introduced in Appendix A as a formal tool to generate a $1/N$ expansion for the four-slave-boson method].

In the expression (10), $z_{i,\sigma}(m, m-1)$ stands for the matrix element of the operator $z_{i,\sigma}$ between coherent states labeled by imaginary times $\tau_m = m\delta$ (on the left) and $\tau_{m-1} = \tau_m - \delta$ (on the right). When $z_{i,\sigma}$ is taken of the general form (4), this matrix element becomes

$$z_{i,\sigma}(m, m') = [e_{i,m}^* s_{i,\sigma,m'} + s_{i,-\sigma,m}^* d_{i,m'}] R_{i,\sigma}(m, m') \quad (11)$$

where $R_{i,\sigma}(m, m')$ is the matrix element of the subsidiary operator $R_{i,\sigma}$ between coherent states at times m and m' . In particular, when the normal-ordered form (5a) is considered, the above matrix element $R_{i,\sigma}(m, m')$ acquires the simple form:

$$R_{i,\sigma}^{KR}(m, m') = \frac{1}{\sqrt{1 - d_{i,m}^* d_{i,m'} - s_{i,\sigma,m}^* s_{i,\sigma,m'}}} \frac{1}{\sqrt{1 - e_{i,m}^* e_{i,m'} - s_{i,-\sigma,m}^* s_{i,-\sigma,m'}}}. \quad (12)$$

This form with $m = m'$ has been constantly used in the previous literature.²¹ In the more general case when the operator $R_{i,\sigma}$ is not explicitly in normal-ordered form, it should be expressed as a sum of normal-ordered terms by suitably commuting the bosonic operators. In practice, for an operator like (5b) this procedure can be implemented in the context of a $1/N$ expansion, as it will be shown in subsection II E.

As remarked in the Introduction, the functional-integral representation of the partition function requires one to keep, in principle, the discretized imaginary time mesh until the end of the calculation.¹⁷ However, it has been common practice in the slave-boson literature to violate this requirement by taking the continuum ($\delta \rightarrow 0$) limit of the action (7) - (10) at the outset, thus effectively transferring the $M \rightarrow \infty$ limit in Eq. (6) under the integral sign. This procedure removes the distinction between the two time labels m and m' in Eqs. (11) and (12). These seemingly formal considerations acquire relevance from the occurrence of the unphysical results obtained in the continuum limit already at the Gaussian level, as shown in the next Section.

Specifically, we argue that taking the continuum limit at the outset is *pathologic* for the slave-boson problems owing to the presence of the slave-boson condensate, as it was already discussed in detail in Ref.¹⁴ for the $U = \infty$ one-slave-boson problem. Accordingly, the $M \rightarrow \infty$ limit has to be properly taken in Eq. (6) *only at the end of the calculation*. Otherwise, wrong results for the free energy (and derived quantities) are obtained when including fluctuation corrections beyond the saddle-point of the functional integral. As it will be clear from the following analysis, these problems stem from a failure of the functional integral to account for the bosonic commutation rules when the continuum limit is taken at the outset.

C. GAUSSIAN FLUCTUATIONS FOR THE FREE ENERGY WITH A DISCRETIZED TIME MESH

The complex boson fields at each discretized imaginary time τ_m entering the functional integral (6) can be represented, alternatively, either via their amplitude and phase or via their real and imaginary parts. The two representations correspond to the so-called ‘‘radial’’ and ‘‘Cartesian’’ gauges, respectively. In this Section, we adopt the

“radial” gauge to evaluate on the same footing both the conventional “continuum” contribution (which was regularly considered in the previous literature) and the novel contribution resulting from a careful handling of the continuum limit of the functional integral (which we shall name “contribution from infinity” from the range of Matsubara frequencies it originates from). Accordingly, each stage of the calculation reported below will be free from infrared singularities which plague instead the “Cartesian” treatment. However, we shall show in Appendix C that use of the “Cartesian” gauge makes the specific calculation of the “contribution from infinity” somewhat simpler than in the “radial” gauge (at least at the Gaussian level we consider). Comparison of the results obtained for the “contribution from infinity” in the two gauges can also serve as a test of the validity of the $1/N$ expansion for the four-slave-boson method presented in Appendix A.

The boson fields in Eq. (6) are represented via their amplitude and phase, by setting

$$\begin{cases} e_{i,m} &= \tilde{e}_{i,m} \exp\{i\varphi_{i,m}^{(e)}\} \\ s_{i,\sigma,m} &= \tilde{s}_{i,\sigma,m} \exp\{i\varphi_{i,m}^{(s_\sigma)}\} \\ d_{i,m} &= \tilde{d}_{i,m} \exp\{i\varphi_{i,m}^{(d)}\}. \end{cases} \quad (13)$$

It is then convenient to transform the Grassmann fields therein as follows:

$$f_{i,\sigma,m} = \tilde{f}_{i,\sigma,m} \exp\{i(\varphi_{i,m}^{(e)} - \varphi_{i,m}^{(s_\sigma)})\}. \quad (14)$$

Entering Eqs. (13) and (14) in the action (7) - (10) makes the boson phases to appear only in certain combinations. It is then convenient to introduce the following alternative variables

$$\begin{cases} \Lambda_{i,m-1}^a = \frac{i}{\delta} (\varphi_{i,m}^{(e)} - \varphi_{i,m-1}^{(e)}) + \lambda_i^a \\ \Lambda_{i,m-1}^a - \Lambda_{i,\sigma,m-1}^b = \frac{i}{\delta} (\varphi_{i,m}^{(s_\sigma)} - \varphi_{i,m-1}^{(s_\sigma)}) + \lambda_i^a - \lambda_{i,\sigma}^b \\ g_{i,m} = i(\varphi_{i,m}^{(e)} + \varphi_{i,m}^{(d)} - \sum_{\sigma} \varphi_{i,m}^{(s_\sigma)}). \end{cases} \quad (15)$$

In this way, the three phases $\varphi_{i,m}^{(e)}$ and $\varphi_{i,m}^{(s_\sigma)}$ (with $\sigma = \pm 1$) are eliminated in favor of the new variables $\Lambda_{i,m}^a$ and $\Lambda_{i,\sigma,m}^b$, which can be considered as time-dependent Lagrange multipliers. The need of keeping in the functional integral an additional independent variable, like $g_{i,m}$ of Eq. (15), has been already pointed out by Jolicœur and Le Guillou (Ref.¹²) [although in the continuum case], by arguing that $\varphi_{i,m}^{(d)}$ cannot be chosen to make $g_{i,m}$ vanishing for each m . For later convenience, we introduce also the variables

$$\begin{cases} \lambda_{i,m-1}^a &= \frac{i}{\delta} (\varphi_{i,m}^{(e)} - \varphi_{i,m-1}^{(e)}) \\ \lambda_{i,m-1}^a - \lambda_{i,\sigma,m-1}^b &= \frac{i}{\delta} (\varphi_{i,m}^{(s_\sigma)} - \varphi_{i,m-1}^{(s_\sigma)}) \end{cases} \quad (16)$$

which, however, are not linearly independent because

$$\sum_{m=0}^{M-1} \lambda_{i,m}^a = \sum_{m=0}^{M-1} \lambda_{i,\sigma,m}^b = 0. \quad (17)$$

To simplify the notation somewhat, we further introduce the dictionary

$$\begin{aligned} \tilde{e} &\leftrightarrow a^{(1)} = b^{(1)}, & g &\leftrightarrow a^{(5)} = b^{(5)}, \\ \tilde{s}_\uparrow &\leftrightarrow a^{(2)} = b^{(2)}, & \lambda_\uparrow^b &\leftrightarrow a^{(6)} = \lambda^{(1)}, \\ \tilde{s}_\downarrow &\leftrightarrow a^{(3)} = b^{(3)}, & \lambda_\downarrow^b &\leftrightarrow a^{(7)} = \lambda^{(2)}, \\ \tilde{d} &\leftrightarrow a^{(4)} = b^{(4)}, & \lambda^a &\leftrightarrow a^{(8)} = \lambda^{(3)}, \end{aligned} \quad (18)$$

with the understanding that the appropriate site and time (or wave vector and frequency) indices (or arguments) will be indicated whenever necessary. In addition, the notation \underline{a} will stand for the set $\{a^{(\alpha)}; \alpha = 1, \dots, 8\}$, \underline{b} for the set $\{b^{(\beta)}; \beta = 1, \dots, 5\}$, and $\underline{\lambda}$ for the set $\{\lambda^{(l)}; l = 1, \dots, 3\}$.

With the above notation, the terms (8)-(10) of the action (7) can be cast in the form:

$$W_{i,m}^{(F)} = \frac{1}{\delta} \sum_{\sigma} \tilde{f}_{i,\sigma,m} \left[\tilde{f}_{i,\sigma,m} - q^\sigma (\lambda_{i,\sigma,m-1}^b, \lambda_{i,\sigma}^b - \mu) \tilde{f}_{i,\sigma,m-1} \right], \quad (19)$$

$$W_{i,m}^{(B)} = \frac{1}{\delta} \sum_{\beta=1}^4 b_{i,m}^{(\beta)*} \left[b_{i,m}^{(\beta)} - h^\beta(\underline{\Delta}_{i,m-1}, \underline{\Delta}_i, g_{i,m} - g_{i,m-1}) b_{i,m-1}^{(\beta)} \right], \quad (20)$$

and

$$W_{i,m}^{(FB)} = t \sum_{\substack{\bar{f}_{i+\Delta,\sigma,m} \\ \underline{\Delta}, \sigma}} \bar{\rho}^\sigma(\underline{q}_{i+\Delta,m}, \underline{q}_{i+\Delta,m-1}) \rho^\sigma(\underline{q}_{i,m}, \underline{q}_{i,m-1}) \bar{f}_{i,\sigma,m-1} \quad . \quad (21)$$

Here, q^σ , h^β , and ρ^σ ($\bar{\rho}^\sigma$) are functions of the bosonic and λ variables, defined respectively by

$$q^\sigma(\lambda_{i,\sigma,m-1}^b, \lambda_{i,\sigma}^b - \mu) = [1 - \delta(\lambda_{i,\sigma}^b - \mu)] \exp\{-\delta\lambda_{i,\sigma,m-1}^b\}, \quad (22)$$

$$h^1(\underline{\Delta}_{i,m-1}, \underline{\Delta}_i, g_{i,m} - g_{i,m-1}) = [1 - \delta\lambda_i^a] \exp\{-\delta\lambda_{i,m-1}^a\}, \quad (23)$$

$$h^{\frac{5-\sigma}{2}}(\underline{\Delta}_{i,m-1}, \underline{\Delta}_i, g_{i,m} - g_{i,m-1}) = [1 - \delta(\lambda_i^a - \lambda_{i,\sigma}^b)] \exp\{-\delta(\lambda_{i,m-1}^a - \lambda_{i,\sigma,m-1}^b)\}, \quad (24)$$

$$\begin{aligned} h^4(\underline{\Delta}_{i,m-1}, \underline{\Delta}_i, g_{i,m} - g_{i,m-1}) &= [1 - \delta(\lambda_i^a - \sum_{\sigma} \lambda_{i,\sigma}^b) - \delta U] \\ &\times \exp\left\{-\delta(\lambda_{i,m-1}^a - \sum_{\sigma} \lambda_{i,\sigma,m-1}^b) - (g_{i,m} - g_{i,m-1})\right\}, \end{aligned} \quad (25)$$

and

$$\begin{aligned} \rho^\sigma(\underline{q}_{i,m}, \underline{q}_{i,m-1}) &= \exp\{-\delta\lambda_{i,m-1}^a\} \mathcal{R}(n_{i,m}^{(e)}, n_{i,m}^{(s_\sigma)}, n_{i,m}^{(s_{\bar{\sigma}})}, n_{i,m}^{(d)}) \\ &\times \left[\tilde{e}_{i,m} \tilde{s}_{i,\sigma,m-1} + \tilde{s}_{i,\bar{\sigma},m} \tilde{d}_{i,m-1} \exp\{g_{i,m-1} + \delta\lambda_{i,\bar{\sigma},m-1}^b\} \right] \end{aligned} \quad (26)$$

with $\bar{\sigma} = -\sigma$ and

$$\begin{cases} n_{i,m}^{(e)} &= \tilde{e}_{i,m} \tilde{e}_{i,m-1} \exp\{-\delta\lambda_{i,m-1}^a\} \\ n_{i,m}^{(s_\sigma)} &= \tilde{s}_{i,\sigma,m} \tilde{s}_{i,\sigma,m-1} \exp\{-\delta(\lambda_{i,m-1}^a - \lambda_{i,\sigma,m-1}^b)\} \\ n_{i,m}^{(d)} &= \tilde{d}_{i,m} \tilde{d}_{i,m-1} \exp\{-\delta(\lambda_{i,m-1}^a - \sum_{\sigma} \lambda_{i,\sigma,m-1}^b) - (g_{i,m} - g_{i,m-1})\} \end{cases} \quad (27)$$

[$\bar{\rho}^\sigma$ is obtained from ρ^σ by interchanging $b_{i,m}^{(\beta)} \leftrightarrow b_{i,m-1}^{(\beta)}$ ($\beta = 1, \dots, 5$) and then letting $g \rightarrow -g$]. In Eq.(26) it is understood that the *subsidiary function* \mathcal{R} is formally obtained from the subsidiary operator $R_{i,\sigma}$ of Eq.(4) by replacing each bosonic occupation number therein with the corresponding c-number argument (27). This prescription holds provided the subsidiary operator R is written as the normal ordering of a function of the bosonic occupation numbers.

Equations (19)-(27) are still exact. We now proceed and expand the action in powers of the fluctuating fields about a chosen mean-field solution, by setting for the bosonic and *static* λ variables

$$\begin{cases} b_{i,m}^{(\beta)} &= b_0^{(\beta)} + \tilde{b}_{i,m}^{(\beta)} & (\beta = 1, \dots, 5), \\ \lambda_i^{(l)} &= \lambda_0^{(l)} + \tilde{\lambda}_i^{(l)} & (l = 1, \dots, 3). \end{cases} \quad (28)$$

The choice (28) entails a *homogeneous* (i.e., site independent) mean-field solution, which will restrict us in the following to the paramagnetic (or else, to the ferromagnetic) case. It also implies that the mean-field solution is *static* (i.e., time-independent).²² Accordingly, the dynamic variables (16) have, by their definition, vanishing mean-field contribution.²³

We next introduce the space and time Fourier transforms of the fluctuating fields, by setting

$$\tilde{b}_{i,m}^{(\beta)} = \sum_{\mathbf{q}} \sum_{\nu=0}^{BZ} \sum_{\tau_m}^{M-1} e^{i(\mathbf{q} \cdot \mathbf{R}_i - \omega_\nu \tau_m)} b^{(\beta)}(\mathbf{q}, \omega_\nu) \quad (\beta = 1, \dots, 5), \quad (29)$$

$$\tilde{\lambda}_{i,m}^{(l)} \equiv \lambda_{i,m}^{(l)} = \sum_{\mathbf{q}} \sum_{\nu=1}^{BZ} \sum_{m=0}^{M-1} e^{i(\mathbf{q} \cdot \mathbf{R}_i - \omega_\nu \tau_m)} \lambda^{(l)}(\mathbf{q}, \omega_\nu) \quad (l = 1, \dots, 3), \quad (30)$$

and

$$\tilde{\lambda}_i^{(l)} = \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}_i} \lambda^{(l)}(\mathbf{q}, 0) \quad (l = 1, \dots, 3). \quad (31)$$

Here, \mathbf{R}_i is the lattice vector associated to site i , \mathbf{q} is a wave vector restricted to the first Brillouin zone (BZ), $\tau_m = m\delta$ ($m = 0, \dots, M-1$), $\omega_\nu = 2\pi\nu/\beta$ is a bosonic Matsubara frequency, and $\lambda^{(l)}(\mathbf{q}, 0) = \lambda^{(l)}(\mathbf{q}, \omega_\nu = 0)$ by our definition. A similar transformation holds for the Grassmann fields:

$$\tilde{f}_{i,\sigma,m} = \sum_{\mathbf{k}} \sum_{s=0}^{BZ} \sum_{m=0}^{M-1} e^{i(\mathbf{k} \cdot \mathbf{R}_i - \omega_s \tau_m)} f_\sigma(\mathbf{k}, \omega_s) \quad (32)$$

where now $\omega_s = 2\pi(s+1/2)/\beta$ is a fermionic Matsubara frequency. Note that the *range* of the Matsubara frequencies remains *bounded* while keeping the discretized time mesh.²⁴

Expanding the action up to quadratic order in the fluctuating fields requires one to consider the first and second derivatives of the functions (22)-(26) with respect to their arguments. By our convention, each argument may represent either a single variable or a set of variables (in the latter case we shall underline the corresponding symbol). To keep the notation compact, we then introduce the following short-hand notation for the required derivatives. We set:

$$\begin{aligned} q_{0;0}^\sigma &= q^\sigma(x, y) \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}, \\ q_{1;0}^\sigma &= \frac{\partial q^\sigma(x, y)}{\partial x} \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}, \\ q_{0;1}^\sigma &= \frac{\partial q^\sigma(x, y)}{\partial y} \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}, \\ q_{(1,1);0}^\sigma &= \frac{\partial^2 q^\sigma(x, y)}{\partial x^2} \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}, \\ q_{0;(1,1)}^\sigma &= \frac{\partial^2 q^\sigma(x, y)}{\partial y^2} \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}, \\ q_{1;1}^\sigma &= \frac{\partial^2 q^\sigma(x, y)}{\partial x \partial y} \Big|_{x=0, y=\lambda_{\sigma,0}^b - \mu}; \end{aligned} \quad (33)$$

$$\begin{aligned} h_{0;0;0}^\beta &= h^\beta(\underline{X}, \underline{Y}, Z) \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{l;0;0}^\beta &= \frac{\partial h^\beta(\underline{X}, \underline{Y}, Z)}{\partial X^{(l)}} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{0;0;1}^\beta &= \frac{\partial h^\beta(\underline{X}, \underline{Y}, Z)}{\partial Z} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{l;l';0}^\beta &= \frac{\partial^2 h^\beta(\underline{X}, \underline{Y}, Z)}{\partial X^{(l)} \partial Y^{(l')}} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{l;0;1}^\beta &= \frac{\partial^2 h^\beta(\underline{X}, \underline{Y}, Z)}{\partial X^{(l)} \partial Z} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{(l,l');0;0}^\beta &= \frac{\partial^2 h^\beta(\underline{X}, \underline{Y}, Z)}{\partial X^{(l)} \partial X^{(l')}} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \\ h_{0;0;(1,1)}^\beta &= \frac{\partial^2 h^\beta(\underline{X}, \underline{Y}, Z)}{\partial Z^2} \Big|_{\underline{X}=\underline{0}, \underline{Y}=\underline{\lambda}_0, Z=0}, \end{aligned} \quad (34)$$

and so on;

$$\begin{aligned}
\rho_{0;0}^\sigma &= \rho^\sigma(\underline{X}, \underline{Y}) \Big|_{\underline{X}=(\underline{b}_0, \underline{0}), \underline{Y}=(\underline{b}_0, \underline{0})}, \\
\rho_{\alpha;0}^\sigma &= \frac{\partial \rho^\sigma(\underline{X}, \underline{Y})}{\partial X^{(\alpha)}} \Big|_{\underline{X}=(\underline{b}_0, \underline{0}), \underline{Y}=(\underline{b}_0, \underline{0})}, \\
\rho_{\alpha; \alpha'}^\sigma &= \frac{\partial^2 \rho^\sigma(\underline{X}, \underline{Y})}{\partial X^{(\alpha)} \partial Y^{(\alpha')}} \Big|_{\underline{X}=(\underline{b}_0, \underline{0}), \underline{Y}=(\underline{b}_0, \underline{0})}, \\
\rho_{(\alpha, \alpha'); 0}^\sigma &= \frac{\partial^2 \rho^\sigma(\underline{X}, \underline{Y})}{\partial X^{(\alpha)} \partial X^{(\alpha')}} \Big|_{\underline{X}=(\underline{b}_0, \underline{0}), \underline{Y}=(\underline{b}_0, \underline{0})},
\end{aligned} \tag{35}$$

and so on. Similar conventions hold for $\overline{\rho}^\sigma$. In particular, the suffices $\underline{X} = (\underline{b}_0, \underline{0})$ and $\underline{Y} = (\underline{b}_0, \underline{0})$ in Eqs.(35) signify that each bosonic field $b_{i,m}^{(\beta)}$ ($\beta = 1, \dots, 5$) is replaced by the associated mean-field value $b_0^{(\beta)}$, while each *dynamic* $\lambda_{i,m}^{(l)}$ field ($l = 1, \dots, 3$) is replaced by zero.

Expanding at this point the action (7) up to quadratic order in the fluctuating bosonic fields, we obtain the following contributions:

$$S_M = \beta \mathcal{N} [S^{(0)} + S_F^{(0)} + S_F^{(1)} + S^{(2)} + S_F^{(2)}]. \tag{36}$$

Here:

$$S^{(0)} = \lambda_0^a \left(\sum_{\beta=1}^4 b_0^{(\beta)2} - 1 \right) - \sum_{\sigma} \lambda_{\sigma,0}^b (b_0^{(4)2} + b_0^{(\frac{5-\sigma}{2})2}) + U b_0^{(4)2} \tag{37}$$

is the constant (mean-field) value of the bosonic part (9) of the action;

$$S_F^{(0)} = \sum_{\mathbf{k}} \sum_{\sigma} \sum_{s=0}^{M-1} \overline{f}_{\sigma}(\mathbf{k}, \omega_s) e^{i\omega_s \delta} G_0^{\sigma}(\mathbf{k}, \omega_s)^{-1} f_{\sigma}(\mathbf{k}, \omega_s) \tag{38}$$

where

$$G_0^{\sigma}(\mathbf{k}, \omega_s)^{-1} = \frac{(e^{-i\omega_s \delta} - 1)}{\delta} + \varepsilon_{\sigma}(\mathbf{k}) \tag{39}$$

is the single-particle mean-field fermionic Green's function corresponding to the band eigenvalue

$$\varepsilon_{\sigma}(\mathbf{k}) = \lambda_{\sigma,0}^b - \mu + t \rho_{0;0}^{\sigma} \overline{\rho}_{0;0}^{\sigma} \gamma(\mathbf{k}) \tag{40}$$

with

$$\gamma(\mathbf{k}) = \sum_{\Delta} \exp\{-i\mathbf{k} \cdot \Delta\}; \tag{41}$$

$$\begin{aligned}
S_F^{(1)} &= \sum_{\mathbf{q}} \sum_{\nu=0}^{M-1} \sum_{\alpha=1}^8 \sum_{\mathbf{k}} \sum_{\sigma} \sum_{s=0}^{M-1} \overline{f}_{\sigma}(\mathbf{k}, \omega_s) e^{i\omega_s \delta} \mathcal{E}^{(1)}(\mathbf{q}, \omega_{\nu}; \mathbf{k}, \sigma | \alpha) \\
&\quad \times a^{(\alpha)}(\mathbf{q}, \omega_{\nu}) f_{\sigma}(\mathbf{k} - \mathbf{q}, \omega_s - \omega_{\nu})
\end{aligned} \tag{42}$$

where

$$\begin{aligned}
\mathcal{E}^{(1)}(\mathbf{q}, \omega_{\nu}; \mathbf{k}, \sigma | \alpha) &= (1 - \delta_{\nu,0}^K \sum_{l=1}^3 \delta_{\alpha, l+5}^K) \\
&\quad \times t \left[\gamma(\mathbf{k}) \overline{\rho}_{0;0}^{\sigma} (\rho_{0;\alpha}^{\sigma} + e^{-i\omega_{\nu} \delta} \rho_{\alpha;0}^{\sigma}) \right. \\
&\quad \left. + \gamma(\mathbf{k} - \mathbf{q}) \rho_{0;0}^{\sigma} (\overline{\rho}_{0;\alpha}^{\sigma} + e^{-i\omega_{\nu} \delta} \overline{\rho}_{\alpha;0}^{\sigma}) \right] \\
&\quad - (\delta_{\alpha,6}^K \delta_{\sigma,+1}^K + \delta_{\alpha,7}^K \delta_{\sigma,-1}^K) \frac{1}{\delta} \left[(1 - \delta_{\nu,0}^K) q_{1;0}^{\sigma} + \delta_{\nu,0}^K q_{0;1}^{\sigma} \right],
\end{aligned} \tag{43}$$

$\delta_{i,j}^K$ (= 1 when $i = j$ and 0 otherwise) being the Kronecker delta function;

$$S^{(2)} = \sum_{\mathbf{q}} \sum_{\nu=0}^{BZ} \sum_{\alpha, \alpha'=1}^{M-1} a^{(\alpha)}(\mathbf{q}, \omega_\nu) \mathcal{B}(\mathbf{q}, \omega_\nu | \alpha, \alpha') a^{(\alpha')}(-\mathbf{q}, -\omega_\nu) \quad (44)$$

where

$$\begin{aligned} \mathcal{B}(\mathbf{q}, \omega_\nu | \alpha, \alpha') &= \delta_{\alpha, \alpha'}^K \sum_{\beta=1}^4 \delta_{\alpha, \beta}^K \frac{1}{\delta} (1 - e^{-i\omega_\nu \delta} h_{0;0;0}^\alpha) \\ &- \frac{1}{2} \frac{(1 + e^{-i\omega_\nu \delta})}{\delta} \sum_{\beta=1}^4 \delta_{\alpha, \beta}^K b_0^{(\alpha)} \left[\delta_{\alpha', 5}^K (e^{i\omega_\nu \delta} - 1) h_{0;0;1}^\alpha \right. \\ &+ \sum_{l'=1}^3 \delta_{\alpha', 5+l'}^K ((1 - \delta_{\nu, 0}^K) h_{l';0;0}^\alpha + \delta_{\nu, 0}^K h_{0;l';0}^\alpha) \left. \right] \\ &- \frac{1}{2} \frac{(1 + e^{i\omega_\nu \delta})}{\delta} \sum_{\beta'=1}^4 \delta_{\alpha', \beta'}^K b_0^{(\alpha')} \left[\delta_{\alpha, 5}^K (e^{-i\omega_\nu \delta} - 1) h_{0;0;1}^{\alpha'} \right. \\ &+ \sum_{l=1}^3 \delta_{\alpha, 5+l}^K ((1 - \delta_{\nu, 0}^K) h_{l;0;0}^{\alpha'} + \delta_{\nu, 0}^K h_{0;l;0}^{\alpha'}) \left. \right] \\ &- \frac{1}{2\delta} \sum_{\beta=1}^4 b_0^{(\beta)2} \left\{ \sum_{l=1}^3 \delta_{\alpha, 5+l}^K \sum_{l'=1}^3 \delta_{\alpha', 5+l'}^K \right. \\ &\times \left[(1 - \delta_{\nu, 0}^K) h_{(l,l');0;0}^\beta + \delta_{\nu, 0}^K h_{0;(l,l');0}^\beta \right] \\ &+ \sum_{l=1}^3 \delta_{\alpha, 5+l}^K \delta_{\alpha', 5}^K (e^{i\omega_\nu \delta} - 1) h_{l;0;1}^\beta \\ &+ \delta_{\alpha, 5}^K \sum_{l'=1}^3 \delta_{\alpha', 5+l'}^K (e^{-i\omega_\nu \delta} - 1) h_{l';0;1}^\beta \\ &\left. + \delta_{\alpha, 5}^K \delta_{\alpha', 5}^K (e^{i\omega_\nu \delta} - 1) (e^{-i\omega_\nu \delta} - 1) h_{0;0;(1,1)}^\beta \right\}; \quad (45) \end{aligned}$$

$$\begin{aligned} S_F^{(2)} &= \sum_{\mathbf{q}} \sum_{\nu=0}^{BZ} \sum_{\alpha, \alpha'=1}^{M-1} a^{(\alpha)}(\mathbf{q}, \omega_\nu) \left[\sum_{\mathbf{k}} \sum_{\sigma} \sum_{s=0}^{M-1} \bar{f}_\sigma(\mathbf{k}, \omega_s) e^{i\omega_s \delta} \right. \\ &\left. \times \mathcal{E}^{(2)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \sigma | \alpha, \alpha') f_\sigma(\mathbf{k}, \omega_s) \right] a^{(\alpha')}(-\mathbf{q}, -\omega_\nu) \quad (46) \end{aligned}$$

where

$$\begin{aligned} \mathcal{E}^{(2)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \sigma | \alpha, \alpha') &= -\delta_{\alpha, \alpha'}^K (\delta_{\alpha, 6}^K \delta_{\sigma, +1}^K + \delta_{\alpha, 7}^K \delta_{\sigma, -1}^K) \\ &\times \frac{1}{2\delta} \left((1 - \delta_{\nu, 0}^K) q_{(1,1);0}^\sigma + \delta_{\nu, 0}^K q_{0;(1,1)}^\sigma \right) \\ &+ (1 - \delta_{\nu, 0}^K) \sum_{l=1}^3 \delta_{\alpha, 5+l}^K (1 - \delta_{\nu, 0}^K) \sum_{l'=1}^3 \delta_{\alpha', 5+l'}^K \\ &\times \frac{t}{2} \left[\gamma(\mathbf{k}) \rho_{0;0}^\sigma (\bar{\rho}_{(\alpha, \alpha')}^\sigma + \bar{\rho}_{0;(\alpha, \alpha')}^\sigma + \bar{\rho}_{\alpha; \alpha'}^\sigma e^{-i\omega_\nu \delta} + \bar{\rho}_{\alpha'; \alpha}^\sigma e^{i\omega_\nu \delta}) \right. \\ &\left. + \gamma(\mathbf{k}) \bar{\rho}_{0;0}^\sigma (\rho_{(\alpha, \alpha')}^\sigma + \rho_{0;(\alpha, \alpha')}^\sigma + \rho_{\alpha; \alpha'}^\sigma e^{-i\omega_\nu \delta} + \rho_{\alpha'; \alpha}^\sigma e^{i\omega_\nu \delta}) \right] \end{aligned}$$

$$\begin{aligned}
& + \gamma(\mathbf{k} - \mathbf{q}) \left(\overline{\rho}_{\alpha;0}^\sigma \rho_{\alpha';0}^\sigma + \overline{\rho}_{0;\alpha}^\sigma \rho_{0;\alpha'}^\sigma + \overline{\rho}_{\alpha;0}^\sigma \rho_{0;\alpha'}^\sigma e^{-i\omega_\nu \delta} + \overline{\rho}_{0;\alpha}^\sigma \rho_{\alpha';0}^\sigma e^{i\omega_\nu \delta} \right) \\
& + \gamma(\mathbf{k} + \mathbf{q}) \left(\overline{\rho}_{\alpha';0}^\sigma \rho_{\alpha;0}^\sigma + \overline{\rho}_{0;\alpha'}^\sigma \rho_{0;\alpha}^\sigma + \overline{\rho}_{\alpha';0}^\sigma \rho_{0;\alpha}^\sigma e^{i\omega_\nu \delta} + \overline{\rho}_{0;\alpha'}^\sigma \rho_{\alpha;0}^\sigma e^{-i\omega_\nu \delta} \right) \Big]. \tag{47}
\end{aligned}$$

Note that in the action (36) we have not considered the linear term in the bosonic field (which originates from the purely bosonic contribution (9)), since this term cancels at self-consistency by definition.²² In addition, only pairs of fermionic (Grassmann) variables with the *same* \mathbf{k} and ω_s have been retained in the contribution (46), because all other pairs would give a vanishing contribution to the following Gaussian calculation.

The fermionic variables are eliminated at this point by performing the functional integration over the action $S_F^{(0)} + S_F^{(1)} + S_F^{(2)}$ which is quadratic in the fermionic variables. Exponentiating the resulting expression and expanding the exponent up to second order in the fluctuating bosonic fields, we eventually obtain the effective action

$$S_{eff} = \beta \mathcal{N} [S^{(0)} + \overline{S}^{(0)} + S^{(2)} + \overline{S}^{(2)}] \tag{48}$$

where $S^{(0)}$ and $S^{(2)}$ are given by (37) and (44), respectively, and

$$\overline{S}^{(0)} = -\frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} \frac{1}{\beta} \sum_{s=0}^{M-1} \ln[\delta e^{i\omega_s \delta} G_0^\sigma(\mathbf{k}, \omega_s)^{-1}], \tag{49}$$

$$\overline{S}^{(2)} = \sum_{\mathbf{q}} \sum_{\nu=0}^{M-1} \sum_{\alpha, \alpha'=1}^8 a^{(\alpha)}(\mathbf{q}, \omega_\nu) \mathcal{C}(\mathbf{q}, \omega_\nu | \alpha, \alpha') a^{(\alpha')}(-\mathbf{q}, -\omega_\nu), \tag{50}$$

with

$$\begin{aligned}
\mathcal{C}(\mathbf{q}, \omega_\nu | \alpha, \alpha') &= \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} \left\{ f_M(\varepsilon_\sigma(\mathbf{k})) \mathcal{E}^{(2)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \sigma | \alpha, \alpha') \right. \\
& - \frac{1}{2} \mathcal{E}^{(1)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \sigma | \alpha) \Pi_M(\varepsilon_\sigma(\mathbf{k}), \varepsilon_\sigma(\mathbf{k} - \mathbf{q}); \nu) \\
& \left. \times \mathcal{E}^{(1)}(-\mathbf{q}, -\omega_\nu; \mathbf{k} - \mathbf{q}, \sigma | \alpha') \right\} \tag{51}
\end{aligned}$$

[cf. Eqs. (39), (43), and (47)]. In expression (51) we have introduced the Fermi function $f_M(\varepsilon)$ and the fermionic polarization function $\Pi_M(\varepsilon, \varepsilon'; \nu)$, which generalize to the case of the discretized time mesh considered in this paper the familiar functions of the Matsubara Green's functions theory, the latter being recovered in the continuum ($\delta \rightarrow 0$) limit. The expressions of $f_M(\varepsilon)$ and $\Pi_M(\varepsilon, \varepsilon'; \nu)$ are reported in Appendix B.

The free energy is obtained by performing the Gaussian integration over the bosonic variables $\{a^{(\alpha)}(\mathbf{q}, \omega_\nu); \alpha = 1, \dots, 8\}$ with action S_{eff} given by Eq. (48). One obtains (per lattice site):

$$F = F_0 + F_1 \tag{52}$$

with

$$F_0 = S^{(0)} + \overline{S}^{(0)} \tag{53}$$

and

$$\begin{aligned}
F_1 &= \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \frac{1}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \left\{ \ln \det \Gamma(\mathbf{q}, \omega_\nu) - \sum_{\beta=1}^4 \ln(4 b_0^{(\beta)2}) \right. \\
& \left. + (1 - \delta_{\nu,0}^K) \ln \left[\frac{\delta^2}{(1 - e^{i\omega_\nu \delta})(1 - e^{-i\omega_\nu \delta})} \right] \right\}, \tag{54}
\end{aligned}$$

where M has been taken, for convenience, to be an odd integer and the matrix $\Gamma(\mathbf{q}, \omega_\nu)$ has elements [cf. Eqs. (45) and (51)]

$$\begin{aligned}
\Gamma(\mathbf{q}, \omega_\nu)_{\alpha, \alpha'} &= \mathcal{B}(\mathbf{q}, \omega_\nu | \alpha, \alpha') + \mathcal{C}(\mathbf{q}, \omega_\nu | \alpha, \alpha') \\
& + \mathcal{B}(-\mathbf{q}, -\omega_\nu | \alpha', \alpha) + \mathcal{C}(-\mathbf{q}, -\omega_\nu | \alpha', \alpha). \tag{55}
\end{aligned}$$

The first term within braces in Eq. (54) has been obtained by the method discussed in Appendix E, which is required since the relevant Gaussian matrix is not Hermitian. The remaining terms within braces in Eq. (54) originate instead from Jacobian contributions which are specific to the “radial” gauge and are included here for convenience of the following calculation. Note also that the frequency sum in Eq. (54) has been symmetrized between positive and negative values, in order to extract directly its “continuum limit” (see below) according to a theorem reported in Appendix B.

The mean-field contribution F_0 to the (site) free energy given by Eq. (53) does not present any pathology in the $\delta \rightarrow 0$ limit. One obtains the familiar expression for an (effective) system of independent particles

$$\lim_{M \rightarrow \infty} \beta \overline{S}^{(0)} = -\frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma}^{BZ} \ln \left(1 + e^{-\beta \varepsilon_{\sigma}(\mathbf{k})} \right) \quad (56)$$

[cf. Eq. (49)], as shown in Appendix B. The fluctuation contribution F_1 to the (site) free energy, on the other hand, has pathologic behavior in the $\delta \rightarrow 0$ limit owing to the presence of the bosonic frequency sum in Eq. (54). It turns out, in fact, that performing the Matsubara frequency sum with the discretized time mesh (i. e., keeping $|\nu| \leq (M-1)/2$ and taking the $M \rightarrow \infty$ limit only *after* having evaluated the sum) gives a different result from the one obtained by interchanging the continuum limit with the frequency sum. The latter procedure requires standard mathematical techniques and has invariably been considered in the previous slave-boson literature.

The pathologic behavior of a bosonic frequency sum of the type (54) has been discussed in detail in Ref.¹⁴ in the context of the simpler $U = \infty$ one-slave-boson problem. Specifically, it has been proved that this frequency sum can be suitably partitioned into a “continuum limit” contribution (where the $\delta \rightarrow 0$ limit is taken *at the outset* in each term of the sum while the Matsubara index ν is extended from $-\infty$ to $+\infty$) plus a “contribution from infinity” which accounts for what is left out by the continuum limit. For the reader’s convenience, we report in Appendix B the statement of a theorem which shows how the “contribution from infinity” can be extracted for a class of bosonic frequency sums that satisfy certain requirements. For a complete proof of the theorem we refer instead to Appendix B of Ref.¹⁴.

It has been also demonstrated in Ref.¹⁴ in the context of the $U = \infty$ one-slave-boson problem that taking into account the “contribution from infinity” (to the bosonic frequency sum entering the Gaussian correction to the free energy) is not only required at a formal level, but it is also *essential* in practice for validating the $1/N$ expansion for the free energy. In the next Section we will show that taking properly into account the “contribution from infinity” to the sum (54) is essential for obtaining meaningful results at the Gaussian level even for the four-slave-boson case. This will hold in spite of the nontrivial additional complications related to the presence of the subsidiary operator R in Eq. (4).

In essence, the reason why taking the continuum limit at the outset in the frequency sum of Eq. (54) leads to incorrect results, is that the bosonic frequency ω_{ν} enters the relevant fluctuation matrix (55) *only* through the phase factor $\exp\{i\omega_{\nu}\delta\}$. By taking the continuum limit, one effectively regards the argument of this phase factor to be small (i. e., $|\omega_{\nu}|\delta \ll 1$) and accordingly replaces $\exp\{i\omega_{\nu}\delta\} \rightarrow 1 + i\omega_{\nu}\delta$. The flaw of this procedure is that, even in the limit $\delta \rightarrow 0$, $|\omega_{\nu}|\delta$ can be comparable to unity since, by definition, $\omega_{\nu}\delta = 2\pi\nu/M$ ($\nu = -(M-1)/2, \dots, (M-1)/2$) and $\max |\omega_{\nu}\delta| \cong \pi$. The replacement $\exp\{i\omega_{\nu}\delta\} \rightarrow 1 + i\omega_{\nu}\delta$ is thus not allowed to obtain the correct value of the bosonic frequency sum in Eq. (54), and the limit $\delta \rightarrow 0$ can be safely taken therein only *after* having performed the frequency sum.

To be more specific, a bosonic frequency sum of the type (54) can be effectively partitioned into two contributions associated with “small” and “large” frequencies, respectively. The contribution from “small” frequencies (such that $|\omega_{\nu}|\delta \ll 1$) corresponds to the usual continuum limit. The contribution from “large” frequencies (such that $|\omega_{\nu}|\delta$ is of order unity) requires instead expanding the argument of the sum in terms of all δ factors not entering the combination $\exp\{i\omega_{\nu}\delta\}$. Specifically, the contribution from “large” frequencies we are concerned with originates from terms $\mathcal{O}(\delta)$ in this power expansion, since the sum of a large (of order M) number of terms each $\mathcal{O}(\delta)$ yields a finite contribution.

According to the general procedure of Appendix B, extraction of the contribution from “large” frequencies (that we have named “contribution from infinity”) amounts to isolating the function g of Eq. (B10) and to determining its constant term g_0 of the expansion (B9). Whenever the terms in the bosonic sum have simple expressions (as for the $U = \infty$ one-slave-boson problem treated in Ref.¹⁴), extraction of the “contribution from infinity” g_0 can be done analytically with moderate effort. In the present four-slave-boson case, however, the expressions of the matrix elements (55) are exceedingly complicated to handle the sum in Eq. (54) analytically. For this reason, we have developed a computer algorithm for symbolic calculations which (i) evaluates explicitly the quantities (33)-(35) in terms of the bosonic mean-field values $a_0^{(\alpha)}$ ($\alpha = 1, \dots, 8$) and of the parameter δ , (ii) sets up the matrix elements (55), and (iii) performs the steps indicated in Appendix B to extract the “contribution from infinity” g_0 .

In this context, we found it convenient to regularize at the outset the matrix (55) for $\nu \neq 0$ in the limit of small δ , by introducing an auxiliary fluctuation matrix $\overline{\Gamma}$ such that

$$\bar{\Gamma}(\mathbf{q}, e^{i\omega\nu\delta}|\delta)_{\alpha,\alpha'} = \delta^{1-\chi_\alpha-\chi_{\alpha'}} \Gamma(\mathbf{q}, \omega\nu)_{\alpha,\alpha'} \quad (57)$$

where $\chi_\alpha = \sum_{l=1}^3 \delta_{\alpha,5+l}^K$. This definition makes the matrix $\bar{\Gamma}$ and its inverse regular in δ about $\delta = 0$ and implies that $\det \bar{\Gamma} = \delta^2 \det \Gamma$. Accordingly, we write (in matrix notation)

$$\bar{\Gamma}(\mathbf{q}, \zeta|\delta) = \bar{\Gamma}_0(\mathbf{q}, \zeta) + \delta \bar{\Gamma}_1(\mathbf{q}, \zeta) + \mathcal{O}(\delta^2) \quad (58)$$

with $\zeta = \exp\{i\omega\nu\delta\}$, and expand

$$\ln \det \bar{\Gamma} = \text{tr} \ln \bar{\Gamma} = \ln \det \bar{\Gamma}_0 + \delta \text{tr} \left(\bar{\Gamma}_0^{-1} \bar{\Gamma}_1 \right) + \mathcal{O}(\delta^2) \quad (59)$$

provided $\bar{\Gamma}_0$ is nonsingular. For the lowest-order term we obtain

$$\det \bar{\Gamma}_0(\zeta) = (1 - \zeta)(1 - \zeta^{-1}) \prod_{\beta=1}^4 4 b_0^{(\beta)2}, \quad (60)$$

which (together with the factor δ^2 from the transformation (57)) cancels the Jacobian contributions on the right-hand side of Eq.(54) (except for a term $-\frac{1}{2\beta} \ln 4 b_0^{(\beta)2}$ that will be added to the $\nu = 0$ component of the fluctuation matrix). We are thus left with extracting the constant term g_0 from the function

$$g_{\mathbf{q}}(\zeta) = \text{tr} [\bar{\Gamma}_0(\zeta)^{-1} \bar{\Gamma}_1(\mathbf{q}, \zeta)] \quad (61)$$

for any given wave vector \mathbf{q} , according to the prescription discussed in Appendix B.

We eventually obtain the following expression for the ‘‘contribution from infinity’’ to the Gaussian free energy (54):

$$\begin{aligned} F_1^{(d)} &= -2\lambda_0^a + 2\lambda_0^b - \frac{U}{2} - \frac{1}{4} \sum_{\beta=1}^4 \frac{\partial F_0}{\partial b_0^{(\beta)2}} \\ &+ \mathcal{F}[\mathcal{R}; \underline{b}_0] \frac{2t}{\mathcal{N}} \sum_{\mathbf{k}}^{BZ} \gamma(\mathbf{k}) f_F(\varepsilon_{\mathbf{k}}) \end{aligned} \quad (62)$$

which holds specifically for the *paramagnetic* case whereby $\lambda_0^b = \lambda_{\sigma,0}^b$ and $\varepsilon_{\mathbf{k}} = \varepsilon_{\sigma}(\mathbf{k})$ are independent of σ . In Eq. (62), $f_F(\varepsilon)$ is the ordinary Fermi function (which is recovered in the present context as the continuum limit of the function $f_M(\varepsilon)$ - cf. Appendix B), F_0 is given by Eq. (53), and $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ depends on the specific form of the subsidiary operator R in Eq.(4). In particular, $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ vanishes in the simplest case when $R = 1$. In all other cases, $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ depends in a nontrivial way on the subsidiary function \mathcal{R} introduced in Eq. (26) and on its first and second derivatives, which have to be calculated with the arguments (27) taken at the mean-field level. Specifically, $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ can be represented in the compact form:

$$\begin{aligned} \mathcal{F}[\mathcal{R}; \underline{b}_0] &= -2z_0 \left[b_0^{(1)} b_0^{(2)} \left(\frac{\partial \mathcal{R}}{\partial n_1} + \frac{\partial \mathcal{R}}{\partial n_2} + \frac{1}{2} \frac{\partial \mathcal{R}}{\partial n_3} + \frac{1}{2} \frac{\partial \mathcal{R}}{\partial n_4} \right) \right. \\ &+ b_0^{(3)} b_0^{(4)} \left(\frac{1}{2} \frac{\partial \mathcal{R}}{\partial n_1} + \frac{1}{2} \frac{\partial \mathcal{R}}{\partial n_2} + \frac{\partial \mathcal{R}}{\partial n_3} + \frac{\partial \mathcal{R}}{\partial n_4} \right) \\ &\left. + (b_0^{(1)} b_0^{(2)} + b_0^{(3)} b_0^{(4)}) \frac{1}{2} \sum_{\beta=1}^4 b_0^{(\beta)2} \frac{\partial^2 \mathcal{R}}{\partial n_\beta^2} \right]. \end{aligned} \quad (63)$$

In this expression, $\mathcal{R} = \mathcal{R}(n_1, n_2, n_3, n_4)$ with $n_\beta = b_0^{(\beta)2}$ ($\beta = 1, \dots, 4$),

$$z_0 = (b_0^{(1)} b_0^{(2)} + b_0^{(3)} b_0^{(4)}) \mathcal{R}(n_1, n_2, n_3, n_4) \quad (64)$$

is the mean-field value of the bosonic operator $z_{i,\sigma}$ given by Eq. (4), and $b_0^{(2)} = b_0^{(3)}$ for the paramagnetic case we are considering.

Equations (62) and (63) are the main results of this subsection. It will be shown in Appendix C how these results can be obtained alternatively within the ‘‘Cartesian’’ gauge. The reason to work here with the ‘‘radial’’ gauge is that

the resulting “continuum limit ” calculation is free from infrared divergences. In particular, the “continuum limit ” contribution to the Gaussian free energy (54) is given by

$$F_1^{(c)} = \frac{1}{2\beta\mathcal{N}} \sum_{\mathbf{q}} \sum_{\nu=-\infty}^{+\infty} \left\{ \ln \left[\frac{\det \Gamma_c(\mathbf{q}, \omega_\nu)}{\delta_{\nu,0}^K + (1 - \delta_{\nu,0}^K) \omega_\nu^2} \right] - \sum_{\beta=1}^4 \ln(4 b_0^{(\beta)2}) \right\} \quad (65)$$

where $\Gamma_c(\mathbf{q}, \omega_\nu)$ is the continuum ($\delta \rightarrow 0$) limit of the matrix (55).

The physical free energy (per lattice site) at the Gaussian level is then given by [cf. Eq.(52)]

$$F = F_0 + F_1^{(c)} + F_1^{(d)} \quad (66)$$

where $F_1^{(c)}$ and $F_1^{(d)}$ are given by Eqs. (65) and (62), respectively, with each contribution evaluated *at self-consistency* by taking the mean-field values for the bosonic variables \underline{b}_0 . In this way, each term $\partial F_0 / \partial b_0^{(\beta)2}$ in Eq.(62) vanishes.²⁵

The “contribution from infinity ” $F_1^{(d)}$ in Eq. (66) is what has been missed in the previous literature on the four-slave-boson approach to the Hubbard model when considering Gaussian corrections beyond mean field. We have attributed the reason for this omission to an improper handling of the continuum limit of the functional integral. We now argue that the occurrence of $F_1^{(d)}$ is intrinsically related to the need of recovering the correct bosonic commutators within the functional integral.

D. INTERPRETATION OF THE “CONTRIBUTION FROM INFINITY”

The “contribution from infinity ” (62), when taken at self-consistency, can be interpreted in an euristic way by the following argument. Let’s consider first the simplest case when $\mathcal{R} = 1$ (and $\mathcal{F}[\mathcal{R}; \underline{b}_0] = 0$, according to Eq.(63)). In this case, noncommuting bosonic operators enter the Hamiltonian only through the number operators $b^{(\beta)\dagger} b^{(\beta)}$. We argue that taking naively the continuum limit of the action at the outset corresponds effectively to replacing each number operator $b^{(\beta)\dagger} b^{(\beta)}$ in the original Hamiltonian as follows

$$b^{(\beta)\dagger} b^{(\beta)} \rightarrow \frac{1}{2} (b^{(\beta)\dagger} b^{(\beta)} + b^{(\beta)} b^{(\beta)\dagger}) = b^{(\beta)\dagger} b^{(\beta)} + \frac{1}{2} [b^{(\beta)}, b^{(\beta)\dagger}], \quad (67)$$

and then treating the action associated with the modified Hamiltonian correctly (that is, by keeping the discretized time mesh until the end of the calculation). To restore the correct original Hamiltonian, one has thus to *subtract* one half of the commutator $[b^{(\beta)}, b^{(\beta)\dagger}]$ whenever the term $b^{(\beta)\dagger} b^{(\beta)}$ occurs in it. However, since bosonic commutators contribute terms of order at least $1/N$ to the action of the functional integral (cf. Appendix A, in particular Eq. (A3)), one half of each commutator has to be subtracted only when fluctuation ($1/N$) corrections are included. Thus, to the terms

$$\begin{aligned} & \lambda_i^a (e_i^\dagger e_i + \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i) \\ & - \sum_{\sigma} \lambda_{i,\sigma}^b (s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i) + U d_i^\dagger d_i \end{aligned} \quad (68)$$

at a given lattice site in the original Hamiltonian, there corresponds *subtraction* of the terms

$$\lambda_0^a \frac{1}{2} 4 - 2\lambda_0^b \frac{1}{2} 2 + U \frac{1}{2} = 2\lambda_0^a - 2\lambda_0^b + \frac{U}{2} \quad (69)$$

from the Gaussian contribution to the (site) free energy calculated in the continuum limit (in the paramagnetic case). In this way, we can account for the presence of the first three terms on the right-hand side of Eq. (62).

In the general case when $\mathcal{R} \neq 1$ (and $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ is nonvanishing), the last term on the right-hand side of Eq. (62) originates from *additional* noncommuting operators which are present in the bosonic (hopping) operator (4) as soon as the subsidiary operator $R_{i,\sigma}$ is different from unity. In this case, noncommuting bosonic operators enter the Hamiltonian also through more general combinations than the number operators $b^{(\beta)\dagger} b^{(\beta)}$.

Quite generally, we argue that taking the continuum limit of the action at the outset corresponds to replacing the original Hamiltonian operator H by a different operator $Q_c(H)$, obtained by a suitable average over the permutations

of the sequence of creation and destruction bosonic operators defining H . To restore the original operator H , one has then to introduce the difference $C_\infty(H)$ between H and $Q_c(H)$ and set

$$H = Q_c(H) + C_\infty(H) . \quad (70)$$

By construction, the difference $C_\infty(H)$ is expressed in terms of bosonic commutators. It thus contributes to the action only terms of order at least $1/N$. In our case this implies that $C_\infty(H)$ contributes to the Gaussian correction to the free energy only its average value $C_\infty^0(H)$ evaluated at the mean-field level.

We can formulate the following hypotheses on the operator transformation Q_c acting on a generic operator P :

- (i) Q_c is a linear transformation, in the sense that $Q_c(P + P') = Q_c(P) + Q_c(P')$ for any given pair of operators P and P' ;
- (ii) When two operators P and P' refer to “different kinds” of particles (i. e., to different bosons at the same or different sites, or to the same bosons at different sites), then $Q_c(P P') = Q_c(P) Q_c(P')$;
- (iii) If K is a c-number term or a fermionic operator, then $Q_c(KP) = K Q_c(P)$.²⁶

With the above hypotheses, we can restrict ourselves to considering the transformation Q_c acting on a monomial operator P entering the expression of the Hamiltonian operator H , of the form

$$P = b^{\dagger n} b^m \quad (71)$$

(with m and n arbitrary integers) for any given kind b of bosons. Accordingly, we might take Q_c of the form

$$Q_c(b^{\dagger n} b^m) = \frac{1}{n_{\mathcal{P}}} \sum_{\{k\}} \mathcal{P}_k(b^{\dagger n} b^m) \quad (72)$$

where k labels the $n_{\mathcal{P}} = (n+m)!/(n!m!)$ permutations \mathcal{P}_k of the product $b^{\dagger n} b^m$. Alternatively, we could consider the simpler form

$$Q'_c(b^{\dagger n} b^m) = \frac{1}{2}(b^{\dagger n} b^m + b^m b^{\dagger n}). \quad (73)$$

For our purposes, the two operators (72) and (73) are equivalent to each other, since the average (mean-field) values $C_\infty^0(P)$ of the corresponding operators $C_\infty(P)$ differ by terms of order at least $(1/N)^2$ with respect to the average value of $b^{\dagger n} b^m$. In the following, we shall thus consider only the simpler form (73).

To evaluate the average (mean-field) value $C_\infty^0(b^{\dagger n} b^m)$, we exploit the relation

$$[b^\dagger, b^m] = -m b^{m-1} , \quad (74)$$

from which

$$\begin{aligned} b^{\dagger n} b^m &= b^m b^{\dagger n} - \frac{1}{1!} \frac{\partial x^n}{\partial x} \Big|_{x=1} \frac{\partial y^m}{\partial y} \Big|_{y=1} b^{\dagger n-1} b^{m-1} \\ &\quad - \frac{1}{2!} \frac{\partial^2 x^n}{\partial x^2} \Big|_{x=1} \frac{\partial^2 y^m}{\partial y^2} \Big|_{y=1} b^{\dagger n-2} b^{m-2} \\ &\quad - \frac{1}{3!} \frac{\partial^3 x^n}{\partial x^3} \Big|_{x=1} \frac{\partial^3 y^m}{\partial y^3} \Big|_{y=1} b^{\dagger n-3} b^{m-3} \\ &\quad - \dots . \end{aligned} \quad (75)$$

Thus:

$$b^{\dagger n} b^m = \frac{1}{2} (b^{\dagger n} b^m + b^m b^{\dagger n}) - \frac{nm}{2} b^{\dagger n-1} b^{m-1} - \dots \quad (76)$$

where the remaining terms originating from the commutator (75) have been omitted since they contribute to $C_\infty^0(P)$ at order at least $(1/N)^2$. *At the relevant $1/N$ order*, comparison of Eq. (76) with Eqs.(70) (written for P in the place of H), (71), and (73) yields eventually

$$C_\infty(b^{\dagger n} b^m) = -\frac{nm}{2} b^{\dagger n-1} b^{m-1} . \quad (77)$$

The corresponding average value C_∞^0 is then obtained from Eq. (77) by replacing b and b^\dagger by their mean-field value b_0 .

With the monomial (71) we can construct the generic (normal-ordered) operators of interest, namely,

$$: f(b^\dagger b) : = \sum_{n=0}^{\infty} f_n b^{\dagger n} b^n, \quad (78)$$

$$: b^\dagger f(b^\dagger b) : = \sum_{n=0}^{\infty} f_n b^{\dagger n+1} b^n, \quad (79)$$

$$: f(b^\dagger b) b : = \sum_{n=0}^{\infty} f_n b^{\dagger n} b^{n+1}. \quad (80)$$

The corresponding values of C_∞^0 are, in the order:

$$\begin{aligned} C_\infty^0(: f(b^\dagger b) :) &= - \sum_{n=1}^{\infty} f_n \frac{n^2}{2} b_0^{2(n-1)} \\ &= - \frac{1}{2} (f'(b_0^2) + b_0^2 f''(b_0^2)), \end{aligned} \quad (81)$$

$$\begin{aligned} C_\infty^0(: b^\dagger f(b^\dagger b) :) &= -b_0 \sum_{n=1}^{\infty} f_n \frac{(n+1)n}{2} b_0^{2(n-1)} \\ &= - \frac{b_0}{2} (2f'(b_0^2) + b_0^2 f''(b_0^2)), \end{aligned} \quad (82)$$

$$C_\infty^0(: f(b^\dagger b) b :) = C_\infty^0(: b^\dagger f(b^\dagger b) :) \quad (83)$$

where we have assumed the series $\sum_{n=0}^{\infty} f_n x^n$ to represent the analytic function $f(x)$.

Thus far we have considered a single kind of bosons. For different kinds of bosons, C_∞^0 can be evaluated by exploiting the following property. Given two operators P_a and P_b referring to bosons a and b , respectively, hypothesis (ii) above together with the definition (70) imply the identity:

$$\begin{aligned} C_\infty(P_a P_b) &= P_a P_b - Q_c(P_a) Q_c(P_b) \\ &= P_a P_b - (P_a - C_\infty(P_a))(P_b - C_\infty(P_b)) \\ &= P_a C_\infty(P_b) + C_\infty(P_a) P_b - C_\infty(P_a) C_\infty(P_b). \end{aligned} \quad (84)$$

Taking the average value of both sides of Eq. (84), we obtain at the leading order in $1/N$

$$C_\infty^0(P_a P_b) = \langle P_a \rangle_0 C_\infty^0(P_b) + \langle P_b \rangle_0 C_\infty^0(P_a) \quad (85)$$

where $\langle P \rangle_0$ signifies that the average value of P is evaluated at the mean-field level.

The compound operators of interest are of the form

$$: f(a^\dagger, a, b^\dagger, b) := \sum_{m,n} f_{mn} : a^{\dagger \mu} a^\nu (a^\dagger a)^m (b^\dagger b)^n b^{\dagger \rho} b^\tau : \quad (86)$$

where the integers μ, ν, ρ , and τ can take the values 0 and 1. In particular, when $\mu = \nu = \rho = \tau = 0$ we obtain from Eqs. (85) and (77):

$$\begin{aligned} C_\infty^0(: f(a^\dagger a, b^\dagger b) :) &= \sum_{m,n} f_{mn} (a_0^{2m} C_\infty^0(b^{\dagger n} b^n) + b_0^{2n} C_\infty^0(a^{\dagger m} a^m)) \\ &= - \frac{1}{2} \sum_{m,n} f_{mn} \left[x^m \left(\frac{\partial}{\partial y} + y \frac{\partial^2}{\partial y^2} \right) y^n + y^n \left(\frac{\partial}{\partial x} + x \frac{\partial^2}{\partial x^2} \right) x^m \right]_{x=a_0^2, y=b_0^2} \\ &= - \frac{1}{2} \left[\left(\frac{\partial}{\partial x} + x \frac{\partial^2}{\partial x^2} \right) f(x, b_0^2) \Big|_{x=a_0^2} + \left(\frac{\partial}{\partial y} + y \frac{\partial^2}{\partial y^2} \right) f(a_0^2, y) \Big|_{y=b_0^2} \right] \\ &= C_\infty^0(: f(a^\dagger a, b_0^2) :) + C_\infty^0(: f(a_0^2, b^\dagger b) :) \end{aligned} \quad (87)$$

where use has been made of Eq.(81) and of the assumption that the series $\sum_{m,n} f_{mn} x^m y^n$ represents the analytic function $f(x, y)$. By the same token, we obtain for the other cases of Eq.(86):

$$C_\infty^0(: f(a^\dagger, a, b^\dagger, b) :) = C_\infty^0(: f(a_0, a_0, b^\dagger, b) :) + C_\infty^0(: f(a^\dagger, a, b_0, b_0) :) . \quad (88)$$

Extension of Eq. (88) to several kinds of bosons is straightforward.

We are now in a position to reproduce the last term on the right-hand side of Eq.(62). This term turns out to be the C_∞^0 contribution originating from the presence of noncommuting bosonic operators in the kinetic part of the Hamiltonian, which occurs only when nontrivial forms of the subsidiary operator in Eq.(4) are considered (i.e., when $R_{i,\sigma} \neq 1$). According to the above prescriptions, we then obtain for the kinetic part of the Hamiltonian:

$$\begin{aligned} C_\infty^0\left(\frac{t}{\mathcal{N}} \sum_{i,\Delta,\sigma} f_{i,\sigma}^\dagger z_{i,\sigma}^\dagger z_{i+\Delta,\sigma} f_{i+\Delta,\sigma}\right) &= \frac{t}{\mathcal{N}} \sum_{i,\Delta,\sigma} \left\langle f_{i,\sigma}^\dagger f_{i+\Delta,\sigma} \right\rangle_0 C_\infty^0(: z_{i,\sigma}^\dagger z_{i+\Delta,\sigma} :) \\ &= \frac{t}{\mathcal{N}} \sum_{i,\Delta,\sigma} \left\langle f_{i,\sigma}^\dagger f_{i+\Delta,\sigma} \right\rangle_0 z_0 \left(C_\infty^0(: z_{i,\sigma}^\dagger :) + C_\infty^0(: z_{i+\Delta,\sigma} :) \right) \end{aligned} \quad (89)$$

where z_0 is given by Eq.(64). In deriving Eq. (89) we have made use of Eq. (85) and of the fact that, at the order of the $1/N$ expansion we are considering, the fermionic average has to be evaluated with the bosons taken at the mean-field level. Equation (89) further simplifies for the homogeneous and paramagnetic mean-field solution we are restricting to. In this case

$$C_\infty^0(: z_{i,\sigma}^\dagger :) = C_\infty^0(: z_{i+\Delta,\sigma} :) = C_\infty^0(: z_\uparrow :) \quad (90)$$

is independent of i and σ . [It is here understood that the operator z_\uparrow corresponds to a given reference site, say i_0]. We obtain eventually:

$$\begin{aligned} C_\infty^0\left(\frac{t}{\mathcal{N}} \sum_{i,\Delta,\sigma} f_{i,\sigma}^\dagger z_{i,\sigma}^\dagger z_{i+\Delta,\sigma} f_{i+\Delta,\sigma}\right) &= 2z_0 C_\infty^0(: z_\uparrow :) \frac{t}{\mathcal{N}} \sum_{i,\Delta,\sigma} \left\langle f_{i,\sigma}^\dagger f_{i+\Delta,\sigma} \right\rangle_0 \\ &= 2z_0 C_\infty^0(: z_\uparrow :) \frac{2t}{\mathcal{N}} \sum_{\mathbf{k}}^{BZ} \gamma(\mathbf{k}) f_F(\varepsilon_{\mathbf{k}}) \end{aligned} \quad (91)$$

with $\gamma(\mathbf{k})$ given by Eq.(41).

We are thus left with evaluating $C_\infty^0(: z_\uparrow :)$. Taking z_\uparrow of the form [cf. Eq.(4)]

$$z_\uparrow = s_\downarrow^\dagger R_\uparrow d + e^\dagger R_\uparrow s_\uparrow \quad (92)$$

with

$$R_\sigma =: \mathcal{R}(e^\dagger e, s_\sigma^\dagger s_\sigma, s_\sigma^\dagger s_{\bar{\sigma}}, d^\dagger d) : \quad (93)$$

by our conventions, and using Eqs. (81)-(83) and (88), we obtain

$$C_\infty^0(: z_\uparrow :) = C_\infty^0(: s_\downarrow^\dagger R_\uparrow d :) + C_\infty^0(: e^\dagger R_\uparrow s_\uparrow :) \quad (94)$$

where [cf. the dictionary (18)]

$$\begin{aligned} C_\infty^0\left(: s_\downarrow^\dagger R_\uparrow d :\right) &= C_\infty^0\left(b_0^{(3)} : \mathcal{R}(b^{(1)\dagger} b^{(1)}, b_0^{(2)2}, b_0^{(3)2}, b_0^{(4)2}) : b_0^{(4)}\right) \\ &\quad + C_\infty^0\left(b_0^{(3)} : \mathcal{R}(b_0^{(1)2}, b^{(2)\dagger} b^{(2)}, b_0^{(3)2}, b_0^{(4)2}) : b_0^{(4)}\right) \\ &\quad + C_\infty^0\left(: b^{(3)\dagger} \mathcal{R}(b_0^{(1)2}, b_0^{(2)2}, b^{(3)\dagger} b^{(3)}, b_0^{(4)2}) : b_0^{(4)}\right) \\ &\quad + C_\infty^0\left(b_0^{(3)} : \mathcal{R}(b_0^{(1)2}, b_0^{(2)2}, b_0^{(3)2}, b^{(4)\dagger} b^{(4)}) b^{(4)} :\right) \\ &= -\frac{1}{2} b_0^{(3)} b_0^{(4)} \left\{ \left[\frac{\partial}{\partial n_1} + b_0^{(1)2} \frac{\partial^2}{\partial n_1^2} + \frac{\partial}{\partial n_2} + b_0^{(2)2} \frac{\partial^2}{\partial n_2^2} \right] \mathcal{R} \right. \\ &\quad \left. + \left[2 \frac{\partial}{\partial n_3} + b_0^{(3)2} \frac{\partial^2}{\partial n_3^2} + 2 \frac{\partial}{\partial n_4} + b_0^{(4)2} \frac{\partial^2}{\partial n_4^2} \right] \mathcal{R} \right\} \end{aligned} \quad (95)$$

with the same notation used in Eq.(63). The other contribution $C_\infty^0 (: e^\dagger R_\uparrow s_\uparrow :)$ can be obtained from Eq.(95) with the replacement $1 \leftrightarrow 4$ and $2 \leftrightarrow 3$ for the boson indices. Comparison of Eqs. (94) and (95) with Eq.(63) identifies eventually

$$\mathcal{F}[\mathcal{R}; \underline{b}_0] = 2z_0 C_\infty^0 (: z_\uparrow :). \quad (96)$$

This result, in turn, implies that the last term on the right-hand side of Eq.(62) coincides with the C_∞^0 contribution (91) from the kinetic part of the Hamiltonian.

The method that we have here provided to rationalize the ‘‘contribution from infinity’’ (62) might also serve as a practical prescription to avoid the burden of keeping *explicitly* the discretized nature of the functional integral until the end of the calculation.²⁷ This method may thus be useful when considering Hamiltonians different from (1) and more general phases (like magnetic ones). However, extension of this procedure to physical quantities other than the free energy and its derivatives (for instance, to the electronic correlation functions) is not straightforward and requires a separate study. This problem will be touched upon in Appendix C in the framework of the ‘‘Cartesian’’ gauge.

E. EXTENSION TO OPERATORS NOT EXPLICITLY IN NORMAL-ORDERED FORM

Thus far we have considered subsidiary operators $R_{i,\sigma}$ that are *explicitly* written in normal-ordered form. In fact, in subsection II C the normal-ordering prescription entered the operative definition of the subsidiary function \mathcal{R} [cf. the comment following Eq. (27)], while in subsection II D the normal-ordering prescription for all terms in the Hamiltonian was assumed throughout [cf. the main result (96) therein]. Nonetheless, it might be also relevant to consider operators, like $R_{i,\sigma}^{SQ}$ given by Eq.(5b), which are *not* explicitly written in normal-ordered form. For instance, it will result from the numerical calculations presented in the next Section that the choice (5b) remedies the unphysical results obtained with its normal-ordered version (5a).²⁸

It is clear that, when adopting a functional-integral formalism based on coherent states, any non normal-ordered form for $R_{i,\sigma}$ should be preliminarily rearranged into a sequence of normal-ordered terms. In general, this rearrangement might result into hardly manageable expressions (or even into divergent expressions when non polynomial operators like (5b) are adopted). This difficulty can be overcome as follows in the spirit of the $1/N$ expansion considered in this paper.

Let’s consider first the rearrangement of the simple bosonic monomial operator $(b^\dagger b)^n$ into a sequence of normal-ordered terms:

$$(b^\dagger b)^n = \sum_{k=0}^n a_{n,k} : (b^\dagger b)^{n-k} :. \quad (97)$$

It is clear that $a_{n,0} = 1$. A recursive relation can be readily obtained for the other coefficients of the expansion (97):

$$a_{n,k} = a_{n-1,k} + (n-k)a_{n-1,k-1} \quad (98)$$

with the initial conditions $a_{n,n+1} = a_{n,-1} = 0$ and $a_{0,0} = 1$. In particular, Eq. (98) gives for $k = 1$

$$a_{n,1} = \frac{n(n-1)}{2}. \quad (99)$$

Knowledge of coefficients with $k > 1$ is not required at the order $1/N$ we are considering in this paper.

For a general bosonic operator we then write

$$f \left(\frac{b^\dagger b}{N} \right) = \sum_{n=0}^{\infty} f_n \left(\frac{b^\dagger b}{N} \right)^n = \sum_{n=0}^{\infty} \sum_{k=0}^n f_n a_{n,k} \frac{1}{N^n} : (b^\dagger b)^{n-k} :, \quad (100)$$

where the expansion (97) has been used and $b^\dagger b$ has been divided by N according to a standard procedure of the $1/N$ expansion [see Appendix A]. The right-hand side of Eq.(100) admits a direct representation in terms of the functional integral, by mapping $: (b^\dagger b)^q :$ onto $(b_m^* b_{m-1})^q$ in the action for any (positive) integer q . In the spirit of the $1/N$ expansion, we then rescale the bosonic variables b_m by setting $b_m = \sqrt{N} \tilde{b}_m$. The operator (100) is thus mapped in the action onto the series $\sum_{k=0}^{\infty} N^{-k} \tilde{f}^{(k)}(\tilde{b}_m^* \tilde{b}_{m-1})$, where

$$\tilde{f}^{(k)}(x) = \sum_{q=0}^{\infty} f_{k+q} a_{k+q,k} x^q. \quad (101)$$

At the first order in $1/N$, only terms $\bar{f}^{(k)}(x)$ with $k = 0$ and 1 have to be retained in the action. Specifically, the term with $k = 0$ will contribute both to the leading term F_0 of the free energy [cf. Eq. (A10)] and to its $1/N$ correction F_1 [cf. Eq. (A13)], by considering its mean-field value and its Gaussian terms, respectively. The term with $k = 1$ will instead contribute only to F_1 , by considering its mean-field value.²⁹ In this way, the contribution to F_1 of the term with $k = 1$ can be effectively reabsorbed into the “contribution from infinity“ to F_1 originating from the term with $k = 0$. Specifically, it turns out that this contribution simply cancels the term containing the second derivative of f in Eq. (81).

Entering Eq. (99) into Eq. (101) we, in fact, obtain for $\bar{f}^{(1)}(x)$:

$$\bar{f}^{(1)}(x) = \sum_{q=0}^{\infty} f_{1+q} a_{1+q,1} x^q = \frac{1}{2} x f''(x), \quad (102)$$

so that

$$C_{\infty}^0(: f(b^\dagger b) :) + \bar{f}^{(1)}(b_0^2) = -\frac{1}{2} f'(b_0^2) \quad (103)$$

owing to Eq. (81). In Eq. (103) we have consistently replaced the argument of the function $\bar{f}^{(1)}(x)$ by b_0^2 and set $N = 1$ eventually. Generalization of the above results to the case of several bosons is straightforward.

In conclusion, for an operator $R_{i,\sigma}$ not *explicitly* in normal-ordered form the above considerations have the effect of modifying the factor $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ in Eq. (62), by (i) dropping the last terms in Eq. (63) containing the second derivatives of \mathcal{R} and (ii) interpreting the function \mathcal{R} in the remaining terms in Eq. (63) (as well as in the expression for the continuum part of the fluctuations) as being associated with $: R_{i,\sigma} :$, i.e., with the normal-ordered component of $R_{i,\sigma}$.

It will be shown in the next Section that, when specified to $R_{i,\sigma}^{SQ}$, the above prescription succeeds in eliminating the unpleasant features occurring for its normal-ordered version $R_{i,\sigma}^{KR}$ [cf. Eq. (5a)]. Namely, it eliminates an unphysical divergence of the ground-state energy when the zero-occupancy limit is approached (making the ground-state energy to correctly vanish in this limit) and completely suppresses the fluctuation corrections to the KR mean-field ground-state energy for $U = 0$ and any filling value.

Finally, we remark that the right-hand side of Eq. (103) could be obtained directly by generalizing the heuristic argument of subsection II D to the case of non normal-ordered operators. To this end, one suitably defines the operator $Q_c(P)$ (and consequently $C_{\infty}(P)$) for a non normal-ordered operator P by extending the “specular” prescription (73), and evaluates C_{∞}^0 accordingly. By this procedure, one is led to interpret the right-hand side of Eq. (103) as the “contribution from infinity ” originating from the non normal-ordered operator $f(b^\dagger b)$.

III. NUMERICAL RESULTS FOR A ONE-LEVEL TWO-SITE MODEL

In the previous Section we have shown that the additional contributions (62) to the Gaussian free energy originate from a careful handling of the continuum time limit of the functional integral. The question naturally arises whether these additional contributions might substantially affect the numerical value of the free energy (and of related physical quantities) in the practical cases of interest, or even modify its behavior in a qualitative way. Specifically, we may inquire whether the additional contributions (62) could serve to overcome the inconsistencies encountered when including Gaussian fluctuations by treating the functional integral in the continuum limit. In this respect, we have found that the *wrong curvature* of the free energy versus U results with the conventional continuum limit treatment, thus producing an unphysical *increase* of the (average) number of doubly occupied sites for increasing U . Additional inconsistencies have been pointed out for the noninteracting ($U = 0$) case in Ref.¹².

In this Section we will show that inclusion of the “contribution from infinity ” (62) indeed succeeds in overcoming the inconsistencies mentioned above. In addition, we will show that relaxing the normal-ordering prescription (5a) of the KR choice for the subsidiary operator, makes the $1/N$ results *coinciding* with the exact (free-particle) solution at $U = 0$ for any filling and number of lattice sites. In this way, the goodness of the KR mean-field solution will not be spoiled by the inclusion of fluctuations.

We shall illustrate the above effects by numerical calculations at a generic value of U for a one-level two-site model, which avoids the complications due to the spatial structure while dealing explicitly with the imaginary time discretization. We expect, however, these effects to hold for a more general multi-site system as well, since the time continuum limit does not depend on the spatial structure [In this respect, we will also present some numerical results for the lattice case when $U = 0$]. The restriction to a two-site model will also enable us to compare the numerical results, obtained within alternative approximations to the functional integral, with the available exact solution discussed in Appendix D.³⁰ In addition, to get a practical insight into the usefulness of a given choice for the bosonic hopping operator z , we compare the results obtained with several alternative choices of z .

A. MEAN-FIELD SOLUTION

At the mean-field level, the free energy (per lattice site) of the paramagnetic solution is given by [cf. Eqs. (53), (37), and (56)]:

$$F_0 = -\frac{1}{\beta} \sum_{p=1}^2 \ln(1 + e^{-\beta \varepsilon_p}) + F_0^{(B)} \quad (104)$$

where

$$F_0^{(B)} = \lambda_0^a (b_0^{(1)2} + 2b_0^{(2)2} + b_0^{(4)2} - 1) - 2\lambda_0^b (b_0^{(2)2} + b_0^{(4)2}) + U b_0^{(4)2} \quad (105)$$

and [cf. Eq. (40)]

$$\begin{cases} \varepsilon_1 = \lambda_0^b - \mu - 2t\rho_0^2 \\ \varepsilon_2 = \lambda_0^b - \mu + 2t\rho_0^2 \end{cases} \quad (106)$$

with the notation

$$\rho_0 = b_0^{(2)} (b_0^{(1)} + b_0^{(4)}) \mathcal{R}(n_1, n_2, n_2, n_4) \quad (107)$$

in the place of z_0 [cf. Eq. (64)]. We have here specified to the two-site model the general expressions reported in Section II for the lattice model, and made use of the paramagnetic *ansatz* $b_0^{(2)} = b_0^{(3)}$.

The parameters $b_0^{(1)}$, $b_0^{(2)}$, $b_0^{(4)}$, λ_0^a , λ_0^b , and μ are determined by minimizing $F_0 + \mu n$ (where n stands for the particle density per lattice site). The resulting mean-field equations are:

$$\frac{\partial F_0}{\partial b_0^{(\beta)}} = 4t(f_F(\varepsilon_2) - f_F(\varepsilon_1))\rho_0 \frac{\partial \rho_0}{\partial b_0^{(\beta)}} + \frac{\partial F_0^{(B)}}{\partial b_0^{(\beta)}} = 0 \quad (\beta = 1, 2, 4), \quad (108)$$

$$\frac{\partial F_0}{\partial \lambda_0^a} = b_0^{(1)2} + 2b_0^{(2)2} + b_0^{(4)2} - 1 = 0, \quad (109)$$

$$\frac{\partial F_0}{\partial \lambda_0^b} = f_F(\varepsilon_1) + f_F(\varepsilon_2) - 2(b_0^{(2)2} + b_0^{(4)2}) = 0, \quad (110)$$

$$-\frac{\partial F_0}{\partial \mu} = f_F(\varepsilon_1) + f_F(\varepsilon_2) = n. \quad (111)$$

In particular, *in the zero-temperature limit* Eq.(111) implies

$$f_F(\varepsilon_1) = 1 \quad , \quad f_F(\varepsilon_2) = n - 1, \quad (112)$$

whenever $n \geq 1$ and ρ_0 is nonvanishing, with the chemical potential jumping from ε_1 to ε_2 across $n = 1$.

At “half filling” (i. e., when $n = 1$) there exists a critical value U_c such that $b_0^{(1)} = b_0^{(4)} = 0$ and $b_0^{(2)} = 1/\sqrt{2}$ for $U \geq U_c$ (and the associated Helmholtz free energy density $F_0 + \mu n$ vanishes in the zero-temperature limit). It can be readily shown from Eqs. (108)-(111) that U_c is given by³¹

$$U_c = 4t\mathcal{R}^2(0, \frac{1}{2}, \frac{1}{2}, 0). \quad (113)$$

In deriving Eq.(113) we have exploited the symmetry properties

$$\mathcal{R}(n_1, n_2, n_2, n_4) = \mathcal{R}(n_4, n_2, n_2, n_1) = \mathcal{R}(n_2, n_1, n_4, n_2) \quad (114)$$

which are satisfied by the choices we shall consider for \mathcal{R} . This transition at $U = U_c$ makes the effective hopping in Eq.(106) vanishing, and it is referred to as a Mott-Hubbard transition.² For the two-site model we are considering this transition is clearly an artifact of the slave-boson approach at the mean-field level, which will be (at least partly) cured by the inclusion of (Gaussian) fluctuations.

For comparison, we also give the results of the conventional Hartree-Fock decoupling. For the one-level two-site model of interest, the Hartree-Fock ground-state energy (per lattice site) in the paramagnetic phase is given by

$$E^{HF} = 2t(f_F(\varepsilon_2^{HF}) - f_F(\varepsilon_1^{HF})) + \left(\frac{n}{2}\right)^2 U \quad (115)$$

where

$$\begin{cases} \varepsilon_1^{HF} = -2t + \frac{n}{2}U - \mu \\ \varepsilon_2^{HF} = 2t + \frac{n}{2}U - \mu \end{cases} \quad (116)$$

with $f_F(\varepsilon_1)$ and $f_F(\varepsilon_2)$ given by Eq. (112) (in the zero-temperature limit for $n \geq 1$). Since ε_p^{HF} ($p = 1, 2$) are independent of U (at fixed particle density), the energy (115) grows linearly without bound for increasing U . Equation (115) also shows that, within the (paramagnetic) Hartree-Fock decoupling, the site probability of double occupancy is given by $(n/2)^2$, irrespective of U . One thus concludes that the (paramagnetic) Hartree-Fock decoupling can be approximately correct only for $U \lesssim t$ (being, in particular, exact when $U = 0$). Numerical comparison of the mean-field ground-state (site) energy $E = F_0 + \mu n$ (in the zero-temperature limit) and of the associated $1/N$ fluctuation results with the Hartree-Fock E^{HF} and with the exact solution will be presented in the following.

B. OVERCOMING THE PROBLEMS ASSOCIATED WITH THE CONTINUUM FLUCTUATIONS BY THE DISCRETIZED FLUCTUATIONS

A naive handling of the functional integral (whereby the continuum limit is taken at the outset) yields, at the Gaussian level, the (site) free energy (66) with the term $F_1^{(d)}$ omitted and $F_1^{(c)}$ given by Eq.(65). In that expression, the continuum fluctuation matrix $\Gamma_c(\mathbf{q}, \omega_\nu)$ is obtained by performing the $\delta \rightarrow 0$ limit of the matrix (55) (with \mathcal{B} and \mathcal{C} given by Eqs.(45) and (51), in the order), i. e., by letting $\delta \rightarrow 0$ *everywhere* δ appears.

In particular, the continuum limit of the matrix \mathcal{B} given by Eq.(45) has elements

$$\begin{aligned} \mathcal{B}_c(\mathbf{q}, \omega_\nu | 1, 1) &= i\omega_\nu + \lambda_0^a, \\ \mathcal{B}_c(\mathbf{q}, \omega_\nu | 1, 2) &= \dots = \mathcal{B}_c(\mathbf{q}, \omega_\nu | 1, 7) = 0, \\ \mathcal{B}_c(\mathbf{q}, \omega_\nu | 1, 8) &= \mathcal{B}_c(\mathbf{q}, \omega_\nu | 8, 1) = b_0^{(1)}, \end{aligned} \quad (117)$$

and so on; the continuum limit of the factors $\mathcal{E}^{(1)}$ entering the expression (51) for the matrix \mathcal{C} is given by

$$\begin{aligned} \mathcal{E}_c^{(1)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \uparrow | \beta) &= tz_0(\gamma(\mathbf{k}) + \gamma(\mathbf{k} - \mathbf{q})) \frac{\partial z_0}{\partial b_0^{(\beta)}}, \quad (\beta = 1, \dots, 4) \\ \mathcal{E}_c^{(1)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \uparrow | 5) &= tz_0 \mathcal{R}(\gamma(\mathbf{k}) - \gamma(\mathbf{k} - \mathbf{q})) b_0^{(2)} b_0^{(4)}, \end{aligned} \quad (118)$$

and so on (with z_0 given by Eq. (64)); the continuum limit of the factors $\mathcal{E}^{(2)}$ entering the expression (51) for the matrix \mathcal{C} is given by

$$\frac{1}{2} \sum_{\sigma} \mathcal{E}_c^{(2)}(\mathbf{q}, \omega_\nu; \mathbf{k}, \sigma | 1, 1) = \frac{t}{2} \left[2z_0 \frac{\partial^2 z_0}{\partial b_0^{(1)2}} \gamma(\mathbf{k}) + \left(\frac{\partial z_0}{\partial b_0^{(1)}} \right)^2 (\gamma(\mathbf{k} - \mathbf{q}) + \gamma(\mathbf{k} + \mathbf{q})) \right], \quad (119)$$

and so on.³² Finally, the continuum limit of the Fermi function $f_M(\varepsilon)$ and of the polarization function $\Pi_M(\varepsilon, \varepsilon'; \nu)$ entering the expression of the matrix \mathcal{C} are given in Appendix B.

The above expressions hold for a general lattice model. The two-site model that we consider for numerical calculations is recovered by restricting the wave vectors to the two values 0 and $\pi/|\Delta|$.³⁰

Proper handling of the functional integral (with the continuum limit taken only at the end of the calculation) adds to the continuum limit (site) free energy $F_0 + F_1^{(c)}$ the ‘‘contribution from infinity’’ $F_1^{(d)}$ given by Eq. (62) with the appropriate form (63) for $\mathcal{F}[\mathcal{R}; \underline{b}_0]$, with or without the terms containing the second derivatives depending on the ordering prescription (cf. subsection II E). Our purpose here is to demonstrate to what extent the contribution $F_1^{(d)}$ modifies the free energy in a quantitative and even in a qualitative way, using the two-site model as a simple prototype system. In this way, the contribution $F_1^{(d)}$ will prove to be important also from a practical point of view.

To proceed further, we have to select an *explicit* form for the subsidiary operator $R_{i,\sigma}$ introduced in Eq.(4). The choice commonly adopted in the four-slave-boson literature is the original KR choice (5a). The associated subsidiary function introduced in Eq.(26) takes the form

$$\mathcal{R}^{KR}(n_e, n_\sigma, n_{\bar{\sigma}}, n_d) = \frac{1}{\sqrt{1 - n_e - n_{\bar{\sigma}}}\sqrt{1 - n_d - n_\sigma}}, \quad (120)$$

which recovers at the mean-field level the (paramagnetic) Gutzwiller approximation for the lattice Hubbard Hamiltonian at any band filling.⁴ However, it will turn out that the normal-ordering prescription leads to results which markedly depart from the free-particle solution at $U = 0$ *even* when the “contribution from infinity” is properly included. In addition, this prescription leads to a divergent free energy in the zero-occupancy limit. These shortcomings can be remedied by suitably relaxing the normal-ordering prescription, as shown in the next subsection.

Figure 1 compares the ground-state energy per lattice site (in units of t) for the one-level two-site model versus U/t at “half filling” ($n = 1.0$) and at $n = 1.2$, as obtained from the exact solution of Appendix D and from alternative (paramagnetic) approximations to the four-slave-boson method with the KR form (5a) for $R_{i,\sigma}$.³³ The Hartree-Fock result (115) is also shown for comparison (HF). The KR mean-field solution (KR) is seen to be in good agreement with the exact solution (EX) for both doping values, while the fluctuation results considerably worsen this agreement *regardless* they are obtained by the incorrect continuum (CFL) or by the correct discretized (DFL) time limiting procedure in the functional integral (i. e., without and with the inclusion of the term $F_1^{(d)}$ of Eq. (66)). The HF result, on the other hand, is in agreement with the exact solution only for small values of U (say, when $U \lesssim 5t$). Note from Fig.1a that at “half filling” both the CFL and DFL curves terminate at a critical value of U ($\cong 6.8t$) where an antiferromagnetic instability develops at the mean-field level, thus preventing the inclusion of paramagnetic fluctuations. Note also the arrow which locates the critical value U_c/t corresponding to the Mott-Hubbard transition for the KR mean-field solution (the choice (120) for \mathcal{R} gives $U_c/t = 16$ according to Eq.(113)).

We conclude from Fig.1 that, with the KR choice (5a) for $R_{i,\sigma}$, the DFL results can be even worse than the CFL results, as they depart from the exact solution more than the mean-field results. This finding could appear surprising, since one would expect a more complete treatment of the functional integral to produce better results. That this is not the case with the KR choice (5a) can definitely be concluded by looking at the DFL free energy in the zero-occupancy limit, which diverges for this choice in this limit.

Before searching for alternative prescriptions for the subsidiary operator $R_{i,\sigma}$ in Eq.(4), it is relevant to verify whether the above unpleasant results were peculiar to the finite-size model. To this end, we have performed the $U = 0$ calculations also for the lattice case versus the doping value $n - 1$ (since in the lattice case the antiferromagnetic instability occurs already at infinitesimal U due to the perfect nesting of the Fermi surface). The results shown in Fig.2 confirm our conclusion that, regardless of its successes at the mean-field level, the KR form of $R_{i,\sigma}$ is not suited for the inclusion of fluctuations. Note, in particular, the divergence of the DFL results when $n = 2$, which was mentioned above for the two-site model.

This conclusion calls for alternative expressions of the subsidiary operator. One could initially resort to the *simplest* possible expression (2) for $z_{i,\sigma}$, for which $R_{i,\sigma} = R_{i,\sigma}^0 = 1$ and $\mathcal{R} = 1$. In this case the factor $\mathcal{F}[\mathcal{R}; \mathbf{l}_0]$ of Eq.(62) vanishes identically [cf. Eq.(63)]. The corresponding results for the ground-state energy (per lattice site) of the one-level two-site model are shown in Fig.3, with the same notations of Fig.1 (except for the labeling of the mean-field curve, which is now MF). Note that the critical value for the Mott-Hubbard transition to occur at “half filling” is now $U_c = 4t$, according to Eq.(113). We see from this figure that the DFL results now improve the agreement with the exact solution with respect to the MF results, while the CFL results considerably worsen the agreement. This finding thus gives us support for treating correctly the time continuum limit of the functional integral within the four-slave-boson approach.

In addition, we note the following *shortcomings of the CFL results*:

- (i) At finite doping ($n > 1$) the CFL result yield the *wrong curvature* of E/t versus U/t , thus producing an *unphysical increase* of the (average) number of doubly occupied sites for increasing U/t .³⁴ This shortcoming is remedied by the DFL results.
- (ii) As mentioned above, in the zero-occupancy ($n = 0$) limit, the ground-state energy has to vanish irrespective of the value of U . The CFL results are instead finite in that limit. (This shortcoming is also shared by the previous KR choice for $R_{i,\sigma}$). The mean-field results MF and HF behave instead correctly in the limit. Once more, the DFL calculation remedies the shortcoming (with the exception of the previous KR choice for $R_{i,\sigma}$ which leads to divergent DFL results in the $n = 0$ limit). The $n = 0$ limit thus provides us with a common *reference level* for comparing alternative results for the ground-state energy.

Although the choice $R_{i,\sigma}^0 = 1$ cures formally all flaws occurring with the KR choice when fluctuation corrections are included, it is seen from Fig.3 that the mean-field solution associated with $R_{i,\sigma}^0 = 1$ constitutes a rather poor starting point for the inclusion of fluctuations. In this respect, even the HF mean field is closer to the exact solution for $U/t \lesssim 8$. In particular, the choice $R_{i,\sigma}^0 = 1$ does not reproduce at the mean-field level the independent-particle

result when $U = 0$. By contrast, the KR form for $R_{i,\sigma}$ has been tuned to reproduce *exactly* the $U = 0$ result at the mean-field level, by introducing the nontrivial factor \mathcal{R}^{KR} just as a “normalization” factor.

It is thus clear from the above discussion that a more sophisticated prescription than $R_{i,\sigma}^0 = 1$ is required for the subsidiary operator, which would preserve the nice features associated with $R_{i,\sigma}^{KR}$ at the mean-field level and, at the same time, would avoid the unphysical behavior resulting from $R_{i,\sigma}^{KR}$ when fluctuations are included.

C. ALTERNATIVE SELECTIONS OF THE SUBSIDIARY OPERATOR R

An appealing feature of the KR (paramagnetic) mean-field solution is that (besides recovering the $U = 0$ limit) it reproduces the Gutzwiller approximation for the single-band (lattice) Hubbard Hamiltonian (at any filling).⁴ This approximation is, in turn, expected to capture the essential electronic correlations for the Hubbard model by reducing the site double occupancy at large U .¹⁰ One would then like to select the form of the operator $R_{i,\sigma}$ in such a way that the Gutzwiller approximation is still recovered at the mean-field level (at least for some particular filling). Recall in this context that the subsidiary operator $R_{i,\sigma}$ of Eq.(4) has to be equivalent to the unit operator in the relevant Fock subspace.

An alternative selection for the operator $R_{i,\sigma}$ might rest on the following criterion which exploits the mean-field constraints (109)-(111) in the zero-temperature limit. In particular, *at half filling* ($n = 1$) the relation $b_0^{(1)2} + b_0^{(2)2} = b_0^{(2)2} + b_0^{(4)2} = 1/2$ holds for any value of U , so that any function \mathcal{R} of $b_0^{(1)2} + b_0^{(2)2}$ and $b_0^{(2)2} + b_0^{(4)2}$ will also be independent of U . This property is satisfied by the KR form (120). For any other form of \mathcal{R} satisfying this property, it is then enough to “normalize” \mathcal{R} in such a way that it coincides with \mathcal{R}^{KR} when $b_0^{(1)2} + b_0^{(2)2} = b_0^{(2)2} + b_0^{(4)2} = 1/2$. This criterion guarantees that this new \mathcal{R} and \mathcal{R}^{KR} give the same mean-field results. Note that the mean-field free energy F_0 is also independent of \mathcal{R} (whenever the property (114) holds) since λ_0^α does not enter F_0 at self-consistency.

A form of the function \mathcal{R} , which reproduces the KR mean-field results at half-filling, is obtained by suitably “linearizing” the expression (120), namely, by setting¹⁵

$$\mathcal{R}^{LIN}(n_e, n_\sigma, n_{\bar{\sigma}}, n_d) = [1 + x(n_e + n_{\bar{\sigma}})][1 + x(n_\sigma + n_d)] \quad (121)$$

with $x = x_0$ such that (in the paramagnetic case)

$$\left(1 + \frac{x_0}{2}\right)^2 = \frac{1}{(1 - \frac{1}{2})} = 2. \quad (122)$$

This gives $x_0 = 2(\sqrt{2} - 1) \cong 0.828$ for the positive solution. Although this particular value of x has been selected at “half filling”, in the following we shall use the same value of x for any filling. Note that the subsidiary function (121) corresponds to the “linearized” subsidiary operator $R_{i,\sigma}^{LIN} = [1 + x(e_i^\dagger e_i + s_{i,-\sigma}^\dagger s_{i,-\sigma})][1 + x(d_i^\dagger d_i + s_{i,\sigma}^\dagger s_{i,\sigma})]$ for which the normal ordering is irrelevant. This simple choice is free from the nonanalyticity problems affecting instead $R_{i,\sigma}^{KR}$.²⁸

The results for the ground-state energy (per lattice site) of the two-site model corresponding to (121) are shown in Fig.4 for filling values $n = 1.0$, $n = 1.2$, and $n = 1.5$. Curves are labeled with the conventions used in Fig.3. Note that the DFL results at “half filling” are now quite close to the exact solution for $U/t \lesssim 8$. In particular, the DFL fluctuation corrections do not change appreciably (i. e., within less than 1%) the exact solution at $U = 0$. (We have verified that this finding remains true also for an infinite system). The agreement between DFL and EX, however, is not so good for U close to the critical value $U_c (= 16t)$ for the Mott-Hubbard transition to occur in the mean-field solution. Note also the presence of a “cusp” about U_c in the fluctuation results. This “cusp” is of no special concern since it is a characteristic feature of the Gaussian corrections near the transition point where higher-order fluctuations are expected to be important. This “cusp”, in fact, quickly disappears as soon as one moves away from half filling (cf. Figs.4b and 4c). Note finally that the exact solution for the ground-state energy approaches a linear trend with respect to U for increasing doping. As a consequence, the HF approximation becomes progressively more reliable for increasing doping.

The behavior of the ground-state energy (per lattice site) versus doping $n - 1$ is shown in Fig. 5 for three characteristic values of U/t with the same “linearized” \mathcal{R}^{LIN} used for Fig. 4. The CFL results, however, have been excluded from Fig. 5 as they depart markedly from the other results. Even in this case, the correct fluctuation contribution (DFL) give quite good overall results. Note that the piecewise linear behavior of the exact solution versus doping is due to the finite size of the system (as well as to the zero-temperature limit), since the exact solution for this system is *constructed* by interpolating between the solutions with $n = 1.0$ and $n = 1.5$ and with $n = 1.5$ and $n = 2.0$. Note, however, from Fig.5a that the free-particle results at $U = 0$ are reproduced by the mean-field solution and by the

fluctuation corrections at “half filling” only (and when $n = 0.0$ or 2.0), while departures from the correct results become more pronounced at finite doping. (Recall that the KR mean field provides instead - by construction - the correct $U = 0$ results at any doping and thus the correct value for the compressibility).

The above shortcoming is obviously due to the fact that the parameter x of the “linearized” \mathcal{R}^{LIN} has been selected at “half filling” according to Eq.(122). Although one might fix x at any selected doping, it is certainly not satisfactory to adjust x to be doping dependent in order to reproduce the independent-particle results at any doping. For this reason the “linearized” form (121) proves to be not completely satisfactory.

The fact that the KR mean field reproduces the ($U = 0$) free-particle results for *any* doping is due to the perfect cancellation of the doping dependence of the factor $b_0^{(2)}(b_0^{(1)} + b_0^{(4)})$ in Eq.(107) with the self-consistent doping dependence of the \mathcal{R}^{KR} factor (120). It is also evident that no “polynomial” generalization of (121) can yield this perfect cancellation for all doping values.

To fully preserve the nice features of the KR mean field, we finally consider the “square root” form $R_{i,\sigma}^{SQ}$ (5b) for the subsidiary operator, whereby the KR normal-ordering prescription in (5a) has been removed. Following the discussion of subsection IIE, this can readily be achieved within the $1/N$ expansion by dropping the last terms in Eq.(63) containing the second derivatives and using \mathcal{R}^{KR} in the rest of the calculation.

The results obtained for the ground-state energy (per lattice site) of the two-site model with the choice $R_{i,\sigma} = R_{i,\sigma}^{SQ}$ are shown in Fig.6 versus U for $n = 1.0$ and $n = 1.2$, where the mean-field (KR) and the complete $1/N$ (SQ) calculations are compared with the exact solution (like in Fig.1, an antiferromagnetic instability develops at “half filling” in SQ when $U \cong 6.8t$). The corresponding results versus doping $n - 1$ are shown in Fig.7 for three characteristic values of U . Note, in particular, from Fig.7a that *the $1/N$ fluctuation corrections are now completely suppressed at $U = 0$ for any doping*. We are thus able to recover exactly the $U = 0$ solution not only at the mean-field level but *also* with the inclusion of fluctuations, without having to adjust any parameter (like, for instance, the x parameter in Eq. (121)). In addition, this finding is not limited to the two-site model but applies also to the lattice case, as shown in Fig.8. In this way, the non normal-ordering SQ prescription (5b) overcomes the difficulties signaled in Ref.¹², without the need of changing the functional form of the bosonic operator z at the leading $1/N$ order beyond mean field. Note, finally, from Figs.6 and 7 that the SQ prescription gives good agreement with the exact solution for the two-site model at any doping *even* at finite U . In particular, for the filled band ($n = 2$) the SQ prescription recovers the exact result $E = U$ for any U [or $E = 0$ for the empty band ($n = 0$)], in contrast with the KR normal-ordering prescription that gives divergent results as $n \rightarrow 2$ (or $n \rightarrow 0$). This divergence resides in the second derivative terms of Eq. (63), which are appropriately eliminated by the non normal-ordering SQ prescription.

IV. CONCLUDING REMARKS

In this paper we have demonstrated the importance of taking correctly the continuum limit of the functional integral for the four-slave-boson method by Kotliar and Ruckenstein, by deriving in detail the additional (ultraviolet) contributions to the free energy associated with a proper handling of the vanishing of the imaginary time step. Although these additional contributions to the free energy have been already derived for the one-slave-boson case in Ref.¹⁴, the presence of several bosons and of a nontrivial bosonic hopping factor z (which is peculiar to the KR method) results into *additional noncommuting terms* in the slave-boson Hamiltonian, which, in turn, make the proper handling of the continuum limit of the functional integral quite more involved. Nonetheless, the rather elaborate mathematical derivations that resulted proved necessary to implement correctly the KR method and make it working properly in practice. We have also provided an “effective” rule to obtain the additional terms in the free energy directly from the original Hamiltonian, without the need of going explicitly through the limiting discretization procedure of the functional integral. The fact that this careful procedure has anyhow produced unphysical results at the $1/N$ order beyond mean field when adopting the conventional KR choice for the bosonic hopping factor z , has further required us to search for alternative forms (or prescriptions) for z . Specifically, we have shown that removing the KR normal-ordering prescription for z enables us to overcome the above difficulties. In particular, we have verified numerically that the non normal-ordering prescription succeeds in suppressing completely the $1/N$ fluctuation corrections to the ground-state energy at $U = 0$ and for any band filling. We regard this finding to be rather compelling to remove the doubts which have been raised on the capability of the KR four-slave-boson method to yield meaningful fluctuation corrections (see, in particular, Ref.¹²).

In this context, some additional features still need, however, to be verified. For instance, it should be verified that removing the normal-ordering prescription from the KR choice of z suppresses the $1/N$ corrections at $U = 0$ also for dynamical quantities (like the fermionic Green’s functions). In this respect, we have developed preliminary arguments which show that the non normal-ordered subsidiary operator (5b) reproduces the exact $U = 0$ results (at

zero temperature) *for any value of N* , thus suppressing the fluctuation corrections to the free energy and to dynamical quantities *exactly* when $U = 0$.³⁵

Although the formal results obtained in this paper are valid even at finite temperature, numerical results have been restricted to the zero-temperature limit throughout. Extension to finite temperature is then in order. Besides, one may also consider multi-band Hubbard-type Hamiltonians (like the Emery model for a CuO_2 layer), for which using our “effective” rule to obtain the additional terms in the free energy should be straightforward.

The numerical results presented in this paper have primarily concerned the two-site model, although results have also been presented for the infinite lattice when $U = 0$. Restriction to $U = 0$ is connected with the paramagnetic *ansatz* we have considered throughout, since the matrix of Gaussian fluctuations develops instabilities for $U = 0^+$ and $n = 1$. Consideration of magnetic phases is thus necessary, at least near “half filling”. We mention in this context that the KR four-slave-boson method, which is not manifestly spin-rotation-invariant, might not properly account for transverse magnetic fluctuations at the order $1/N$. To this end, it would be necessary to include additional “angular” variables associated with transverse fluctuations. This could be achieved by the spin-rotation-invariant method of Ref.⁷ where two additional “s” bosons are introduced at the outset. Resorting to the method of Ref.⁷, in turn, requires one to assess preliminarily the effects of the proper handling of the time continuum limit of the functional integral at the order $1/N$ that have been discussed in the present paper. Work along these lines is in progress.

ACKNOWLEDGMENTS

We are indebted to C. Castellani and R. Raimondi for discussions. One of us (E. A.) would also like to thank P. Fulde for his support and interest in this work.

APPENDIX A: $1/N$ EXPANSION WITH THE FOUR-SLAVE-BOSON METHOD

In this Appendix we show how a suitable $1/N$ expansion can be constructed for the four-slave-boson problem. The need to organize the theory by means of a $1/N$ expansion originates from the lack of an intrinsic small parameter, in powers of which a more conventional perturbation theory could be defined. In addition, the introduction of the parameter $1/N$ enables one to establish a meaningful comparison of the results obtained via different representations of the integration variables in the functional integral (i.e., by using either the “radial” or the “Cartesian” gauges).

As for the one-slave-boson problem,¹⁴ also in the present context the integer $2N$ represents the number of spin components of the fermionic field coupled to the slave bosons. Also in this case, it turns out that the mean-field solution becomes exact in the $N \rightarrow \infty$ limit and that the leading $1/N$ corrections to the free energy are associated with the Gaussian fluctuations. For physical quantities different from the free energy, however, the leading $1/N$ corrections require also the inclusion of higher-order fluctuations (which is equivalent to a $1/N$ shift of the mean-field parameters).

Since the physical case of interest corresponds to the value $N = 1$, one may wonder whether including only the $1/N$ corrections to the mean-field solution might be sufficient to obtain in practice sensible results when $N = 1$. In this respect, the numerical results presented in Section III for a simple model system give us confidence that extrapolating the $1/N$ results down to $N = 1$ can work rather accurately for practical purposes (provided the form of the subsidiary operator is chosen appropriately).³⁶

A meaningful $1/N$ expansion for the four-slave-boson problem can be introduced in the following way:³⁷

- (i) To begin with, the fermionic spin label (which in the original action (7)-(10) was restricted to the two values ± 1) is formally extended to run over the $2N$ values $S = \sigma n$ with $\sigma = \pm 1$ and $n = 1, 2, \dots, N$.
- (ii) In order not to proliferate the number of slave bosons in the action (7)-(10) (thus keeping consistently the number of mean-field equations independent of N), we retain only two “magnetic” bosons $s_{\sigma=+1}$ and $s_{\sigma=-1}$, where now $s_{\sigma=+1}$ is associated with fermions with positive ($S > 0$) spin projection and $s_{\sigma=-1}$ with fermions with negative ($S < 0$) spin projection. This corresponds to generalizing the constraints (3) as follows:

$$d_i^\dagger d_i + \sum_{\sigma=\pm 1} s_{i,\sigma}^\dagger s_{i,\sigma} + e_i^\dagger e_i = N, \quad (\text{A1})$$

$$\sum_{S=\sigma}^{\sigma N} f_{i,S}^\dagger f_{i,S} - s_{i,\sigma}^\dagger s_{i,\sigma} - d_i^\dagger d_i = 0 \quad (\sigma = \pm 1). \quad (\text{A2})$$

In this way, the “spin” label σ of the bosonic variables $\lambda_{i,\sigma}^b$ and $z_{i,\sigma}$ in Eqs. (8)-(10) is maintained. Note that the replacement $1 \rightarrow N$ on the right-hand-side of Eq. (A1) is necessary since the mean value of the fermionic

term in Eq. (A2) is of order N . By the same token, the unity in the square roots in Eq. (5b) (and consequently in its “linearized” version discussed in Section III) has also to be replaced by N .

(iii) To keep the mean-field bosonic parameters independent of N , we rescale the bosonic fields by letting

$$e_{i,m} \longrightarrow \sqrt{N}e_{i,m} , \quad (\text{A3})$$

and similarly for $s_{i,\sigma,m}$ ($\sigma = \pm 1$) and $d_{i,m}$.

(iv) Requiring the kinetic term (10) to be homogeneous in N of the same order as the other two terms (8) and (9) of the action, leads to suitably rescaling the hopping integral t depending on the choice of the subsidiary factor $R_{i,\sigma}$ in Eq. (11). In particular, $t \rightarrow t/N^2$ when $R_{i,\sigma} = 1$; $t \rightarrow t$ with the KR choice (12); $t \rightarrow t/N^6$ with the “linearized” choice corresponding to (121).

With the above prescriptions, the action S_M is generalized as follows:

$$S_M^{(N)} = \sum_{m=0}^{M-1} \sum_{n=1}^N \sum_{\sigma=\pm 1} \sum_{\langle i,j \rangle} \bar{f}_{i,\sigma n,m} \mathcal{G}_{i,m;j,m-1}[\underline{b}; \sigma] f_{j,\sigma n,m-1} + N\mathcal{B}[\underline{b}] \quad (\text{A4})$$

where $\langle i,j \rangle$ limits the lattice sum to nearest-neighbor sites. \mathcal{G} and \mathcal{B} in Eq. (A4) are functionals of the bosonic fields \underline{b} (including now the Lagrange multipliers) which, by our assumptions, are *independent of N* . [For the non normal-ordering prescription for $R_{i,\sigma}$, however, \mathcal{G} is itself written as a power series in $1/N$ - see subsection IIE and footnote 29]. When $N = 1$ the action (A4) consistently reduces to the form (7)-(10) considered in the text.

It is important to emphasize that the N -component generalization of the slave-boson Hamiltonian (which has led to the action (A4)) is equivalent to the N -component generalization of the *original* fermionic Hamiltonian (1) *only for $N = 1$* . The resulting $1/N$ expansion acquires thus physical meaning only when N is eventually set equal to 1. However, this should not be considered to be an inconvenience of the present approach since the N -component slave-boson Hamiltonian has not been conceived to study a physical system with truly large spin; rather, the resulting $1/N$ expansion must be considered as a purely formal tool to control the approximations systematically.

The lack of correspondence of the two (purely fermionic and fermionic-bosonic) Hamiltonian problems when $N > 1$ results from (i) the constraints (A1) and (A2) no longer providing (in general) a one-to-one correspondence between the Fock spaces on which the two Hamiltonians respectively act, and (ii) the matrix elements of a given operator being different even for pairs of corresponding states. As an example, let's consider the case $N = 2$. In this case, to the original configuration $\tilde{f}_{i,+3/2}^\dagger \tilde{f}_{i,-1/2}^\dagger |0\rangle$, for instance, the constraints (A1) and (A2) associate the two distinct configurations $d_i^\dagger e_i^\dagger f_{i,+3/2}^\dagger f_{i,-1/2}^\dagger |0\rangle$ and $s_{i,+1}^\dagger s_{i,-1}^\dagger f_{i,+3/2}^\dagger f_{i,-1/2}^\dagger |0\rangle$. On the other hand, to the original configuration $\tilde{f}_{i,+3/2}^\dagger \tilde{f}_{i,+1/2}^\dagger |0\rangle$ there corresponds the only configuration $(2)^{-1/2} (s_{i,+1}^\dagger)^2 f_{i,+3/2}^\dagger f_{i,+1/2}^\dagger |0\rangle$. [Note that the mapping between the two Fock spaces (i.e., with and without slave bosons) preserves the fermionic configurations (specified by the operators f^\dagger and \tilde{f}^\dagger , in the order) and adjusts the bosonic configurations to satisfy the constraints]. For the latter state the average value of the interaction term $U d_i^\dagger d_i$ vanishes, while for the corresponding original configuration the average value of the original interaction term $U \sum_{S>S'} \tilde{f}_{i,S}^\dagger \tilde{f}_{i,S'}^\dagger \tilde{f}_{i,S'} \tilde{f}_{i,S}$ equals U (with S and S' taking the $2N$ values $-N, \dots, -1, +1, \dots, +N$). Obviously, when $N = 1$ both the one-to-one correspondence between states and the equality of the matrix elements is fully preserved.

Returning to the action (A4), we carry out the associated $1/N$ expansion in the usual way by first integrating out the fermion (Grassmann) fields. The action (A4) is then replaced by

$$S_{eff}^{(N)} = -N(\text{tr} \log \mathcal{G}[\underline{b}; \sigma = +1] + \text{tr} \log \mathcal{G}[\underline{b}; \sigma = -1]) + N\mathcal{B}[\underline{b}] \equiv NS[\underline{b}] \quad (\text{A5})$$

where the trace is taken over the indices (i,j,m) of Eq. (A4) and $S[\underline{b}]$ is independent of N . Note that $S_{eff}^{(N)}$ depends on N *only through the explicit factor N* on the right-hand side of Eq. (A5), as a consequence of the assumptions (i)-(iv) spelled out above. [Apart from the non normal-ordering prescription for $R_{i,\sigma}$, for which $S[\underline{b}]$ of Eq.(A5) is itself written as a power series in $1/N$ - see footnote 29]. By this remark, the following procedure is completely analogous to the standard method for the one-slave-boson case (cf. Ref.¹⁴).

We then expand schematically $S[\underline{b}]$ in Eq. (A5) in powers of the deviation $\tilde{\underline{b}}$ of the bosonic field \underline{b} from its mean-field value \underline{b}_0 as follows:

$$\begin{aligned}
S[\underline{b}] &= S[\underline{b}_0] + \sum_{r_1} \Gamma_{r_1}^{(1)}[\underline{b}_0] \tilde{b}_{r_1} + \sum_{r_1 r_2} \Gamma_{r_1 r_2}^{(2)}[\underline{b}_0] \tilde{b}_{r_1} \tilde{b}_{r_2} \\
&+ \sum_{r_1 r_2 r_3} \Gamma_{r_1 r_2 r_3}^{(3)}[\underline{b}_0] \tilde{b}_{r_1} \tilde{b}_{r_2} \tilde{b}_{r_3} \\
&+ \sum_{r_1 r_2 r_3 r_4} \Gamma_{r_1 r_2 r_3 r_4}^{(4)}[\underline{b}_0] \tilde{b}_{r_1} \tilde{b}_{r_2} \tilde{b}_{r_3} \tilde{b}_{r_4} + \dots, \tag{A6}
\end{aligned}$$

where

$$\Gamma_{r_1 \dots r_k}^{(k)}[\underline{b}_0] = \frac{1}{k!} \frac{\partial^k S}{\partial b_{r_1} \dots \partial b_{r_k}} \Big|_{\underline{b}_0} \tag{A7}$$

and \underline{b}_0 is chosen as usual according to the condition

$$\Gamma_r^{(1)}[\underline{b}_0] = \frac{\partial S}{\partial b_r} \Big|_{\underline{b}_0} = 0 \tag{A8}$$

for all values of r . For convenience, in the above expressions the indices r_1, \dots, r_k label the whole set of bosonic variables (that is, including also the static and homogeneous variables) to be integrated over in the functional integral. For the partition function we obtain accordingly

$$\begin{aligned}
\mathcal{Z} &= e^{-NS[\underline{b}_0]} \int \prod_r (\sqrt{N} d\tilde{b}_r) \exp \left\{ -N \sum_{k=2}^{\infty} \sum_{r_1 \dots r_k} \Gamma_{r_1 \dots r_k}^{(k)}[\underline{b}_0] \tilde{b}_{r_1} \dots \tilde{b}_{r_k} \right\} \\
&= e^{-NS[\underline{b}_0]} \int \prod_r dx_r \exp \left\{ - \sum_{k=2}^{\infty} N^{\frac{2-k}{2}} \sum_{r_1 \dots r_k} \Gamma_{r_1 \dots r_k}^{(k)}[\underline{b}_0] x_{r_1} \dots x_{r_k} \right\} \tag{A9}
\end{aligned}$$

where the factor \sqrt{N} in front of $d\tilde{b}_r$ originates from the rescaling (A3) and we have defined $x = \sqrt{N}\tilde{b}$ (that affects the fluctuating part only). It is then evident from Eq. (A9) that only the term with $k = 2$ gives the leading $1/N$ correction to the mean-field free energy, namely,

$$F_0 = N \frac{S[\underline{b}_0]}{\beta}, \tag{A10}$$

which justifies keeping only the Gaussian fluctuations to calculate the $1/N$ corrections to the free energy.

Besides the free energy, let's consider a physical quantity (or correlation function) which can be expressed as

$$\begin{aligned}
\phi &= \frac{\int \prod_r d\tilde{b}_r \phi(\underline{b}) e^{-NS[\underline{b}]}}{\int \prod_r d\tilde{b}_r e^{-NS[\underline{b}]}} \\
&= \phi(\underline{b}_0) + \frac{1}{\mathcal{Z}} \int \prod_r dx_r \left[\frac{1}{\sqrt{N}} \sum_{r_1} \frac{\partial \phi}{\partial b_{r_1}} \Big|_{\underline{b}_0} x_{r_1} \right. \\
&\quad \left. + \frac{1}{2N} \sum_{r_1 r_2} \frac{\partial^2 \phi}{\partial b_{r_1} \partial b_{r_2}} \Big|_{\underline{b}_0} x_{r_1} x_{r_2} + \dots \right] e^{-NS[\underline{b}]}. \tag{A11}
\end{aligned}$$

Since $\phi(\underline{b}_0)$ is of order $(1/N)^0$, evaluation of its $1/N$ corrections requires one to keep also the cubic terms in the expansion (A6). In particular, the $1/N$ corrections to ϕ derive from (i) the quadratic term in the expansion (A11) (which is itself proportional to $1/N$) integrated only with the Gaussian term in the expansion (A6), and (ii) the linear term in the expansion (A11) (which is proportional to $1/\sqrt{N}$) integrated by keeping also the cubic term in the expansion (A6). In the latter case, one needs to expand the exponential of the cubic term in Eq. (A6) and keep only the leading term in $1/\sqrt{N}$ of this expansion. [The normalization factor \mathcal{Z} of Eq. (A11) should be consistently taken only up to the Gaussian order]. Correction (i) to $\phi(\underline{b}_0)$ is just the ordinary Gaussian contribution, while correction (ii) is equivalent to considering the $1/N$ shift of the mean-field parameters \underline{b}_0 in $\phi(\underline{b}_0)$. To show this, we rewrite correction (ii) in the following way:

$$\begin{aligned}
& -\frac{1}{N} \sum_{r_1 \dots r_4} \Gamma_{r_1 r_2 r_3}^{(3)}[\underline{b}_0] \frac{\partial \phi}{\partial b_{r_4}} \Big|_{\underline{b}_0} \frac{\int \prod_r dx_r (x_{r_1} x_{r_2} x_{r_3} x_{r_4}) \exp \left\{ -\sum_{r_5 r_6} \Gamma_{r_5 r_6}^{(2)}[\underline{b}_0] x_{r_5} x_{r_6} \right\}}{\int \prod_r dx_r \exp \left\{ -\sum_{r_5 r_6} \Gamma_{r_5 r_6}^{(2)}[\underline{b}_0] x_{r_5} x_{r_6} \right\}} \\
& = -\frac{1}{N} \sum_{r_1 \dots r_4} \Gamma_{r_1 r_2 r_3}^{(3)}[\underline{b}_0] \frac{\partial \phi}{\partial b_{r_4}} \Big|_{\underline{b}_0} \frac{3}{4} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_1 r_2} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_3 r_4} \\
& = -\frac{1}{N} \sum_{r_1 \dots r_4} \left(\frac{\partial}{\partial b_{r_3}} \Gamma_{r_2 r_1}^{(2)}[\underline{b}] \right)_{\underline{b}_0} \frac{\partial \phi}{\partial b_{r_4}} \Big|_{\underline{b}_0} \frac{1}{4} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_1 r_2} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_3 r_4} \\
& = -\frac{1}{N} \sum_{r_3 r_4} \left(\frac{\partial}{\partial b_{r_3}} \frac{1}{2} \text{tr} \ln \Gamma^{(2)}[\underline{b}] \right)_{\underline{b}_0} \frac{\partial \phi}{\partial b_{r_4}} \Big|_{\underline{b}_0} \frac{1}{2} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_3 r_4} \\
& = -\frac{1}{N} \sum_{r_3 r_4} \left(\frac{\partial}{\partial b_{r_3}} \beta F_1[\underline{b}] \right)_{\underline{b}_0} \frac{\partial \phi}{\partial b_{r_4}} \Big|_{\underline{b}_0} \frac{1}{2} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_3 r_4}, \tag{A12}
\end{aligned}$$

where we have used the definition (A7) and recalled that the $1/N$ correction to the free energy is given by (cf. Eq.(54))

$$F_1 = \frac{1}{2\beta} \text{tr} \ln \Gamma^{(2)}[\underline{b}_0]. \tag{A13}$$

In fact, owing to space and time translational invariance, the wave vector and frequency labels $q(r)$ of the integration variables in Eq. (A12) are related by

$$q(r_1) + q(r_2) + q(r_3) = q(r_1) + q(r_2) = q(r_3) + q(r_4) = 0, \tag{A14}$$

which gives $q(r_3) = q(r_4) = 0$. For these static and homogeneous variables we can write

$$\Gamma^{(2)}[\underline{b}_0]_{r_3 r_4} = \frac{1}{N} \frac{\beta}{2} \frac{\partial^2 F_0[\underline{b}]}{\partial b_{r_3} \partial b_{r_4}} \Big|_{\underline{b}_0} \tag{A15}$$

and recognize in the expression

$$b_{r_4}^{(1)} = -\frac{1}{N} \frac{\beta}{2} \sum_{r_3} \left(\Gamma^{(2)}[\underline{b}_0]^{-1} \right)_{r_4 r_3} \left(\frac{\partial}{\partial b_{r_3}} F_1[\underline{b}] \right)_{\underline{b}_0} \tag{A16}$$

the $1/N$ shift of the mean-field parameter $b_{r_4}^{(0)}$ [cf., e.g., Appendix C of Ref.¹⁴]. Expression (A12) thus reduces to $\sum_{r_4} (\partial \phi / \partial b_{r_4})_{\underline{b}_0} b_{r_4}^{(1)}$ and corresponds to shifting $\underline{b}_0 \rightarrow \underline{b}_0 + \underline{b}^{(1)}$ in the argument of $\phi(\underline{b}_0)$, as anticipated above.³⁸

Finally, we comment briefly on how the $1/N$ expansion discussed above can be combined with the procedure to restore the spin-rotation invariance in the results obtained via the KR four-slave-boson method. To this end, we will essentially follow the procedure used in Appendix B of Ref.³⁹ for the physical case $N = 1$, albeit with some modifications.

The problems originating from using a slave-boson method which is not manifestly spin-rotation invariant can be evidenced when considering, for instance, spin correlation functions of the type

$$\tilde{\chi}_{\alpha, \alpha'}(i, j; \tau) = \langle T_\tau [\tilde{S}_i^{(\alpha)}(\tau) \tilde{S}_j^{(\alpha')}(0)] \rangle \tag{A17}$$

($\alpha, \alpha' = x, y, z$), where $T_\tau[\dots]$ is the time-ordering operator for imaginary time τ and the spin operators

$$\tilde{S}_i^{(\alpha)} = \frac{1}{2} \sum_{\sigma, \sigma' = \pm 1} \tilde{f}_{i, \sigma}^\dagger \sigma_{\sigma, \sigma'}^{(\alpha)} \tilde{f}_{i, \sigma'} \tag{A18}$$

are defined in terms of the physical spin $\frac{1}{2}$ fermion operators ($\sigma^{(\alpha)}$ being a Pauli matrix). Violation of spin-rotation invariance occurs in (A17) when considering the slave-boson replacement $\tilde{f}_{i, \sigma} \rightarrow f_{i, \sigma} z_{i, \sigma}$. For instance, in the paramagnetic case the (z, z) element of the tensor (A17) differs from the (x, x) and (y, y) elements when the mean-field approximation for the slave bosons is considered.

In Eqs. (A17) and (A18) the spin label σ refers to a given quantization axis (say \hat{z}), which is common to all sites. Spin-rotation invariance can be restored upon averaging over all possible quantization axes, which are identified by

the spherical angle $\Omega = (\theta, \varphi)$ common to all lattice sites. In this respect, we follow Ref.³⁹ and introduce the rotated fermion operators

$$\tilde{g}_{i,\xi} = \sum_{\sigma=\pm 1} [\mathcal{R}^\dagger(\Omega)]_{\xi,\sigma} \tilde{f}_{i,\sigma} \quad (\text{A19})$$

where $\xi = \pm 1$ and

$$\mathcal{R}(\Omega) = e^{-i(\varphi/2)\sigma_z} e^{-i(\theta/2)\sigma_y} \quad (\text{A20})$$

is the relevant rotation operator. Introducing at this point the slave-boson mapping $\tilde{g}_{i,\xi} \rightarrow z_{i,\xi} g_{i,\xi}$ where now the bosonic operators refer to the new quantization axis identified by Ω , the spin operator (A18) becomes

$$\begin{aligned} \tilde{S}_i^{(\alpha)} &= T_{\alpha z}(\Omega) \frac{1}{2} \sum_{\xi,\xi'=\pm 1} g_{i,\xi}^\dagger \boldsymbol{\sigma}_{\xi,\xi'}^{(z)} g_{i,\xi'} \\ &+ \sum_{\beta=x,y} T_{\alpha\beta}(\Omega) \frac{1}{2} \sum_{\xi,\xi'=\pm 1} z_{i,\xi}^\dagger g_{i,\xi}^\dagger \boldsymbol{\sigma}_{\xi,\xi'}^{(\beta)} g_{i,\xi'} z_{i,\xi'} \end{aligned} \quad (\text{A21})$$

with $T_{\alpha\beta}(\Omega)$ defined by

$$\mathcal{R}^\dagger(\Omega) \boldsymbol{\sigma}^{(\alpha)} \mathcal{R}(\Omega) = \sum_{\beta} T_{\alpha\beta}(\Omega) \boldsymbol{\sigma}^{(\beta)}. \quad (\text{A22})$$

Note that the pair of bosonic operators at the same site with equal spin labels ($\xi = \xi'$) have been consistently replaced by unity in Eq. (A21). Note also that, within the mean-field approximation for the slave bosons, the remaining bosonic operators in Eq. (A21) can be replaced by the spin-independent factor z in the paramagnetic phase we are considering.

To evaluate the average over Ω , it is necessary to transform back to the old \hat{z} quantization axis, by using the transformation

$$g_{i,\xi} = \sum_{\sigma=\pm 1} [\mathcal{R}^\dagger(\Omega)]_{\xi,\sigma} f_{i,\sigma} \quad (\text{A23})$$

for the pseudo fermion operators. The operator (A21) then reads

$$\begin{aligned} \tilde{S}_i^{(\alpha)} &= (1 - z^2) T_{\alpha z}(\Omega) \sum_{\beta} \left(\frac{1}{2} \sum_{\sigma,\sigma'=\pm 1} f_{i,\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'}^{(\beta)} f_{i,\sigma'} \right) T_{\beta z}(\Omega) \\ &+ z^2 \frac{1}{2} \sum_{\sigma,\sigma'=\pm 1} f_{i,\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'}^{(\alpha)} f_{i,\sigma'}. \end{aligned} \quad (\text{A24})$$

Extension to arbitrary $N (> 1)$ is performed by adding an additional label $n (= 1, 2, \dots, N)$ to the fermionic operators and considering the action in the form (A5) (which does not depend on Ω). Accordingly, $\tilde{S}_i^{(\alpha)}$ of Eq.(A24) is replaced by

$$\tilde{S}_i^{(\alpha)}(N) = (1 - z^2) T_{\alpha z}(\Omega) \sum_{\beta} S_i^{(\beta)}(N) T_{\beta z}(\Omega) + z^2 S_i^{(\alpha)}(N) \quad (\text{A25})$$

with the notation

$$S_i^{(\alpha)}(N) = \frac{1}{2N} \sum_{n=1}^N \sum_{\sigma,\sigma'=\pm 1} f_{i,\sigma,n}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'}^{(\alpha)} f_{i,\sigma',n}. \quad (\text{A26})$$

Entering the expression (A25) into the correlation function (A17) in the place of $S_i^{(\alpha)}$ and averaging over the spherical angle Ω , we obtain for the averaged spin correlation function:

$$\begin{aligned}
& \int \frac{d\Omega}{4\pi} \langle T_\tau [\tilde{S}_i^{(\alpha)}(N; \tau) \tilde{S}_j^{(\alpha')} (N; 0)] \rangle \\
&= (1 - z^2)^2 \sum_{\beta\beta'} \chi_{\beta\beta'}^{(N)}(i, j; \tau) \int \frac{d\Omega}{4\pi} T_{\alpha z}(\Omega) T_{\alpha' z}(\Omega) T_{\beta z}(\Omega) T_{\beta' z}(\Omega) \\
&+ (1 - z^2) z^2 \sum_{\beta} \chi_{\beta\alpha'}^{(N)}(i, j; \tau) \int \frac{d\Omega}{4\pi} T_{\alpha z}(\Omega) T_{\beta z}(\Omega) \\
&+ z^2 (1 - z^2) \sum_{\beta'} \chi_{\alpha\beta'}^{(N)}(i, j; \tau) \int \frac{d\Omega}{4\pi} T_{\alpha' z}(\Omega) T_{\beta' z}(\Omega) \\
&+ z^4 \chi_{\alpha\alpha'}^{(N)}(i, j; \tau)
\end{aligned} \tag{A27}$$

where

$$\chi_{\alpha\alpha'}^{(N)}(i, j; \tau) \equiv \langle T_\tau [S_i^{(\alpha)}(N; \tau) S_j^{(\alpha')} (N; 0)] \rangle \tag{A28}$$

is a diagonal tensor with equal diagonal elements (at the mean-field level for the slave bosons). Equation (A27) then reduces to

$$\begin{aligned}
& \int \frac{d\Omega}{4\pi} \langle T_\tau [\tilde{S}_i^{(\alpha)}(N; \tau) \tilde{S}_j^{(\alpha')} (N; 0)] \rangle \\
&= \delta_{\alpha, \alpha'} \left\{ (1 - z^2)^2 \sum_{\beta} \chi_{\beta\beta}^{(N)}(i, j; \tau) \int \frac{d\Omega}{4\pi} T_{\alpha z}(\Omega)^2 T_{\beta z}(\Omega)^2 \right. \\
&+ \left. \left[\frac{2}{3} z^2 (1 - z^2) + z^4 \right] \chi_{\alpha\alpha}^{(N)}(i, j; \tau) \right\} \\
&= \delta_{\alpha, \alpha'} \frac{[(1 - z^2)^2 + 2z^2(1 - z^2) + 3z^4]}{3} \chi_{\alpha\alpha}^{(N)}(i, j; \tau) = \delta_{\alpha, \alpha'} \left(\frac{1 + 2z^4}{3} \right) \chi_{\alpha\alpha}^{(N)}(i, j; \tau).
\end{aligned} \tag{A29}$$

In this way spin-rotation invariance for the spin correlation functions has been restored at arbitrary values of N .⁴⁰

APPENDIX B: SUMMARY OF THE RELEVANT MATHEMATICAL EXPRESSIONS INVOLVING MATSUBARA FREQUENCY SUMS WITH A DISCRETIZED TIME MESH

The Fermi function and the fermionic polarization function introduced in Section II for the case of a discretized (imaginary) time mesh are defined, respectively, as follows:

$$f_M(E) = -\frac{1}{\beta} \sum_{s=0}^{M-1} \frac{1}{E - (1 - e^{-i\omega_s \delta})/\delta}, \tag{B1}$$

$$\begin{aligned}
\Pi_M(E, E'; \nu) &= \Pi_M(E', E; -\nu) \\
&= -\frac{1}{\beta} \sum_{s=0}^{M-1} \frac{1}{E - (1 - e^{-i\omega_s \delta})/\delta} \frac{1}{E' - (1 - e^{-i(\omega_s - \omega_\nu) \delta})/\delta}
\end{aligned} \tag{B2}$$

with $\omega_s = 2\pi(s + 1/2)/\beta$ and $\omega_\nu = 2\pi\nu/\beta$ ($\nu = 0, 1, \dots, M - 1$). The fermionic frequency sums in Eqs. (B1) and (B2) can be evaluated according to the method developed in Appendix B of Ref.¹⁴. For the reader's convenience we report here the results:

$$\begin{aligned}
f_M(E) &= \frac{1}{1 - (\beta E)/M} \frac{1}{1 + (1 - (\beta E)/M)^{-M}} \\
&\xrightarrow{M \rightarrow \infty} \frac{1}{1 + e^{\beta E}} = f_F(E),
\end{aligned} \tag{B3}$$

$$\begin{aligned}
\Pi_M(E, E'; \nu) &= \frac{\beta}{M} \frac{e^{i\omega_\nu \delta} f_M(E') - f_M(E)}{e^{i\omega_\nu \delta} \beta E/M - \beta E'/M + 1 - e^{i\omega_\nu \delta}} \\
&\xrightarrow{M \rightarrow \infty} \frac{f_F(E') - f_F(E)}{E - E' - i\omega_\nu},
\end{aligned} \tag{B4}$$

where the limiting expressions for $M \rightarrow \infty$ recover the standard finite-temperature Matsubara results.

Similarly, extraction of the “contribution from infinity” to a given bosonic frequency sum can be obtained according to a theorem proved in Appendix B of Ref.¹⁴. Since that procedure constitutes an essential step to obtain the novel results of Section II (and of Appendix C below), we summarize it here for convenience. According to this theorem, a bosonic frequency sum of the type

$$S_M = \frac{1}{\beta} \sum_{\nu=-(M-1)/2}^{(M-1)/2} h(e^{i\omega_\nu \delta}, \delta) \quad (\text{B5})$$

can be evaluated as the sum of its “continuum limit” S_c plus a “contribution from infinity” g_0 :

$$S_M = S_c + g_0. \quad (\text{B6})$$

In this expression

$$S_c = \frac{1}{\beta} \sum_{\nu=-\infty}^{+\infty} h_c(\omega_\nu) \quad (\text{B7})$$

is an ordinary Matsubara bosonic frequency sum, where

$$h_c(z) = \lim_{\delta \rightarrow 0} h(e^{iz\delta}, \delta) \quad (\text{B8})$$

is the continuum limit of the function h of Eq.(B5), and g_0 is the constant term of the function

$$g(\zeta) = \sum_{s=-S}^{-1} g_s \zeta^s + g_0 + \sum_{s=1}^S g_s \zeta^s \quad (\text{B9})$$

(with $\zeta = \exp\{iz\delta\}$) which enters the expansion

$$h(\zeta, \delta) = \delta g(\zeta) + \mathcal{O}(\delta^2). \quad (\text{B10})$$

The result (B6) holds under some restrictions on the function h , which have been spelled out in detail in Appendix B of Ref.¹⁴. These restrictions are definitely satisfied by the functions of interest considered in Section II (and in Appendix C). It is important to recall here that the function $h(e^{i\omega_\nu \delta}, \delta)$ in Eq. (B5) has to be taken to be even in ω_ν (at last, by suitably symmetrizing it), so that the associated continuum limit function $h_c(\omega_\nu)$ vanishes at least like $|\omega_\nu|^{-2}$ when $|\omega_\nu| \rightarrow \infty$.

We conclude this Appendix by remarking that the result (B3) can also be used to evaluate the contribution from the level E to the fermionic free energy, namely,

$$F_M(E) = -\frac{1}{\beta} \sum_{s=0}^{M-1} \ln(1 - e^{i\omega_s \delta} (1 - \delta E)). \quad (\text{B11})$$

In fact, differentiating both sides of (B11) with respect to E we obtain

$$\frac{\partial F_M(E)}{\partial E} = f_M(E) \quad (\text{B12})$$

according to the definition (B1). On the other hand, the result (B3) can be rewritten in the form

$$f_M(E) = -\frac{1}{\beta} \frac{d}{dE} \ln(1 + (1 - \delta E)^M) \quad (\text{B13})$$

with $\delta = \beta/M$. Comparison of (B12) with (B13) defines $F_M(E)$ up to a constant, which can be determined by noting from (B11) that $F_M(1/\delta) = 0$ for any M . We thus obtain:

$$F_M(E) = -\frac{1}{\beta} \ln(1 + (1 - \delta E)^M) \quad (\text{B14})$$

which recovers the known result

$$F_\infty(E) = -\frac{1}{\beta} \ln(1 + e^{-\beta E}) \quad (\text{B15})$$

in the continuum ($M \rightarrow \infty$) limit. This result has been used to derive Eq.(56) of the text.

APPENDIX C: OBTAINING THE CONTRIBUTION FROM INFINITY IN THE CARTESIAN GAUGE

The “radial” gauge was used in the text to represent the bosonic fields in the functional integral . This choice has enabled us to deal with expressions which are free from infrared divergences in the continuum ($\delta \rightarrow 0$) limit. The price we had to pay was that the calculation of the “contribution from infinity ” to the free energy turned out to be rather involved in the “radial” gauge (cf. Section II). On the other hand, we expect that the “contribution from infinity ” can be obtained equivalently in any other gauge at a given order in $1/N$, provided a separate $1/N$ expansion holds in both discretized and continuum versions of the functional integral .

We shall show in this Appendix that the “contribution from infinity ” to the free energy (62)-(64) taken at self-consistency can alternatively be obtained at the same $1/N$ order in the “Cartesian” gauge, when one takes the real and imaginary parts of the complex bosonic fields as integration variables.⁴¹ It will turn out that the derivation of the “contribution from infinity ” in the “Cartesian” gauge is considerably simpler than in the “radial” gauge, a result which contrasts the situation for the continuum limit expressions that are plagued by infrared divergences in the “Cartesian” gauge. This result gives support to the validity of the $1/N$ expansion discussed in Appendix A, and suggests at the same time that, at least at the order $1/N$ we are explicitly considering, it would be convenient to evaluate a given physical quantity by representing alternatively its continuum limit in the “radial” gauge and the associated “contribution from infinity ” in the “Cartesian” gauge. To this end, besides recovering the “contribution from infinity ” (62)-(64) to the free energy using the “Cartesian” gauge, in the following we shall also indicate how the calculation can be extended to other physical quantities (such as correlation functions) by working out explicitly a simple example.

We begin by rewriting the discretized action (7) in the compact form:

$$\begin{aligned}
 S_M = & \sum_{m=0}^{M-1} \sum_i \left\{ \sum_{\sigma} \bar{f}_{i,\sigma,m} [f_{i,\sigma,m} - (1 - \delta q_{i,\sigma}) f_{i,\sigma,m-1}] \right. \\
 & + \sum_{\beta=1}^4 b_{i,m}^{(\beta)*} [b_{i,m}^{(\beta)} - (1 - \delta h_i^{(\beta)}) b_{i,m-1}^{(\beta)}] \\
 & \left. + \delta t \sum_{\Delta,\sigma} \bar{f}_{i+\Delta,\sigma,m} z_{i+\Delta,\sigma}^*(m-1, m) z_{i,\sigma}(m, m-1) f_{i,\sigma,m-1} - \delta \lambda_i^a \right\} \quad (C1)
 \end{aligned}$$

where the site-dependent coefficients $q_{i,\sigma}$ and $h_i^{(\beta)}$ can be readily read off Eqs. (8) and (9). In the “Cartesian” gauge we set:⁴¹

$$b_{i,m}^{(\beta)} = b_0^{(\beta)} + \tilde{b}_{i,m}^{(\beta)} \quad , \quad b_{i,m}^{(\beta)*} = b_0^{(\beta)} + \tilde{b}_{i,m}^{(\beta)*} \quad (C2)$$

($\beta = 1, \dots, 4$), and expand the action (C1) up to quadratic order in the “small” quantities $\tilde{b}_{i,m}^{(\beta)}$. Introducing the (normalized) Fourier transform

$$\tilde{b}_{i,m}^{(\beta)} = \frac{1}{\sqrt{MN}} \sum_{\mathbf{q}} \sum_{\nu=1}^{M-1} e^{i(\mathbf{q} \cdot \mathbf{R}_i - \omega_{\nu} \tau_m)} b^{(\beta)}(\mathbf{q}, \omega_{\nu}) \quad (C3)$$

[cf. expression (29) of the text] and a similar transformation for the Grassmann fields, the relevant part of the action (C1) becomes:

$$\begin{aligned}
 S_M = & \beta \mathcal{N} S^{(0)} + \sum_{\mathbf{k}} \sum_{\sigma} \sum_{s=0}^{M-1} \bar{f}_{\sigma}(\mathbf{k}, \omega_s) [1 - e^{i\omega_s \delta} (1 - \delta \varepsilon_{\sigma}(\mathbf{k}))] f_{\sigma}(\mathbf{k}, \omega_s) \\
 & + \sum_{\mathbf{q}} \sum_{\beta=1}^4 \sum_{\nu=1}^{M-1} b^{(\beta)}(\mathbf{q}, \omega_{\nu})^* [1 - e^{i\omega_{\nu} \delta} (1 - \delta h_0^{(\beta)})] b^{(\beta)}(\mathbf{q}, \omega_{\nu}) \\
 & + \delta \frac{1}{\sqrt{MN}} \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma} \sum_{\beta=1}^4 \sum_{s=0}^{M-1} \sum_{\nu=1}^{M-1} e^{i\omega_s \delta} \\
 & \times \left\{ \bar{f}_{\sigma}(\mathbf{k}, \omega_s) \varepsilon_1(\mathbf{q}; \mathbf{k}, \sigma | \beta) b^{(\beta)}(\mathbf{q}, \omega_{\nu}) f_{\sigma}(\mathbf{k} - \mathbf{q}, \omega_s - \omega_{\nu}) \right.
 \end{aligned}$$

$$\begin{aligned}
& + \bar{f}_\sigma(\mathbf{k} - \mathbf{q}, \omega_s - \omega_\nu) \bar{\varepsilon}_1(\mathbf{q}; \mathbf{k}, \sigma | \beta) b^{(\beta)}(\mathbf{q}, \omega_\nu)^* f_\sigma(\mathbf{k}, \omega_s) \Big\} \\
& + \delta \frac{1}{MN} \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma} \sum_{\beta, \beta'=1}^4 \sum_{s=0}^{M-1} \sum_{\nu=1}^{M-1} \bar{f}_\sigma(\mathbf{k}, \omega_s) e^{i\omega_s \delta} f_\sigma(\mathbf{k}, \omega_s) \\
& \times \left\{ \varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') e^{i\omega_\nu \delta} b^{(\beta)}(\mathbf{q}, \omega_\nu)^* b^{(\beta')}(\mathbf{q}, \omega_\nu) \right. \\
& + \varepsilon_{12}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') b^{(\beta)}(\mathbf{q}, \omega_\nu)^* b^{(\beta')}(-\mathbf{q}, -\omega_\nu)^* \\
& \left. + \varepsilon_{21}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') b^{(\beta)}(\mathbf{q}, \omega_\nu) b^{(\beta')}(-\mathbf{q}, -\omega_\nu) \right\}. \tag{C4}
\end{aligned}$$

In this expression, $S^{(0)}$ is given by Eq.(37), the single-particle eigenvalue $\varepsilon_\sigma(\mathbf{k})$ is given by Eq.(40), $h_0^{(\beta)}$ are mean-field values (which are spin-independent in the *paramagnetic* phase we are considering),⁴² $(\varepsilon_1, \bar{\varepsilon}_1)$ contain the first derivatives of the bosonic hopping factor while $(\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{21})$ contain the second derivatives. Note that, similarly to the expression (46) in the ‘‘radial’’ gauge, in the last term on the right-hand side of Eq.(C4) only pairs of fermionic variables with the same \mathbf{k} and ω_s have been retained (owing to space and time translational invariance).

After integration of the Grassmann variables, the terms in Eq.(C4) containing $(\varepsilon_1, \bar{\varepsilon}_1)$ will be $\mathcal{O}(\delta^2)$ due to the fact that the function Π_M given by Eq.(B4) is of $\mathcal{O}(\delta)$ and can thus be ignored. By the same token, we can avoid reporting the expressions for ε_{12} and ε_{21} since they contribute at $\mathcal{O}(\delta^2)$. In fact, to the $\mathcal{O}(\delta)$ we are concerned here we need only the symmetry properties

$$\begin{aligned}
\varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') &= \varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta', \beta) \\
\varepsilon_{21}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') &= \varepsilon_{12}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \\
\varepsilon_{21}(-\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') &= \varepsilon_{21}(\mathbf{q}; \mathbf{k}, \sigma | \beta', \beta)
\end{aligned} \tag{C5}$$

as well as the explicit expression of ε_{11} for $\beta = \beta'$:

$$\begin{aligned}
\varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta) &= t \left\{ \gamma(\mathbf{k}) z_0 \left(\frac{\partial^2 z_{j,\sigma}^*(m-1, m)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} + \frac{\partial^2 z_{j,\sigma}(m, m-1)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} \right) \right. \\
& + \gamma(\mathbf{k} + \mathbf{q}) \frac{\partial z_{j,\sigma}^*(m-1, m)}{\partial b_{j,m}^{(\beta)*}} \Big|_{\underline{b}_0} \frac{\partial z_{j,\sigma}(m, m-1)}{\partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} \\
& \left. + \gamma(\mathbf{k} - \mathbf{q}) \frac{\partial z_{j,\sigma}^*(m-1, m)}{\partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} \frac{\partial z_{j,\sigma}(m, m-1)}{\partial b_{j,m}^{(\beta)*}} \Big|_{\underline{b}_0} \right\} \tag{C6}
\end{aligned}$$

where z_0 and $\gamma(\mathbf{k})$ are given by Eqs.(64) and (41) of the text, respectively, and \underline{b}_0 stands for the set $\{b_0^{(\beta)}; \beta = 1, \dots, 4\}$ of Eq.(C2). These are, in essence, the simplifying features which make it easier obtaining the ‘‘contribution from infinity’’ to the free energy in the ‘‘Cartesian’’ gauge.

Integrating out the Grassmann variables, expanding the resulting logarithm up to quadratic order in the bosonic fields, and keeping only terms up to $\mathcal{O}(\delta)$ (while preserving, however, the full exponential $\exp\{i\omega_\nu \delta\}$ - cf. Section II), we obtain the effective action:

$$\begin{aligned}
S_{eff} &= \beta \mathcal{N} F_0 + \delta \sum_{\mathbf{q}} \sum_{\nu=1}^{BZ} \sum_{\beta, \beta'=1}^{M-1} \left\{ b^{(\beta)}(\mathbf{q}, \omega_\nu)^* \left[\delta_{\beta, \beta'} \frac{1 - e^{i\omega_\nu \delta}}{\delta} \right. \right. \\
& + e^{i\omega_\nu \delta} \left(\delta_{\beta, \beta'} h_0^{(\beta)} + \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \right) \Big] b^{(\beta')}(\mathbf{q}, \omega_\nu) \\
& + b^{(\beta)}(\mathbf{q}, \omega_\nu)^* \left[\frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{12}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \right] b^{(\beta')}(-\mathbf{q}, -\omega_\nu)^* \\
& \left. + b^{(\beta)}(\mathbf{q}, \omega_\nu) \left[\frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{21}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \right] b^{(\beta')}(-\mathbf{q}, -\omega_\nu) \right\} \tag{C7}
\end{aligned}$$

with F_0 given by Eq.(53) of the text. It is convenient to introduce at this point the column vector

$$\underline{a}(\mathbf{q}, \omega_\nu) = \begin{pmatrix} b^{(1)}(\mathbf{q}, \omega_\nu) \\ \vdots \\ b^{(4)}(\mathbf{q}, \omega_\nu) \\ b^{(1)}(-\mathbf{q}, -\omega_\nu)^* \\ \vdots \\ b^{(4)}(-\mathbf{q}, -\omega_\nu)^* \end{pmatrix} \quad (\text{C8})$$

and its adjoint $\underline{a}^\dagger(\mathbf{q}, \omega_\nu) = (b^{(1)}(\mathbf{q}, \omega_\nu)^*, \dots, b^{(4)}(\mathbf{q}, \omega_\nu)^*, b^{(1)}(-\mathbf{q}, -\omega_\nu), \dots, b^{(4)}(-\mathbf{q}, -\omega_\nu))$, which allow to rewrite Eq. (C7) in the compact form

$$S_{eff} = \beta \mathcal{N} F_0 + \frac{1}{2} \sum_{\mathbf{q}} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \underline{a}^\dagger(\mathbf{q}, \omega_\nu) \mathbf{\Gamma}(\mathbf{q}, \omega_\nu) \underline{a}(\mathbf{q}, \omega_\nu) \quad (\text{C9})$$

(excluding the $\nu = 0$ term). The fluctuation matrix in (C9) can be conveniently decomposed as follow:

$$\mathbf{\Gamma}(\mathbf{q}, \omega_\nu) = \mathbf{\Gamma}_0(\omega_\nu) + \delta \mathbf{\Gamma}_1(\mathbf{q}, \omega_\nu) \quad (\text{C10})$$

where

$$\mathbf{\Gamma}_0(\omega_\nu) = \begin{pmatrix} (1 - e^{i\omega_\nu \delta}) \mathbf{1} & 0 \\ 0 & (1 - e^{-i\omega_\nu \delta}) \mathbf{1} \end{pmatrix} \quad (\text{C11})$$

($\mathbf{1}$ being the 4×4 unit matrix) and $\mathbf{\Gamma}_1$ has the block form

$$\mathbf{\Gamma}_1(\mathbf{q}, \omega_\nu) = \begin{pmatrix} \mathbf{A}(\mathbf{q}, \omega_\nu) & \mathbf{B}(\mathbf{q}, \omega_\nu) \\ \mathbf{B}(-\mathbf{q}, -\omega_\nu) & \mathbf{A}(-\mathbf{q}, -\omega_\nu) \end{pmatrix}. \quad (\text{C12})$$

In this expression:

$$\mathbf{A}(\mathbf{q}, \omega_\nu)_{\beta\beta'} = e^{i\omega_\nu \delta} \left(\delta_{\beta,\beta'} h_0^{(\beta)} + \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \right) \quad (\text{C13})$$

and

$$\mathbf{B}(\mathbf{q}, \omega_\nu)_{\beta\beta'} = \frac{2}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{12}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta') \quad (\text{C14})$$

are 4×4 matrices. Note that the block structure in (C12) has been obtained by exploiting the symmetry properties (C5).

The “contribution from infinity” to the (site) free energy can now be obtained from the effective action (C9) in the following way. Performing the Gaussian integration over the bosonic variables $\{\underline{a}(\mathbf{q}, \omega_\nu)\}$ according to the method of Appendix E and expanding the result up to $\mathcal{O}(\delta)$, yields

$$\begin{aligned} & \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \frac{1}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \text{tr} \ln(\mathbf{\Gamma}_0(\omega_\nu) + \delta \mathbf{\Gamma}_1(\mathbf{q}, \omega_\nu)) \\ &= \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \frac{1}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \text{tr} (\ln \mathbf{\Gamma}_0(\omega_\nu) + \mathbf{\Gamma}_0(\omega_\nu)^{-1} \delta \mathbf{\Gamma}_1(\mathbf{q}, \omega_\nu) + \mathcal{O}(\delta^2)) \\ &= \frac{1}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \ln \det \mathbf{\Gamma}_0(\omega_\nu) + \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \frac{1}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \\ & \times \left(\frac{\delta}{1 - e^{i\omega_\nu \delta}} \text{tr} \mathbf{A}(\mathbf{q}, \omega_\nu) + \frac{\delta}{1 - e^{-i\omega_\nu \delta}} \text{tr} \mathbf{A}(-\mathbf{q}, -\omega_\nu) \right) \end{aligned}$$

$$\begin{aligned}
&= \frac{4}{\beta} \sum_{\nu=1}^{\frac{M-1}{2}} \ln(1 - e^{i\omega_\nu \delta})(1 - e^{-i\omega_\nu \delta}) \\
&+ \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \frac{BZ}{2\beta} \sum_{\nu=-\frac{M-1}{2}}^{\frac{M-1}{2}} \sum_{\beta=1}^4 \left(\frac{\delta e^{i\omega_\nu \delta}}{1 - e^{i\omega_\nu \delta}} E_\beta(\mathbf{q}) + \frac{\delta e^{-i\omega_\nu \delta}}{1 - e^{-i\omega_\nu \delta}} E_\beta(-\mathbf{q}) \right) \\
&= \frac{4}{\beta} \ln M - \frac{1}{2} \sum_{\beta=1}^4 \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} E_\beta(\mathbf{q})
\end{aligned} \tag{C15}$$

where the ‘‘quasi-particle’’ energies $E_\beta(\mathbf{q})$ are given by the diagonal elements of the matrix (C13) (apart from the factor $\exp\{i\omega_\nu \delta\}$):

$$E_\beta(\mathbf{q}) = h_0^{(\beta)} + \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} \sum_{\sigma}^{BZ} f_F(\varepsilon_\sigma(\mathbf{k})) \varepsilon_{11}(\mathbf{q}; \mathbf{k}, \sigma | \beta, \beta). \tag{C16}$$

The first term on the right-hand side of Eq.(C15) can be absorbed into the overall normalization factor of the functional integral, while the second term gives the desired ‘‘contribution from infinity’’ $F_1^{(d)}$ to the free energy. Upon recalling the expression (C6) for ε_{11} , as well as the property

$$\sum_{\mathbf{q}}^{BZ} \gamma(\mathbf{k} \pm \mathbf{q}) = 0 \tag{C17}$$

[cf. Eq.(41)], we obtain eventually:

$$\begin{aligned}
F_1^{(d)} &= -\frac{1}{2} \sum_{\beta=1}^4 h_0^{(\beta)} - \frac{1}{2} t z_0 \sum_{\beta=1}^4 \sum_{\sigma} \left(\frac{\partial^2 z_{j,\sigma}^*(m-1, m)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} + \frac{\partial^2 z_{j,\sigma}(m, m-1)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} \right) \\
&\quad \times \frac{1}{\mathcal{N}} \sum_{\mathbf{k}}^{BZ} f_F(\varepsilon_\sigma(\mathbf{k})) \gamma(\mathbf{k}).
\end{aligned} \tag{C18}$$

There remains to verify that the result (C18) obtained within the ‘‘Cartesian’’ gauge coincides *at self-consistency* (i.e., when $\partial F_0 / \partial b_0^{(\beta)2} = 0$ for each β) with the result (62) obtained within the ‘‘radial’’ gauge. To this end, we get by comparing Eqs. (C1) and (9)

$$-\frac{1}{2} \sum_{\beta=1}^4 h_0^{(\beta)} = -2\lambda_0^a + 2\lambda_0^b - \frac{U}{2} \tag{C19}$$

(in the paramagnetic phase), which indeed coincides with the result (62) evaluated at self-consistency for the choice $\mathcal{R} = 1$ (so that $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ vanishes according to Eq. (63)). To verify the complete equivalence of the expressions (C18) and (62) at self-consistency for *any* choice of \mathcal{R} , it is thus enough to show that

$$\begin{aligned}
\mathcal{F}[\mathcal{R}; \underline{b}_0] &= -\frac{z_0}{4} \sum_{\beta=1}^4 \sum_{\sigma} \left(\frac{\partial^2 z_{j,\sigma}^*(m-1, m)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} + \frac{\partial^2 z_{j,\sigma}(m, m-1)}{\partial b_{j,m}^{(\beta)*} \partial b_{j,m-1}^{(\beta)}} \Big|_{\underline{b}_0} \right) \\
&= -z_0 \sum_{\beta=1}^4 \frac{\partial^2 z_\uparrow}{\partial b^{(\beta)*} \partial b^{(\beta)}} \Big|_{\underline{b}_0}
\end{aligned} \tag{C20}$$

for the paramagnetic phase, where

$$z_\uparrow = \left(b^{(1)*} b^{(2)} + b^{(3)*} b^{(4)} \right) \mathcal{R} \left(b^{(1)*} b^{(1)}, b^{(2)*} b^{(2)}, b^{(3)*} b^{(3)}, b^{(4)*} b^{(4)} \right). \tag{C21}$$

For instance, when $\beta = 1$ we obtain

$$\begin{aligned} \left. \frac{\partial^2 z_{\uparrow}}{\partial b^{(1)*} \partial b^{(1)}} \right|_{b_0} &= \left(2 b_0^{(1)} b_0^{(2)} + b_0^{(3)} b_0^{(4)} \right) \frac{\partial \mathcal{R}}{\partial n_1} \\ &+ \left(b_0^{(1)} b_0^{(2)} + b_0^{(3)} b_0^{(4)} \right) b_0^{(1)2} \frac{\partial^2 \mathcal{R}}{\partial n_1^2}, \end{aligned} \quad (\text{C22})$$

with similar expressions for $\beta = 2, 3, 4$. Comparison with Eq.(63) thus enables us to verify that Eq.(C20) holds. This completes the proof. [Recall that, as for Eq.(63), the above derivation holds for a subsidiary operator $R_{i,\sigma}$ in Eq.(4) which is explicitly in normal-ordered form].

Although we have focused thus far in the calculation of the free energy (and derived quantities), this is not the only physical quantity of interest. In particular, it will be relevant to extend the methods developed in this paper to the calculation of correlation functions. Similarly to what we have shown for the free energy, we expect that taking the continuum limit at the outset in the functional integral might miss important contributions also for the correlation functions. In principle, one would have to carry out the calculation of correlation functions via the functional integral formulation with the discretized time mesh and to take consistently the continuum limit only at the end of the calculation. In practice, one could exploit the experience that has been developed for the calculation of the free energy and try to formulate simpler alternative methods for the calculation of the correlation functions. Specifically, developing a suitable diagrammatic theory for the correlation functions could enable one to focus directly on those diagrams which admit “contributions from infinity”. In this respect, there exist significant differences between the “Cartesian” and the “radial” gauge, since in the latter keeping the discretized time mesh results in additional vertices of the diagrammatic theory which vanish identically in the continuum limit. However, the results obtained in the two gauges should coincide order by order in the $1/N$ expansion. For this reason, we expect the calculation of the “contribution from infinity” for the correlation functions to be less involved in the “Cartesian” than in the “radial” gauge, in analogy to what we have just shown for the free energy. One might thus envisage calculating diagrammatically the “contribution from infinity” to a given correlation function (at least at the order $1/N$) in the “Cartesian” gauge and the corresponding continuum contribution in the “radial” gauge since this is not plagued by infrared singularities. To this end, it will be necessary to determine, for each elementary propagator and vertex of the diagrammatic structure, the associated order in the time step δ , in order to select directly those diagrams which have a nonvanishing “contribution from infinity”.⁴³

A rigorous classification of the diagrammatic theory associated with correlation functions is beyond the scope of this paper. Nonetheless, we illustrate the above arguments by working out in detail one example for a physical quantity which can also be derived alternatively from the free energy. This example will explicitly show that a suitable handling of the diagrammatic structure in the “Cartesian” gauge can provide the correct “contribution from infinity” at the order $1/N$.

Let’s consider the average number $\langle d^\dagger d \rangle$ of doubly occupied sites, defined by

$$\langle d^\dagger d \rangle = \frac{1}{\mathcal{N}} \sum_i \frac{1}{M} \sum_{m=0}^{M-1} \langle d_{i,m}^* d_{i,m-1} \rangle \quad (\text{C23})$$

(in the limit $M \rightarrow \infty$) where the average $\langle \dots \rangle$ is evaluated with the action (7). Equation (C23) can be interpreted as the $\mathbf{q} = 0$ and $\omega_\nu = 0$ component of a correlation function; alternatively, it can be obtained as the (total) derivative of the free energy (per lattice site):

$$\langle d^\dagger d \rangle = \frac{dF}{dU}. \quad (\text{C24})$$

We are specifically interested in the “contribution from infinity” to $\langle d^\dagger d \rangle$ at the order $1/N$. We may therefore write

$$\langle d^\dagger d \rangle_\infty = \frac{dF_1^{(d)}}{dU} \quad (\text{C25})$$

with $F_1^{(d)}$ given by Eq. (C18), the derivative being evaluated *at self-consistency* for the mean-field parameters.

With the simplest choice $\mathcal{R} = 1$, $F_1^{(d)}$ is given by Eq. (C19). We obtain in this case

$$\langle d^\dagger d \rangle_\infty = -\frac{1}{2} \sum_{\beta=1}^4 \frac{dh_0^{(\beta)}}{dU} = -\frac{1}{2} \left(\sum_{l=1}^3 v_l \frac{d\lambda^{(l)}}{dU} + 1 \right) \quad (\text{C26})$$

with the use of the dictionary (18) for the Lagrange multipliers, where $v_1 = v_2 = -2$ and $v_3 = 4$. [The magnitude of each v_l represents the number of vertices in the action (7) containing the associated $\lambda^{(l)}$ and any bosonic number operator $b^\dagger b$, while the sign of a given v_l corresponds to the sign of those vertices in that action]. Connection of Eq. (C26) with the diagrammatic structure is then obtained by expressing the derivatives $d\lambda^{(l)}/dU$ therein as follows:

$$\frac{d\lambda^{(l)}}{dU} = \sum_{\alpha=1}^8 G_B(\mathbf{q} = 0, \omega_\nu = 0)_{5+l, \alpha} \frac{\partial^2 F_0}{\partial a_0^{(\alpha)} \partial U} = 2d_0 G_B(\mathbf{q} = 0, \omega_\nu = 0)_{5+l, 4} \quad (\text{C27})$$

where $d_0 = a_0^{(4)}$ and the $\mathbf{q} = 0$ and $\omega_\nu = 0$ bosonic propagator matrix G_B is defined in terms of the inverse of the matrix of the second derivatives of F_0 [cf. Eq. (A15)]. Equation (C26) thus becomes:

$$\langle d^\dagger d \rangle_\infty = -\frac{1}{2} \left(2d_0 \sum_{l=1}^3 v_l G_B(\mathbf{q} = 0, \omega_\nu = 0)_{5+l, 4} + 1 \right). \quad (\text{C28})$$

This result can be obtained directly from the diagrammatic structure, with the provision of associating with *each* bosonic loop (of the type $b^\dagger b$) a ‘‘contribution from infinity’’ equal to $-1/2$. To identify the bosonic loops associated with $\langle d^\dagger d \rangle$ at the order $1/N$, we rewrite the definition (C23) in terms of Eqs.(C2) and (C3):

$$\begin{aligned} \langle d^\dagger d \rangle &= d_0^2 + 2d_0 \frac{1}{\mathcal{N}} \sum_i \frac{1}{M} \sum_{m=0}^{M-1} \langle \tilde{d}_{i,m} \rangle + \frac{1}{\mathcal{N}} \sum_i \frac{1}{M} \sum_{m=0}^{M-1} \langle \tilde{d}_{i,m}^* \tilde{d}_{i,m-1} \rangle \\ &= d_0^2 + 2d_0 d^{(1)} + \frac{1}{\mathcal{N}} \sum_{\mathbf{q}}^{BZ} \frac{1}{M} \sum_{\nu=0}^{M-1} e^{i\omega_\nu \delta} \langle d(\mathbf{q}, \omega_\nu)^* d(\mathbf{q}, \omega_\nu) \rangle \end{aligned} \quad (\text{C29})$$

where $d^{(1)}$ is the $1/N$ shift of the mean-field parameter d_0 (cf. Appendix A). According to our prescription, the bosonic loop given by the last term of Eq.(C29) supplies the term $-1/2$ to $\langle d^\dagger d \rangle_\infty$. Additional bosonic loops, however, are hidden in the definition of $d^{(1)}$. We can, in fact, write [cf. Eq. (A16)]

$$d^{(1)} = \sum_{\alpha=1}^8 G_B(\mathbf{q} = 0, \omega_\nu = 0)_{4, \alpha} \frac{\partial F_1}{\partial a^{(\alpha)}} \quad (\text{C30})$$

and identify $|v_l|$ loops in $\partial F_1 / \partial a^{(\alpha)}$ for $\alpha = 5 + l$ associated with a vertex $\lambda^{(l)} b^* b$. Taking also into account the sign of these vertices in the action, we obtain for the ‘‘contribution from infinity’’ to $d^{(1)}$ the expression

$$d_\infty^{(1)} = \sum_{l=1}^3 G_B(\mathbf{q} = 0, \omega_\nu = 0)_{4, 5+l} v_l \left(-\frac{1}{2} \right) \quad (\text{C31})$$

according to our prescription. We have thus verified that the ‘‘contribution from infinity’’ obtained from the diagrammatic structure of the correlation function (C29) coincides with the result (C28), at least for the simplest choice $\mathcal{R} = 1$ of the subsidiary function.

When \mathcal{R} is not unity, $F_1^{(d)}$ is given by (C18) and not simply by (C19). Besides the terms (C26), there exists thus the following additional contribution to $\langle d^\dagger d \rangle_\infty$:

$$\begin{aligned} \frac{d}{dU} \left(\mathcal{F}[\mathcal{R}; \underline{b}_0] \frac{2t}{\mathcal{N}} \sum_{\mathbf{k}}^{BZ} \gamma(\mathbf{k}) f_F(\varepsilon_{\mathbf{k}}) \right) &= \\ = 2d_0 \sum_{\alpha=1}^8 \frac{\partial}{\partial a_0^{(\alpha)}} \left(\mathcal{F}[\mathcal{R}; \underline{b}_0] \frac{2t}{\mathcal{N}} \sum_{\mathbf{k}}^{BZ} \gamma(\mathbf{k}) f_F(\varepsilon_{\mathbf{k}}) \right) G_B(\mathbf{q} = 0, \omega_\nu = 0)_{\alpha, 4} \end{aligned} \quad (\text{C32})$$

since $\mathcal{F}[\mathcal{R}; \underline{b}_0]$ and $\varepsilon_{\mathbf{k}}$ depend on U only through \underline{a}_0 (with \mathcal{F} given by Eq. (C20)). The derivatives on the right-hand side of Eq.(C32), which act alternatively on the bosonic or the fermionic factor, are associated with two different classes of diagrams each containing the relevant (i.e., $b^* b$) bosonic loops. It is clear that these diagrams represent additional contributions to the $1/N$ shift $d^{(1)}$ [cf. Eq. (C30)], and that the relevant bosonic loops therein arise from the ‘‘vertex’’ (C20) and its derivatives. One can readily verify that the result (C32) is eventually recovered by following again our prescription of assigning a ‘‘contribution from infinity’’ equal to $-\frac{1}{2}$ to each bosonic loop of the type $b^\dagger b$ identified in the diagrammatic structure.⁴⁴

APPENDIX D: EXACT SOLUTION FOR A ONE-LEVEL TWO-SITE MODEL

The one-level two-site model Hamiltonian, which was considered in Section III for numerical calculations with the functional integral approach, can readily be diagonalized. For the physical case of spin 1/2, the energy eigenvalue ε_l ($l = 1, 2, \dots, 10$) and the associated degeneracy factor g_l for the l -th level with particle number N_l ($= 0, 1, \dots, 4$) [or, equivalently, with particle density per lattice site $n_l (= 0, 1/2, 1, 3/2, 2)$] are reported in Table I, where

$$\varepsilon_{\pm} = \frac{U}{2} \pm \sqrt{\left(\frac{U}{2}\right)^2 + (4t)^2}. \quad (\text{D1})$$

States with $g_l = 1, 2, 3$ correspond to spin singlet, doublet, and triplet in the order. Note that, due to the use of periodic boundary condition, the “effective” hopping between the two sites is $2t$ and not t .³⁰

Once the set $(N_l, \varepsilon_l, g_l)$ is known, the grand-canonical partition function can be obtained from its definition

$$\mathcal{Z} = \sum_l g_l \exp\{-\beta(\varepsilon_l - \mu N_l)\} \quad (\text{D2})$$

for given β and μ . The chemical potential can be then eliminated in favor of the mean particle density n by setting

$$2n = \frac{1}{\mathcal{Z}} \sum_l g_l N_l \exp\{-\beta(\varepsilon_l - \mu N_l)\}. \quad (\text{D3})$$

In this way, the canonical (site) free energy \bar{F} (and thus the site ground-state energy E in the zero-temperature limit) can be obtained as

$$2\bar{F} = -\frac{1}{\beta} \ln \mathcal{Z} + 2n\mu \xrightarrow{\beta \rightarrow \infty} 2E \quad (\text{D4})$$

for arbitrary (even noninteger) values of $2n$. [We refer the reader to Ref.¹⁴ for a discussion about the equivalence between the grand-canonical and canonical ensembles for a finite-size system in the limit $\beta \rightarrow \infty$].

The result (D4) obtained by exact diagonalization for the finite-size system can be compared quantitatively with the approximate results obtained for the same system by the slave-boson approach discussed in the text. This comparison is shown in Section III.

APPENDIX E: GAUSSIAN INTEGRATION WITH A NON HERMITIAN MATRIX

The Gaussian matrices, which we have dealt with by considering the functional-integral representation of the partition function, are not Hermitian (and not even normal). Therefore, integration of the associated quadratic form cannot be performed in a straightforward way by direct matrix diagonalization. Nonetheless, it is possible to readily generalize the procedure for Gaussian integration to the cases of interest, for which the action can be cast in the form

$$S(\underline{x}, \underline{y}) = \underline{x}^T M \underline{x} + 2i \underline{x}^T Q \underline{y} + \underline{y}^T N \underline{y} = (\underline{x}^T, \underline{y}^T) \begin{pmatrix} M & iQ \\ iQ^T & N \end{pmatrix} \begin{pmatrix} \underline{x} \\ \underline{y} \end{pmatrix}. \quad (\text{E1})$$

In this expression, \underline{x} and \underline{y} are sets of n real variables each, M and N are real and symmetric matrices, and Q is a real (but not necessarily symmetric) matrix.⁴⁵ Note that the presence of the factor i (instead of $-i$) in front of Q^T makes the Gaussian matrix in (E1) non Hermitian.

The Gaussian integral

$$I = \int d\underline{x} d\underline{y} e^{-S(\underline{x}, \underline{y})} \quad (\text{E2})$$

with action (E1) can be evaluated by iteration, performing the integration over, say, the variables \underline{y} first. To this end, we assume that all eigenvalues of the matrix N are positive⁴⁶ and exploit the identity

$$\int d\underline{y} \exp\{-\underline{y}^T N \underline{y} - 2i \underline{x}^T Q \underline{y}\} = [\det(N/\pi)]^{-1/2} \exp\{-\underline{x}^T Q N^{-1} Q^T \underline{x}\} \quad (\text{E3})$$

which can be readily proved by diagonalizing the matrix N . The effective action in the variables \underline{x} then reads

$$S_{eff}(\underline{x}) = \underline{x}^T (M + QN^{-1}Q^T) \underline{x} \quad (\text{E4})$$

with an effective Gaussian matrix which is now real and symmetric. Assuming the eigenvalues of this matrix to be all positive,⁴⁶ we obtain eventually

$$I = [\det(N/\pi)]^{-1/2} \cdot [\det(M + QN^{-1}Q^T)/\pi]^{-1/2} . \quad (\text{E5})$$

There remains to show how the product of the two determinants in (E5) is related to the determinant of the original Gaussian matrix in (E1). To this end, we introduce the notation

$$P = M + QN^{-1}Q^T \quad (\text{E6})$$

and use the familiar properties of the determinants, to obtain:

$$\begin{aligned} \det \begin{pmatrix} M & iQ \\ iQ^T & N \end{pmatrix} &= \det \begin{pmatrix} P - QN^{-1}Q^T & iQ \\ iQ^T & N \end{pmatrix} \\ &= \det \begin{pmatrix} P & iQN^{-1} \\ 0 & \mathbf{1} \end{pmatrix} \cdot \det \begin{pmatrix} \mathbf{1} & 0 \\ iQ^T & N \end{pmatrix} \\ &= \det P \cdot \det N = \det(M + QN^{-1}Q^T) \cdot \det N . \end{aligned} \quad (\text{E7})$$

In conclusion, we obtain for the Gaussian integral (E2):

$$I = \left[\det \frac{1}{\pi} \begin{pmatrix} M & iQ \\ iQ^T & N \end{pmatrix} \right]^{-1/2} . \quad (\text{E8})$$

Note that the same result would have been formally obtained if the original Gaussian matrix were Hermitian. By the same token, it can be proved that Wick's theorem for pairwise contractions holds also for a non Hermitian Gaussian matrix of the form (E1).

There remains to show that the Gaussian actions considered in this paper can be cast in the form (E1). We consider the ‘‘radial’’ and ‘‘Cartesian’’ gauges separately.

1. RADIAL GAUGE

Quite generally, the Gaussian part of the action in the ‘‘radial’’ gauge reads

$$R = \sum_q' \left(\underline{r}^T(q), \underline{\lambda}^T(q) \right) \begin{pmatrix} \Gamma_{rr}^g(q) & i\Gamma_{r\lambda}^g(q) \\ i\Gamma_{\lambda r}^g(q) & -\Gamma_{\lambda\lambda}^g(q) \end{pmatrix} \begin{pmatrix} \underline{r}(-q) \\ \underline{\lambda}(-q) \end{pmatrix} , \quad (\text{E9})$$

where $q = (\mathbf{q}, \omega_\nu)$ is restricted to half the available values (say, $\omega_\nu > 0$), $\underline{r}(q)$ and $\underline{\lambda}(q)$ are four-component vectors (corresponding to the components $\alpha = 1, \dots, 4$ and $\alpha = 5, \dots, 8$, respectively, of the vector $\underline{a}(q)$ in Eqs. (44) and (50)), and the 4×4 block matrices $\Gamma_{rr}^g, \Gamma_{r\lambda}^g, \Gamma_{\lambda r}^g$, and $\Gamma_{\lambda\lambda}^g$ are defined in terms of the 8×8 matrix

$$\Gamma^g(q)_{\alpha, \alpha'} = \Gamma(q)_{\alpha, \alpha'} + \Gamma^T(-q)_{\alpha, \alpha'} \quad (\text{E10})$$

with T standing for the transposed matrix and with

$$\Gamma(q)_{\alpha, \alpha'} = \mathcal{B}(q|\alpha, \alpha') + \mathcal{C}(q|\alpha, \alpha') \quad (\text{E11})$$

[cf. Eq. (55)]. The matrix (E11) (and thus the matrix (E10), too) satisfies the symmetry property

$$\Gamma(\mathbf{q}, \omega_\nu)_{\alpha, \alpha'} = \Gamma(-\mathbf{q}, \omega_\nu)_{\alpha, \alpha'} = \Gamma(-\mathbf{q}, -\omega_\nu)_{\alpha, \alpha'}^* \quad (\text{E12})$$

for a lattice with inversion symmetry. [The modes with $\omega_\nu = 0$ and any \mathbf{q} can be treated separately in a straightforward way].

Note that in Eq.(E9) we have restored the imaginary unit i whenever necessary to identify $\underline{\lambda}(q)$ as the Fourier transform of *real* variables.²⁰ Writing

$$\begin{aligned} \underline{r}(q) &= \underline{x}(q) + i\underline{y}(q) \quad , \quad \underline{r}(-q) = \underline{r}(q)^* = \underline{x}(q) - i\underline{y}(q) \\ \underline{\lambda}(q) &= \underline{\xi}(q) + i\underline{\eta}(q) \quad , \quad \underline{\lambda}(-q) = \underline{\lambda}(q)^* = \underline{\xi}(q) - i\underline{\eta}(q) \end{aligned} \quad (\text{E13})$$

where $\underline{x}(q)$, $\underline{y}(q)$, $\underline{\xi}(q)$, and $\underline{\eta}(q)$ are independent real variables, the Gaussian action (E9) reads:

$$R = \sum'_q \left(\underline{x}^T(q), \underline{y}^T(q), \underline{\xi}^T(q), \underline{\eta}^T(q) \right) \begin{pmatrix} M(q) & iQ(q) \\ iQ^T(q) & N(q) \end{pmatrix} \begin{pmatrix} \underline{x}(q) \\ \underline{y}(q) \\ \underline{\xi}(q) \\ \underline{\eta}(q) \end{pmatrix}. \quad (\text{E14})$$

In this expression,

$$M(q) = U \begin{pmatrix} \Gamma_{rr}^g(q) & \mathbf{0} \\ \mathbf{0} & \Gamma_{rr}^g(q)^T \end{pmatrix} U^\dagger \quad (\text{E15})$$

$$Q(q) = U \begin{pmatrix} \Gamma_{r\lambda}^g(q) & \mathbf{0} \\ \mathbf{0} & \Gamma_{\lambda r}^g(q)^T \end{pmatrix} U^\dagger \quad (\text{E16})$$

$$N(q) = U \begin{pmatrix} -\Gamma_{\lambda\lambda}^g(q) & \mathbf{0} \\ \mathbf{0} & -\Gamma_{\lambda\lambda}^g(q)^T \end{pmatrix} U^\dagger \quad (\text{E17})$$

are 8×8 matrices⁴⁷ with

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ i\mathbf{1} & -i\mathbf{1} \end{pmatrix}, \quad (\text{E18})$$

$\mathbf{1}$ being the 4×4 unit matrix. The matrices $M(q)$ and $N(q)$ are real and symmetric, while the matrix $Q(q)$ is real but not symmetric. The quadratic form (E14) is thus of the type (E1). The associated Gaussian integral then becomes:

$$I_R = \prod'_q \left[\det \frac{1}{\pi} \begin{pmatrix} M(q) & iQ(q) \\ iQ^T(q) & N(q) \end{pmatrix} \right]^{-1/2} = \prod'_q \left[\det \frac{1}{\pi} \begin{pmatrix} \Gamma_{rr}^g(q) & i\Gamma_{r\lambda}^g(q) \\ i\Gamma_{\lambda r}^g(q) & -\Gamma_{\lambda\lambda}^g(q) \end{pmatrix} \right]^{-1} \quad (\text{E19})$$

where (E7) has been used to derive the last expression. Note that the same result would have been formally obtained by considering naively the determinant of the original Gaussian matrix in Eq.(E9) twice.

2. CARTESIAN GAUGE

Similarly, the Gaussian part of the action in the ‘‘Cartesian’’ gauge can be cast in the general form [cf. Eqs. (C8) and (C9)]

$$C = \sum'_q \left(\underline{b}^T(q)^*, \underline{b}^T(-q) \right) \begin{pmatrix} A(q) & B(q) \\ B(-q) & A(-q) \end{pmatrix} \begin{pmatrix} \underline{b}(q) \\ \underline{b}(-q)^* \end{pmatrix}, \quad (\text{E20})$$

where $\underline{b}(q)$ and $\underline{b}(-q)$ are four-component vectors and the 4×4 block matrices satisfy the symmetry properties

$$A(q) = A^T(q) = A(-q)^* \quad (\text{E21})$$

$$B(q) = B^T(q) = B(-q) = B(q)^* \quad (\text{E22})$$

for a lattice with inversion symmetry. Introducing the unitary transformation

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & -\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{pmatrix}, \quad (\text{E23})$$

we write

$$V \begin{pmatrix} \underline{b}(q) \\ \underline{b}(-q)^* \end{pmatrix} = \begin{pmatrix} \underline{X}(q) + i\underline{W}(q) \\ \underline{Y}(q) + i\underline{Z}(q) \end{pmatrix} \quad (\text{E24})$$

where $\underline{X}(q)$, $\underline{Y}(q)$, $\underline{W}(q)$, and $\underline{Z}(q)$ are independent real variables, and set

$$V \begin{pmatrix} A(q) & B(q) \\ B(-q) & A(-q) \end{pmatrix} V^\dagger = \begin{pmatrix} M(q) & iQ(q) \\ iQ^T(q) & N(q) \end{pmatrix}. \quad (\text{E25})$$

In this expression

$$M(q) = \frac{1}{2}(A(q) + A(q)^*) - B(q) \quad (\text{E26})$$

$$N(q) = \frac{1}{2}(A(q) + A(q)^*) + B(q) \quad (\text{E27})$$

$$Q(q) = \frac{1}{2i}(A(q) - A(q)^*) \quad (\text{E28})$$

are now all real and symmetric 4×4 matrices. The Gaussian action (E20) thus reads:

$$C = \sum'_q (\underline{X}^T(q), \underline{Y}^T(q), \underline{W}^T(q), \underline{Z}^T(q)) \begin{pmatrix} M(q) & iQ(q) & & \mathbf{0} \\ iQ^T(q) & N(q) & & \\ & & M(q) & iQ(q) \\ \mathbf{0} & & iQ^T(q) & N(q) \end{pmatrix} \begin{pmatrix} \underline{X}(q) \\ \underline{Y}(q) \\ \underline{W}(q) \\ \underline{Z}(q) \end{pmatrix}) \quad (\text{E29})$$

which is just the sum of two quadratic forms of the type (E1). The associated Gaussian integral then becomes

$$I_C = \prod'_q \left[\det \frac{1}{\pi} \begin{pmatrix} M(q) & iQ(q) \\ iQ^T(q) & N(q) \end{pmatrix} \right]^{-1} = \prod'_q \left[\det \frac{1}{\pi} \begin{pmatrix} A(q) & B(q) \\ B(-q) & A(-q) \end{pmatrix} \right]^{-1}. \quad (\text{E30})$$

Again, this result would have been formally obtained by considering simply the determinant of the original Gaussian matrix in Eq. (E20) twice.

¹ A recent review on strong-coupling approaches can be found in P. Fulde, *Electron Correlations in Molecules and Solids* (Springer, Berlin, 1991).

² The requirement of projection can be considered as the central theme of any strong-coupling approach. See, e. g., D. Vollhardt, *Lecture Notes for the International School of Physics "Enrico Fermi" on "Perspectives in Many-Particle Physics"*, Varenna, July 1992.

³ The slave-boson method has been originally introduced by S. E. Barnes [J. Phys. F**6**, 1375 (1976)] and P. Coleman [Phys. Rev. B **29**, 3035(1984)] in the context of the Anderson impurity model.

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

⁵ See, e. g., *Materials and Mechanisms of Superconductivity - High-Temperature Superconductors III*, edited by M. Tachiki, Y. Muto, and Y. Syono (North-Holland, Amsterdam, 1991), Part III.

⁶ M. Lavagna, Phys. Rev. B **41**, 142 (1990); J. W. Rasul and T. Li, J.Phys.C **21**, 5119 (1988).

⁷ A manifestly spin-rotation-invariant formulation of the KR method has been proposed by T. Li, P. Wölfle, and P. J. Hirschfeld, Phys. Rev. B **40**, 6817 (1989). See also R. Frésard and P. Wölfle, Int. J. Mod. Phys. B **6**, 685(1992), and A. Sudbø and A. Houghton, Phys. Rev. B **42**, 4105(1990). The original version of this spin-rotation-invariant formulation was plagued by a drawback related to the normalization of the singly occupied states (at a given site) expressed in terms of the bosonic spin matrix operator, which affected the mean-field solution (in particular, one did not recover the free-particle results at $U = 0$). Although this drawback has been later suitably overcome (see R. Frésard and P. Wölfle, *Erratum*, Int. J. Mod. Phys. B **6**, 3087 (1992)), we prefer to adopt here for simplicity the original KR formulation with a simpler two-component bosonic spinor operator.

⁸ L. Lilly, A. Muramatsu, and W. Hanke, Phys. Rev. Lett. **65**, 1379 (1990).

⁹ M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963), and Phys. Rev. A **137**, 1726 (1965).

¹⁰ See, e. g., Ref.² and references quoted therein.

¹¹ E. Arrigoni, G. C. Strinati, and C. Castellani, Phys. Rev. B **41**, 4838 (1990). See also C. Balseiro *et al.*, Phys. Rev. Lett. **62**, 2624 (1989).

¹² Th. Jolicœur and J. C. Le Guillou, Phys. Rev. B **44**, 2403 (1991).

¹³ L. Zhang, J. K. Jain, and V. J. Emery, Phys. Rev. B **46**, 5599 (1992).

¹⁴ E. Arrigoni, C. Castellani, M. Grilli, R. Raimondi, and G. C. Strinati, Phys. Reports **241**, 291 (1994); see also E. Arrigoni, C. Castellani, R. Raimondi, and G. C. Strinati, Phys. Rev. B **50**, 2700 (1994).

- ¹⁵ E. Arrighoni and G. C. Strinati, Phys. Rev. Lett. **71**, 3178 (1993).
- ¹⁶ R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (Mc Graw-Hill, New York, 1965).
- ¹⁷ L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981), Chapt. 27; see also J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, 1988), Chapt.s 1-2.
- ¹⁸ Cf., e. g., G. Rickayzen, *Green's Functions and Condensed Matter* (Academic, New York, 1980).
- ¹⁹ We set the Boltzmann's constant k_B and Planck's constant \hbar equal to unity throughout.
- ²⁰ Consistently with the notation used in Eqs. (7)-(9), the Lagrange multipliers are understood to be formally integrated from $-i\infty$ to $+i\infty$ in Eq. (6), in order to enforce the constraints (3) correctly. A method to evaluate in practice the associated Gaussian integral will be discussed in Appendix E.
- ²¹ A provision equivalent to taking the normal-ordered operator (5a) has been discussed by K. Schönhammer [Phys. Rev. B **42**, 2591 (1990)], although with the equal-time restriction $m = m'$.
- ²² In this paper, we shall let *all* variables (including the static and homogeneous ones) to fluctuate on equal footing. This procedure entails expanding the action about the leading mean-field solution (i. e., the lowest-order mean field in the $1/N$ expansion). The next-to-leading order ($1/N$) correction to this mean field shows up in the $1/N$ corrections to the mean values of bosonic operators, as discussed in Appendix A. No such correction is, however, needed for the next-to-leading (Gaussian) correction to the free energy discussed in this Section.
- ²³ It can also be readily verified that $g_0 = b_0^{(5)} = 0$ is the only possible solution of the mean-field equations. The value $b_0^{(5)} = 0$ will be thus understood throughout.
- ²⁴ Transformations (29)-(32) are not unitary. This can be compensated by introducing a Jacobian in the functional integral, namely, a factor $(\mathcal{N}M)^{\frac{1}{2}}$ for each bosonic and a factor $(\mathcal{N}M)^{-\frac{1}{2}}$ for each fermionic integration element, \mathcal{N} being the number of lattice sites.
- ²⁵ The terms $\frac{\partial F_0}{\partial b_0^{(5)2}}$ in Eq. (62) are instead important to evaluate the $1/N$ corrections to the mean-field values \underline{b}_0 (cf. Appendix A).
- ²⁶ The fermionic (Grassmann) variables in the functional integral do not pose any problem even in the continuum limit. For this reason, their effects are factored out in the present analysis.
- ²⁷ Alternatively, the "contribution from infinity" (62) can be obtained by the method discussed in Appendix C using the "Cartesian" gauge.
- ²⁸ It can be argued also at a formal level that an operator $R_{i,\sigma}$ not explicitly in normal-ordered form can be more suited for a functional-integral representation than its normal-ordered component $:R_{i,\sigma}:$, whenever $R_{i,\sigma}$ is constructed from an analytic function $f(x)$ with *bounded* radius of convergence. The argument goes schematically as follows. It was pointed out in Ref.¹⁵ that the presence of two different time labels in the expression $f(b_m^* b_{m-1})$, which is associated in the action with the normal-ordered operator $:f(b^\dagger b):$, makes the magnitude of the argument of f unbound irrespective of the presence of operator constraints on $b^\dagger b$. For this reason, the integration domain has always nonvanishing overlap with the complement of the analyticity domain of the function f , yielding questionable results for the functional integral. A possible solution to this problem might result by the heuristic argument of subsection IID, whereby one assumes the existence of an operator transformation Q_c such that, given a function g , the operator $Q_c(g(b^\dagger b))$ is associated with the continuum limit $g(b^*(\tau)b(\tau))$ in the functional integral. To represent $:f(b^\dagger b):$ by a continuum functional integral one has then to find the function g such that $Q_c(g(b^\dagger b)) = :f(b^\dagger b):$. However, for reasonable choices of the transformation Q_c , it turns out that the power series representation of the function g has *vanishing* radius of convergence whenever the corresponding f has finite radius of convergence. This formal finding supports the occurrence of unphysical results obtained when using a normal-ordered operator like $R_{i,\sigma}^{KR}$. On the other hand, by taking $f(b^\dagger b)$ not explicitly in normal-ordered form, we have verified that the corresponding function g has finite radius of convergence, at least for a specific form of Q_c . This formal argument could explain why the unphysical results obtained with the normal-ordered $R_{i,\sigma}^{KR}$ are removed by considering $R_{i,\sigma}^{SQ}$, already at the order $1/N$.
- ²⁹ Specifically, we assume here that the action $S[\underline{b}]$ on the right-hand side of Eq. (A5) is itself written as a power series in $1/N$, namely, $S[\underline{b}] = S_0[\underline{b}] + \frac{1}{N}S_1[\underline{b}] + \dots$. In this way, the partition function becomes at the relevant $1/N$ order:

$$Z = \int \mathcal{D}\underline{b} e^{-(NS_0[\underline{b}] + S_1[\underline{b}])} \simeq Z_0 e^{-\langle S_1[\underline{b}] \rangle_0}$$

where

$$Z_0 = \int \mathcal{D}\underline{b} e^{-NS_0[\underline{b}]} = e^{-\beta F_0}$$

and $\langle S_1[\underline{b}] \rangle_0$ is the average value of $S_1[\underline{b}]$ with weight $\exp\{-NS_0[\underline{b}]\}$. At the relevant $1/N$ order, $\langle S_1[\underline{b}] \rangle_0$ can be then replaced by the mean-field value $S_1[\underline{b}_0]$, yielding $F_0 + S_1[\underline{b}_0]/\beta$ for the total free energy.

- ³⁰ The Hamiltonian (1) refers to an arbitrary number of lattice sites \mathcal{N} with *periodic* boundary conditions. For the two-site model we are considering for numerical calculations, this implies that the effective hopping between sites 1 and 2 is $2t$ and not t , as it will be explicitly taken into account in the exact results of Appendix D. The expressions needed in this Section are consistently recovered from the general expressions of Section II by restricting all wave vectors to the two values 0 and

$\pi/|\Delta|$, where $|\Delta|$ is the distance between the two sites. This restriction gives for the dispersion $\gamma(\mathbf{k})$ of Eq. (41) the values 2 and -2 , in the order.

- ³¹ In the lattice case, the corresponding value of U_c can be formally obtained from Eq. (113) by replacing $4t \rightarrow 32t/\pi^2 (\cong 3.24t)$.
- ³² A complete tabulation of the elements of the matrices \mathcal{B} and \mathcal{C} can be supplied on request.
- ³³ In the numerical calculation of the partition function, the zero-temperature limit has been approached down to a temperature $\beta \cong 10^{-5}t$ and the “half filling” condition has been approached down to a doping level $n - 1 \cong 10^{-3}$.
- ³⁴ The wrong curvature of E/t versus U/t occurs even more prominently with the KR choice for $R_{i,\sigma}$ (cf. Fig.1b).
- ³⁵ E. Arrigoni and G. C. Strinati (unpublished).
- ³⁶ Detailed comparison of the $1/N$ results with the exact results available when $N = 1, 2, \dots, 8$ for a simple model system has been presented in Ref.¹⁴ for the one-slave-boson case.
- ³⁷ A similar $1/N$ expansion for the spin-rotation-invariant method has been introduced in Ref.⁷.
- ³⁸ When a non normal-ordering prescription for $R_{i,\sigma}$ is considered, two additional terms have to be retained on the right-hand side of Eq.(A11) at the order $1/N$. In this case, in fact, $S[\underline{b}]$ is expanded as $NS_0[\underline{b}] + S_1[\underline{b}] + \dots$ (cf. footnote 29) and the linear term in the expansion (A11) can be contracted with the linear term $N^{-1/2} \sum_{r_1} (\partial S_1[\underline{b}]/\partial b_{r_1})_{\underline{b}_0} x_{r_1}$ in the action, which is nonvanishing since it originates from $S_1[\underline{b}]$. One ends up eventually with an additional contribution to the $1/N$ shift $\underline{b}^{(1)}$ of the form (A16), where one replaces F_1 with the $1/N$ correction $S_1[\underline{b}]/\beta$ of the free energy due to the non normal-ordering prescription. The second contribution to (A11), originating at the order $1/N$ from a non normal-ordering prescription for $R_{i,\sigma}$, arises instead from the direct rearrangement of the operator $\phi(b)$ itself as the sum of normal-ordered terms. This provides an extra $1/N$ term of the form $(1/N)\phi_1(\underline{b}_0)$ evaluated at the mean field.
- ³⁹ E. Arrigoni and G. C. Strinati, Phys. Rev. B **44**, 7455 (1991).
- ⁴⁰ The averaging procedure adopted here relies on a spherical angle which is common to the two sites i and j of Eq. (A29), and thus differs from the procedure used in Appendix B of Ref.³⁹.
- ⁴¹ It should be kept in mind that, even in the “Cartesian” gauge, the static part of the bosonic fields has to be represented in polar coordinates. This remark does not obviously affect the calculation of the “contribution from infinity” which originates from “large” frequencies ($\omega_\nu \delta \simeq 1$).
- ⁴² In the “Cartesian” gauge, integration over the Lagrange multipliers involves only zero-frequency terms which are inessential to obtain the “contribution from infinity” we are after.
- ⁴³ Consistently with what it has been done for the free energy, we classify the “contribution from infinity” and the corresponding continuum contribution in the light of the assumptions of the theorem reported in Appendix B [cf. Eqs. (B5)-(B10)]. To this end, the continuum frequency sum (B7) has to be ultraviolet convergent without introducing extra convergence factors. For the “Cartesian” gauge this remark implies, in particular, that each bosonic loop has to be understood to be associated with the symmetrized propagator $\langle (b_\omega^* b_\omega + b_{-\omega}^* b_{-\omega}) \rangle / 2$ that vanishes like ω^{-2} for large $|\omega|$.
- ⁴⁴ This prescription can be maintained even when a non-normal ordered operator $R_{i,\sigma}$ is considered. In this case, one writes $z =: z_{(0)} : + (1/N) : z_{(1)} : + \dots$ where $: z_{(1)} :$ results into additional $1/N$ vertex corrections in the diagrammatic structure. These additional terms can, in turn, be cast in the form of the $1/N$ shift (C30), with F_1 replaced by S_1/β in this case.
- ⁴⁵ More general cases, with the vectors \underline{x} and \underline{y} having different numbers of components, can be considered by the following treatment.
- ⁴⁶ This condition needs to be verified at the outset, being related to the stability of the saddle-point solution.
- ⁴⁷ The expression for $M(q)$ could be somewhat simplified since it can be proved that $\Gamma_{rr}^g(q)$ is a symmetric matrix.

l	1	2	3	4	5	6	7	8	9	10
N_l	0	1	1	2	2	2	2	3	3	4
ε_l	0	$-2t$	$2t$	ε_-	0	U	ε_+	$U - 2t$	$U + 2t$	$2U$
g_l	1	2	2	1	3	1	1	2	2	1

TABLE I. Energy value ε_l and degeneracy factor g_l for the l -th level of the one-level two-site model Hamiltonian corresponding to particle number N_l . ε_\pm are given by Eq. (D1). For given N_l , the levels are ordered for increasing energy. The “empty” ($N_l = 0$) state has been taken as the reference level with $\varepsilon_l = 0$.

FIG. 1. Ground-state energy (in units of t) for the one-level two-site model versus U/t when (a) $n = 1.0$ and (b) $n = 1.2$, obtained by the exact solution and with the KR choice (5a), as explained in the text.

FIG. 2. Ground-state energy (in units of t) per lattice site for the lattice model versus doping $n - 1$ at $U = 0$, obtained with the KR choice (5a). Conventions are explained in the text. Note the change of scale between positive and negative values of E .

FIG. 3. Same as in Fig. 1, with the choice $R_{i,\sigma} = 1$.

FIG. 4. Ground-state energy (in units of t) for the one-level two-site model versus U/t when (a) $n = 1.0$, (b) $n = 1.2$, and (c) $n = 1.5$, with the “linearized” \mathcal{R}^{LIN} given by (121) with $x = x_0$. Conventions are explained in the text. Note the change of scale and the consequent step in the HF solution in (a).

FIG. 5. Ground-state energy (in units of t) for the one-level two-site model versus doping $n - 1$ when (a) $U/t = 0.0$ (b) $U/t = 2.0$, and (c) $U/t = 5.0$, with the choice \mathcal{R}^{LIN} .

FIG. 6. Same as in Fig.1, with the non normal-ordering prescription (5b). Conventions are explained in the text.

FIG. 7. Same as in Fig.5, with the non normal-ordering prescription (5b). Conventions are explained in the text.

FIG. 8. Same as in Fig.2, with the non normal-ordering prescription (5b). Conventions are explained in the text.

(a)

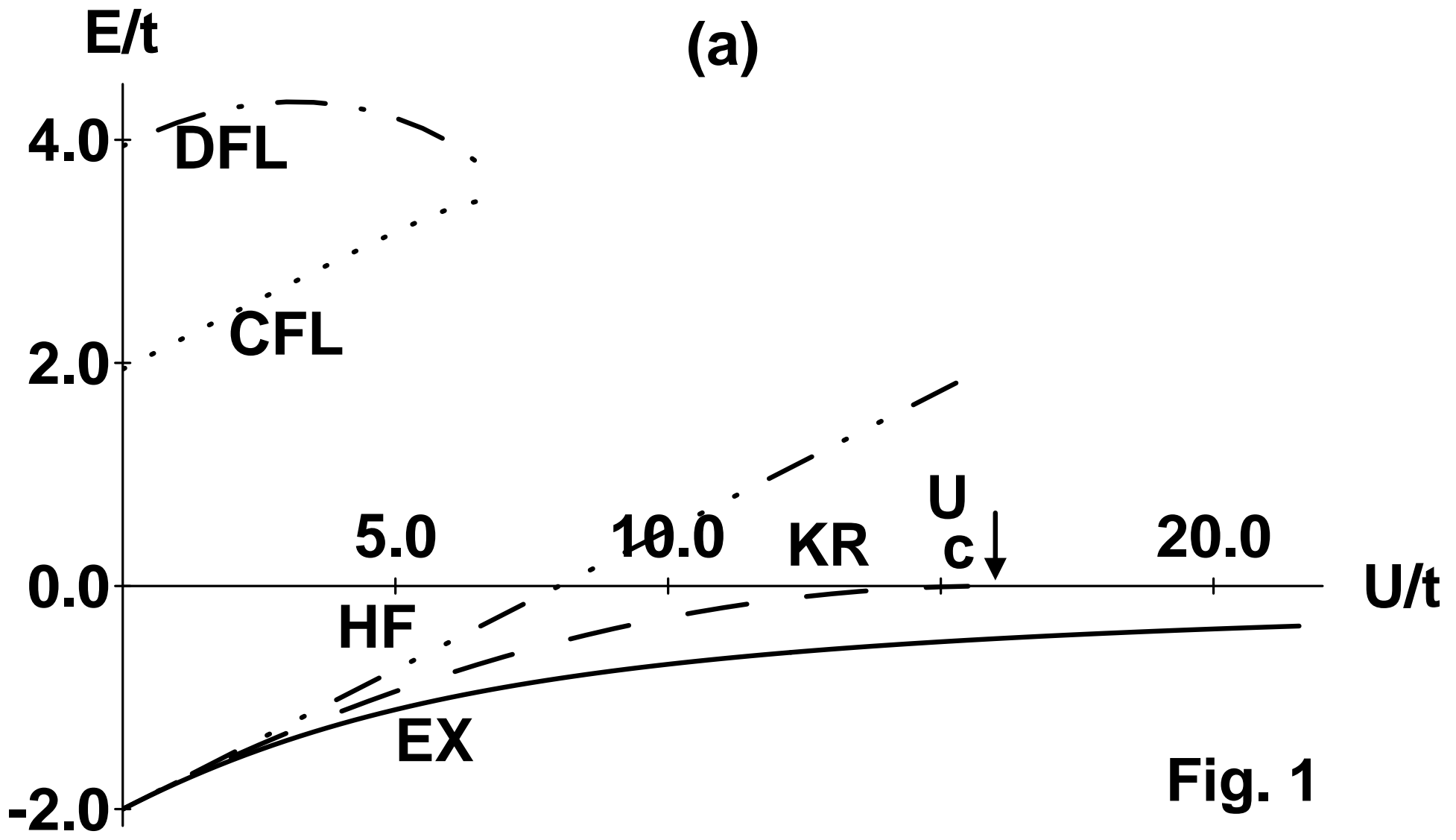


Fig. 1

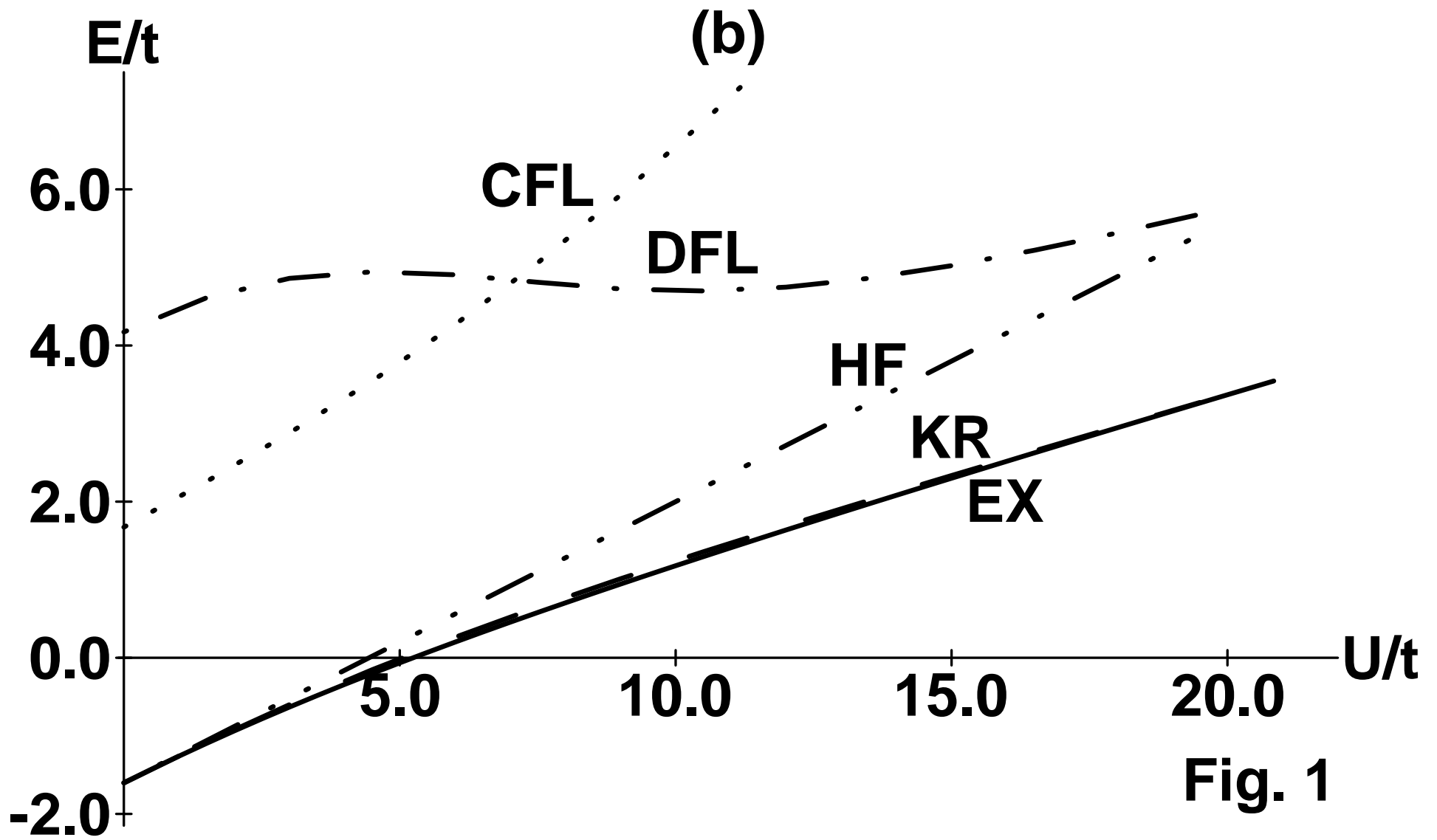


Fig. 1

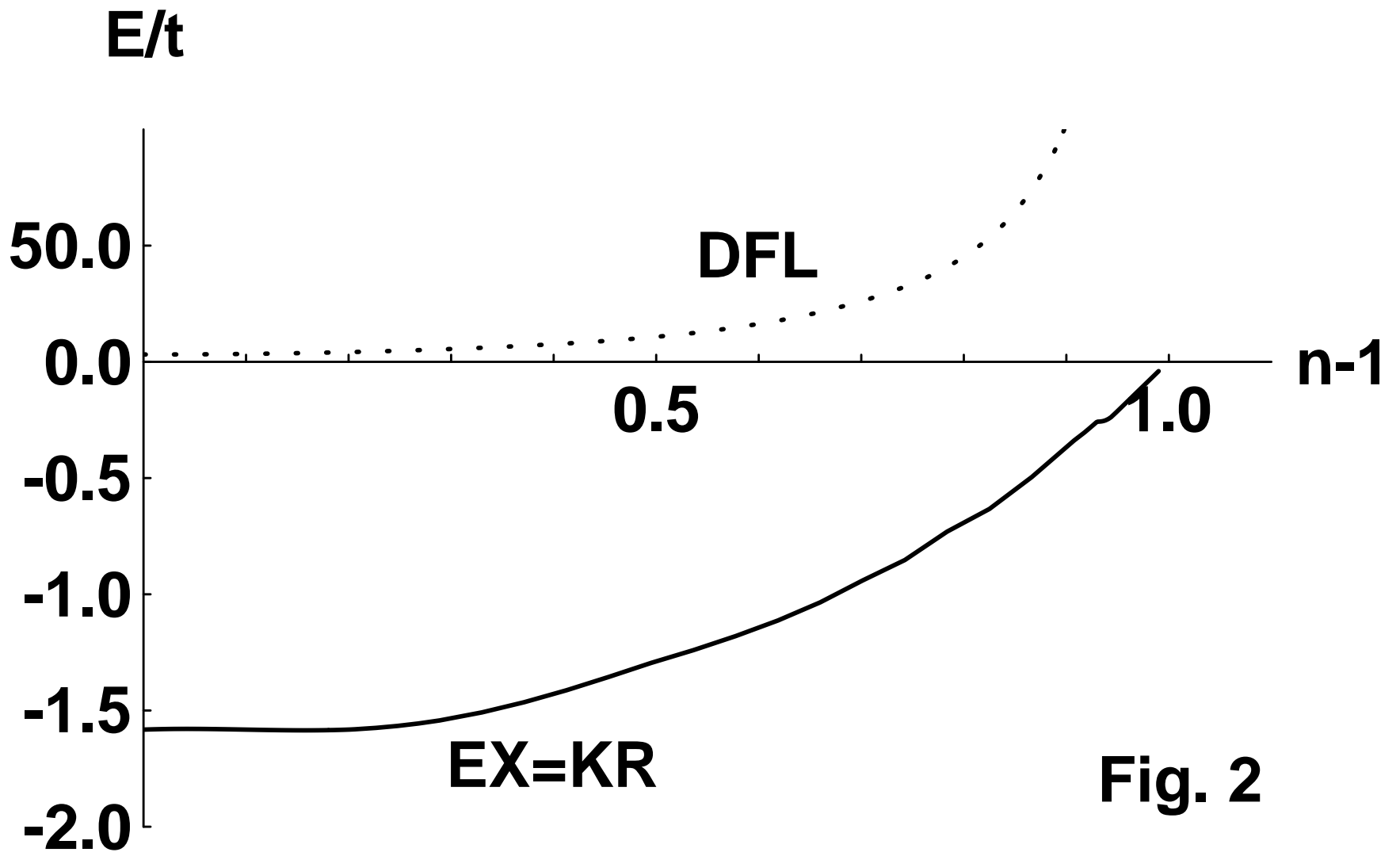


Fig. 2

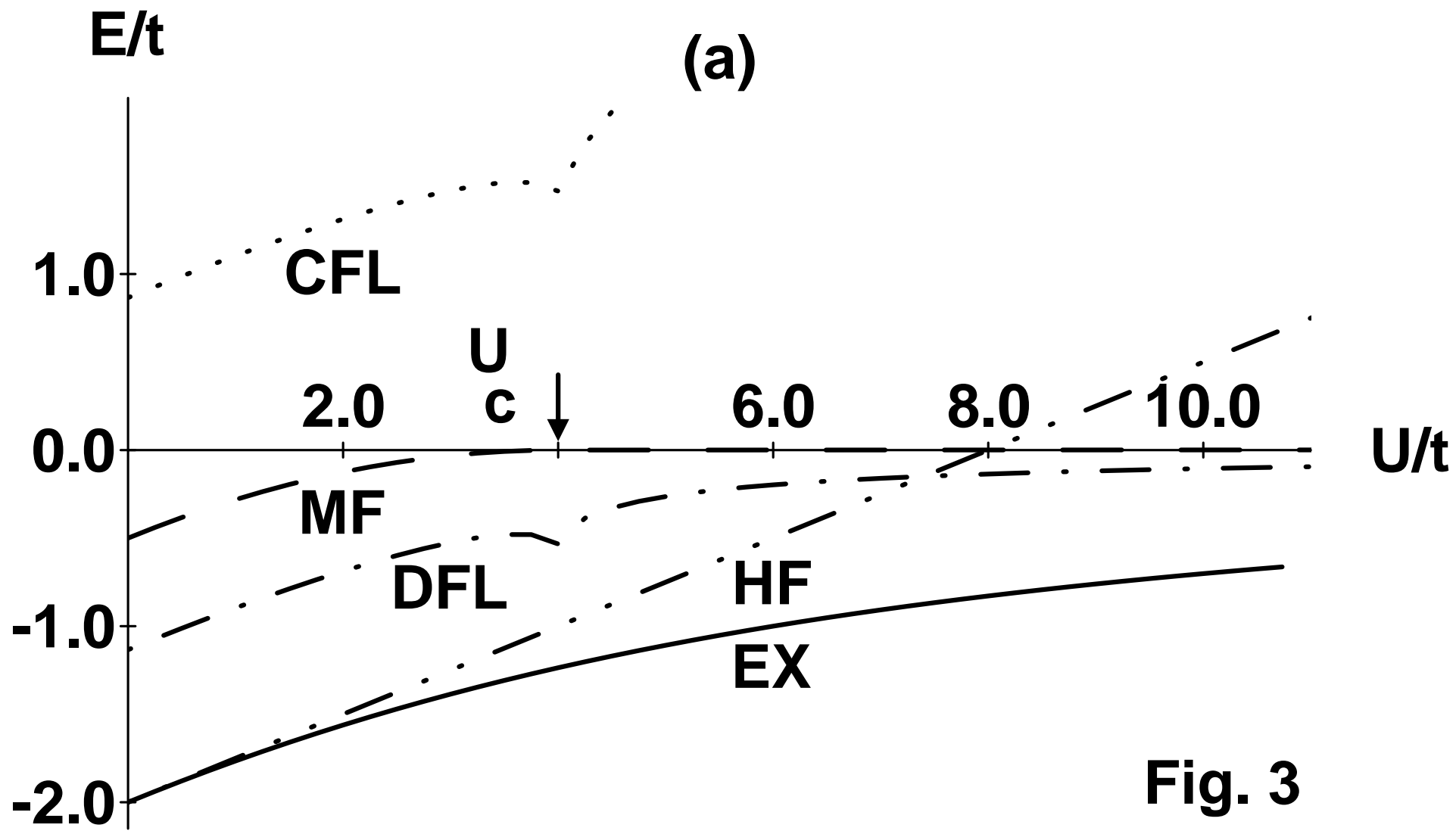
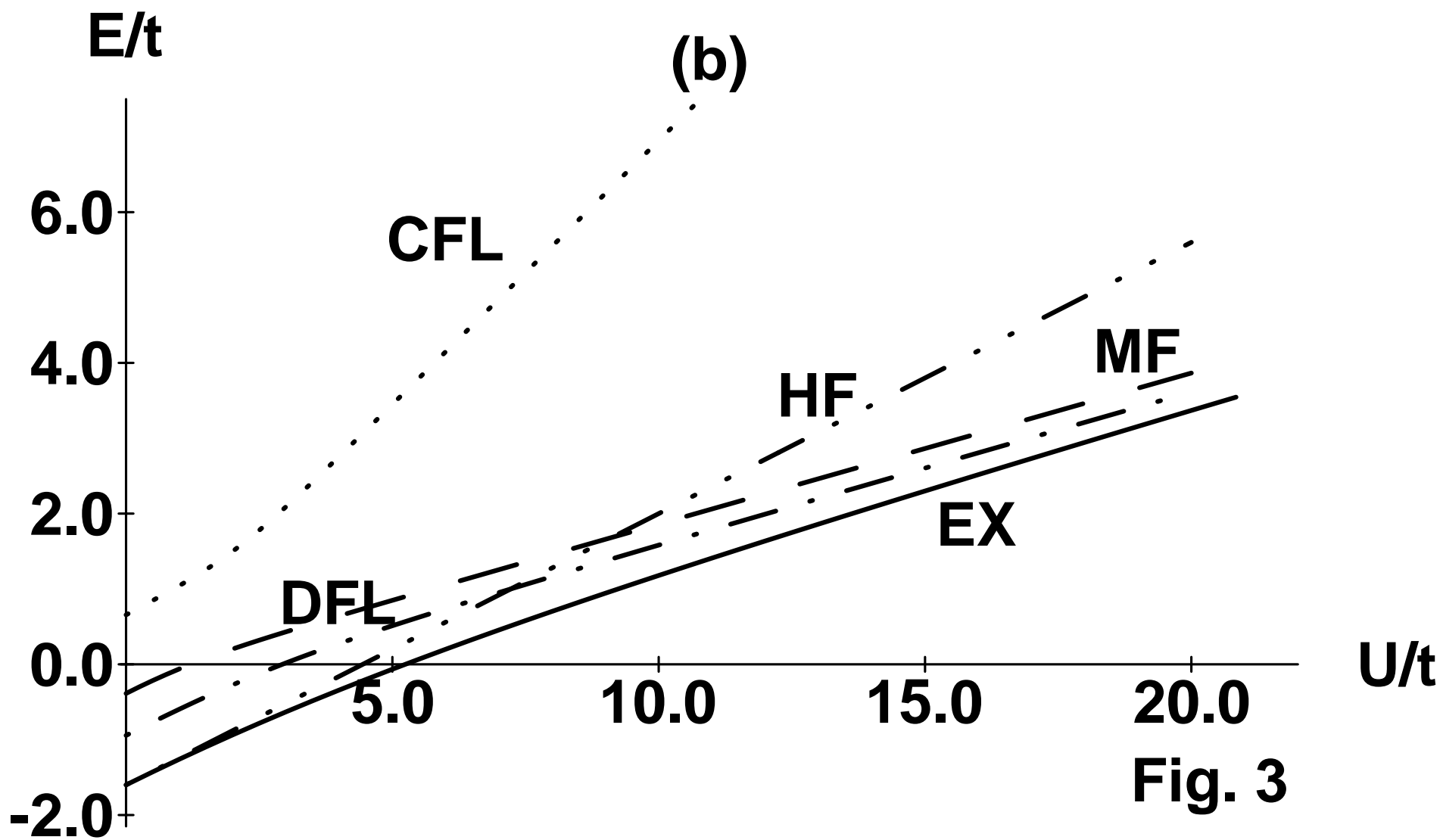
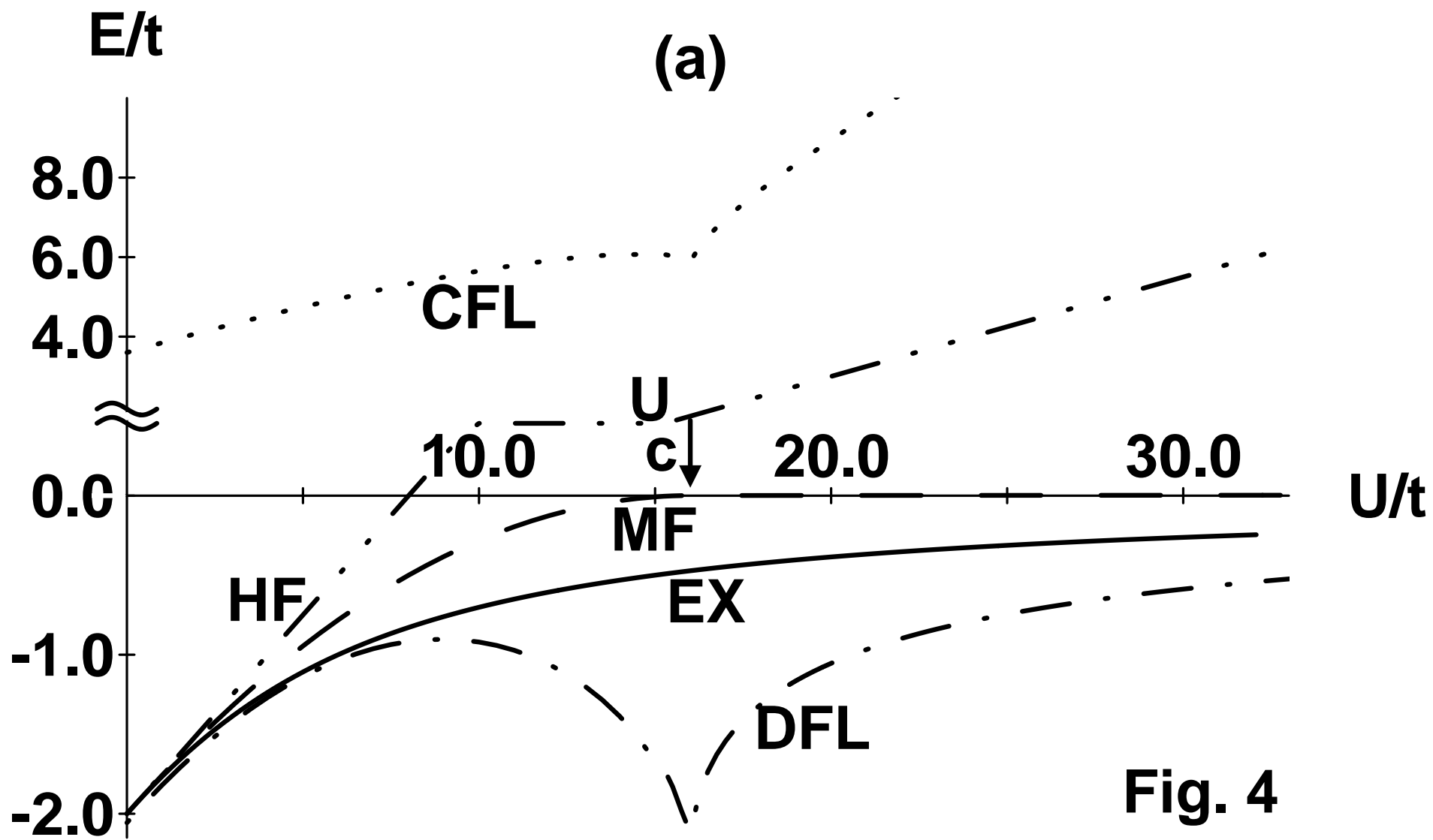
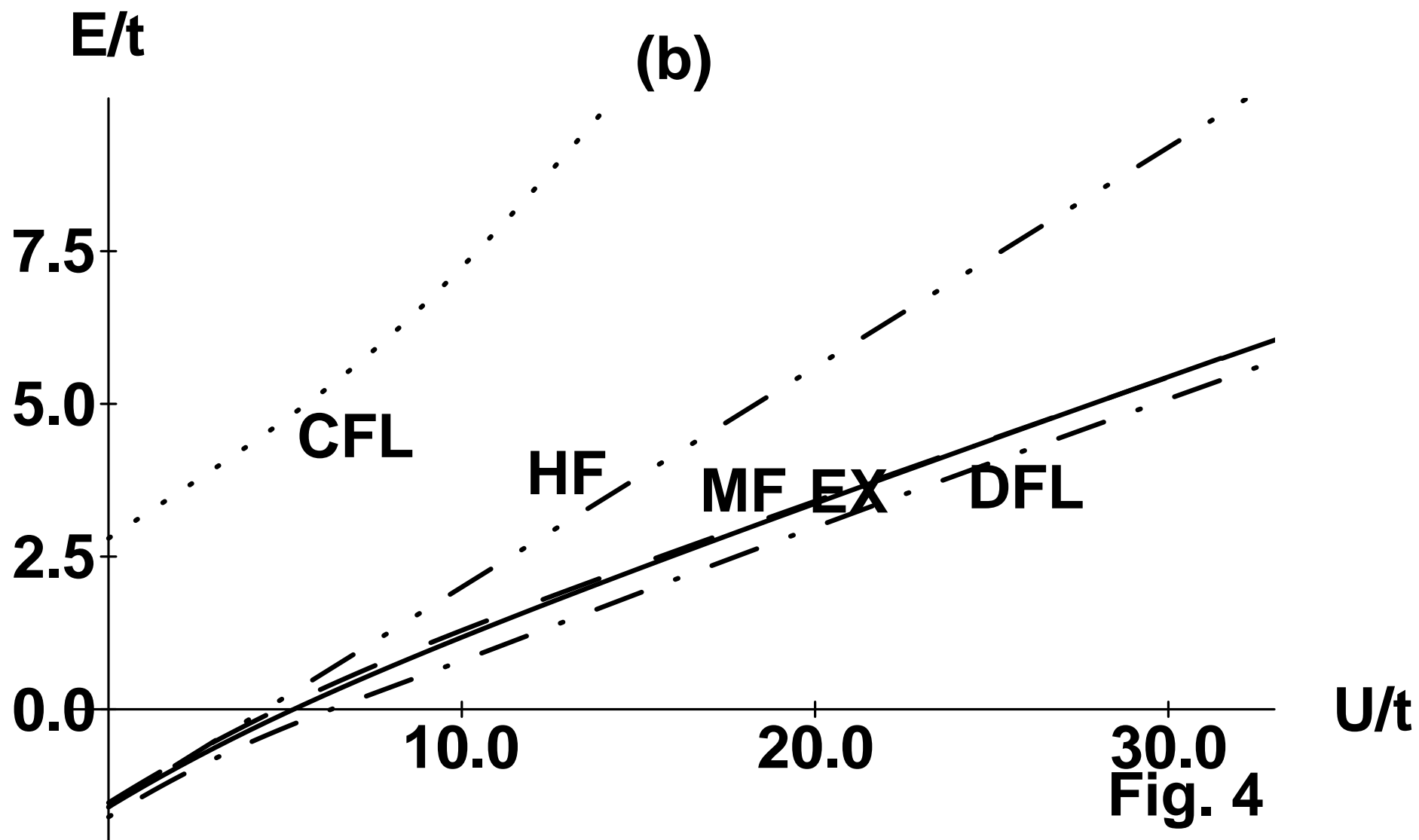
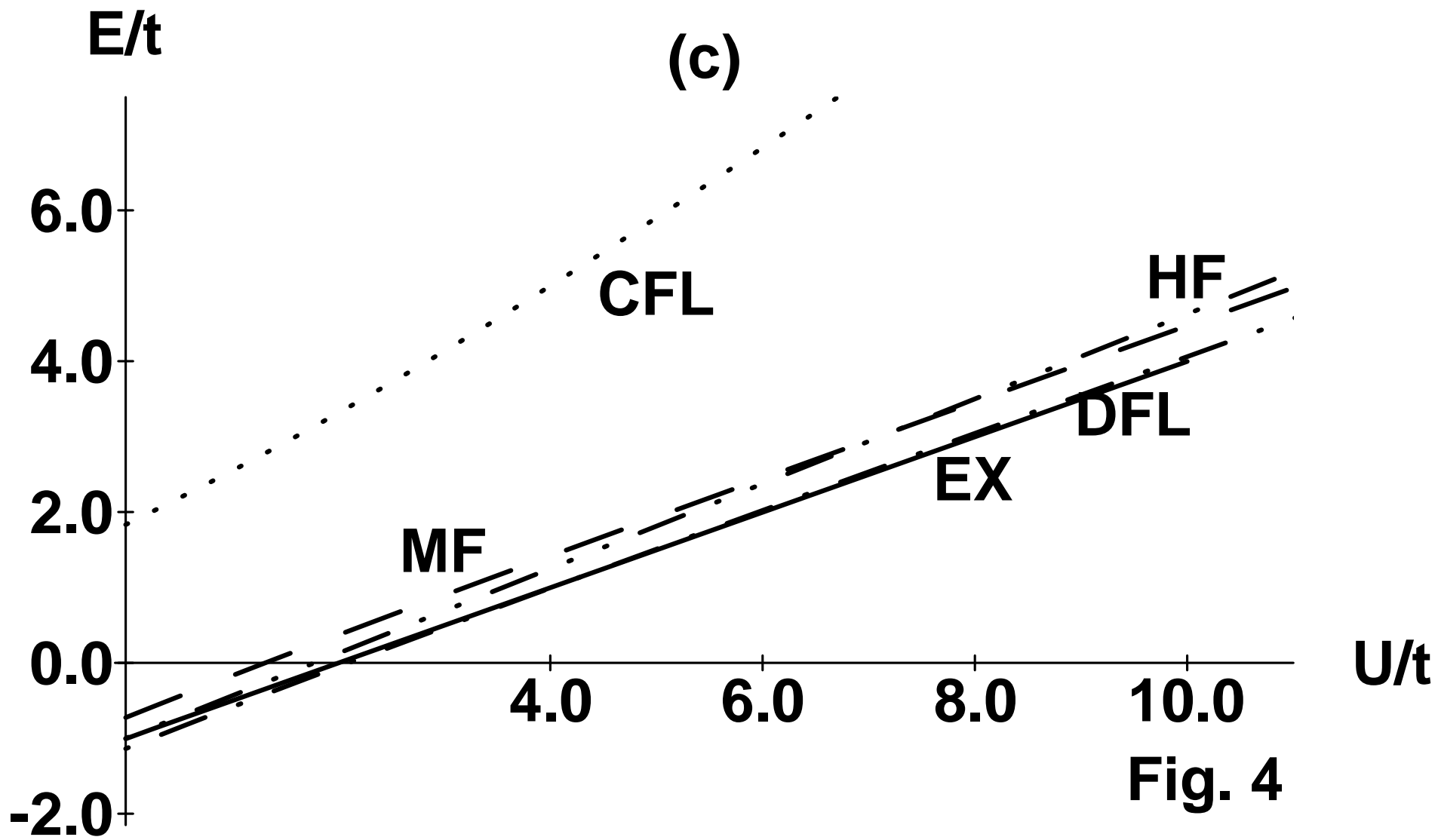


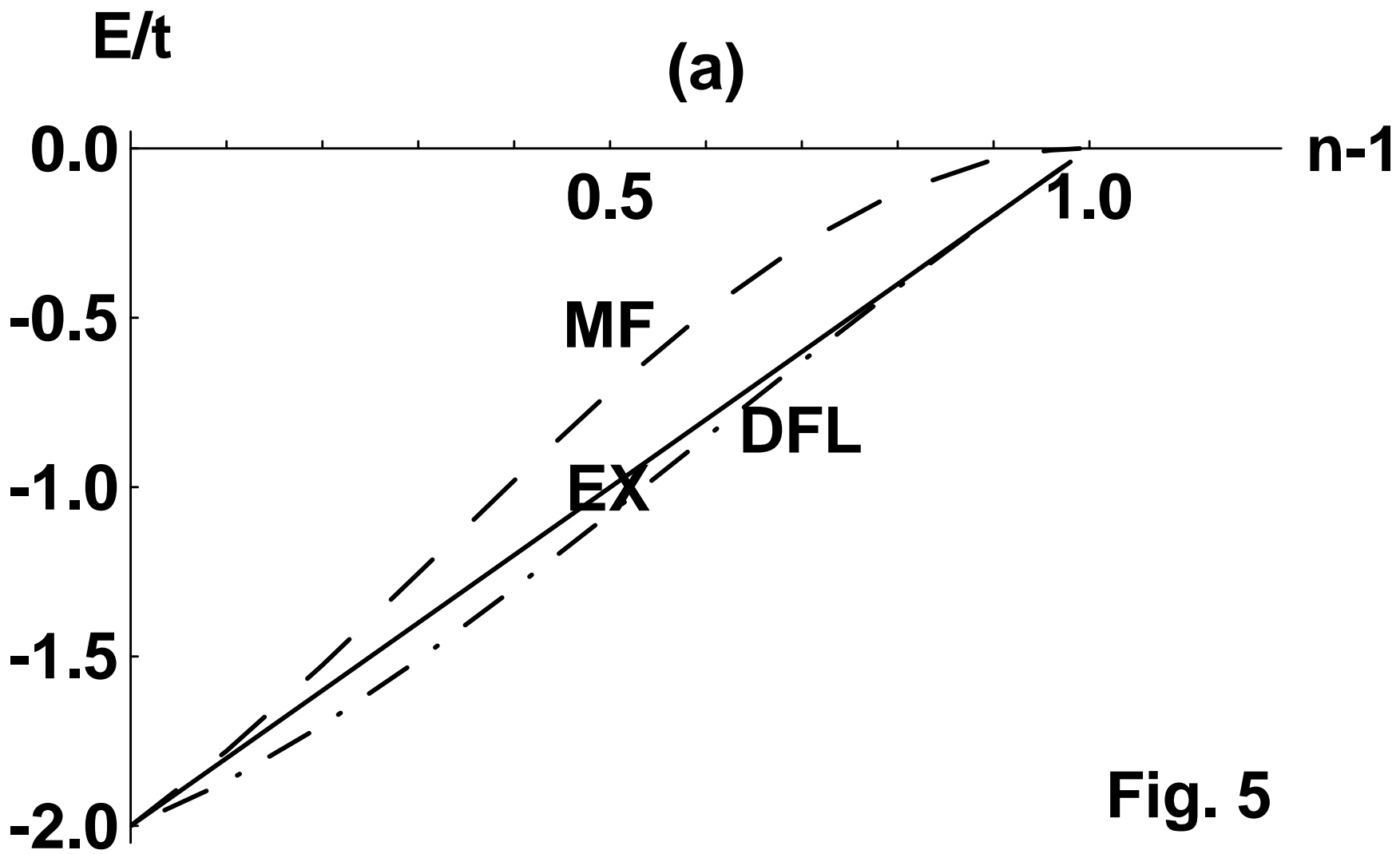
Fig. 3





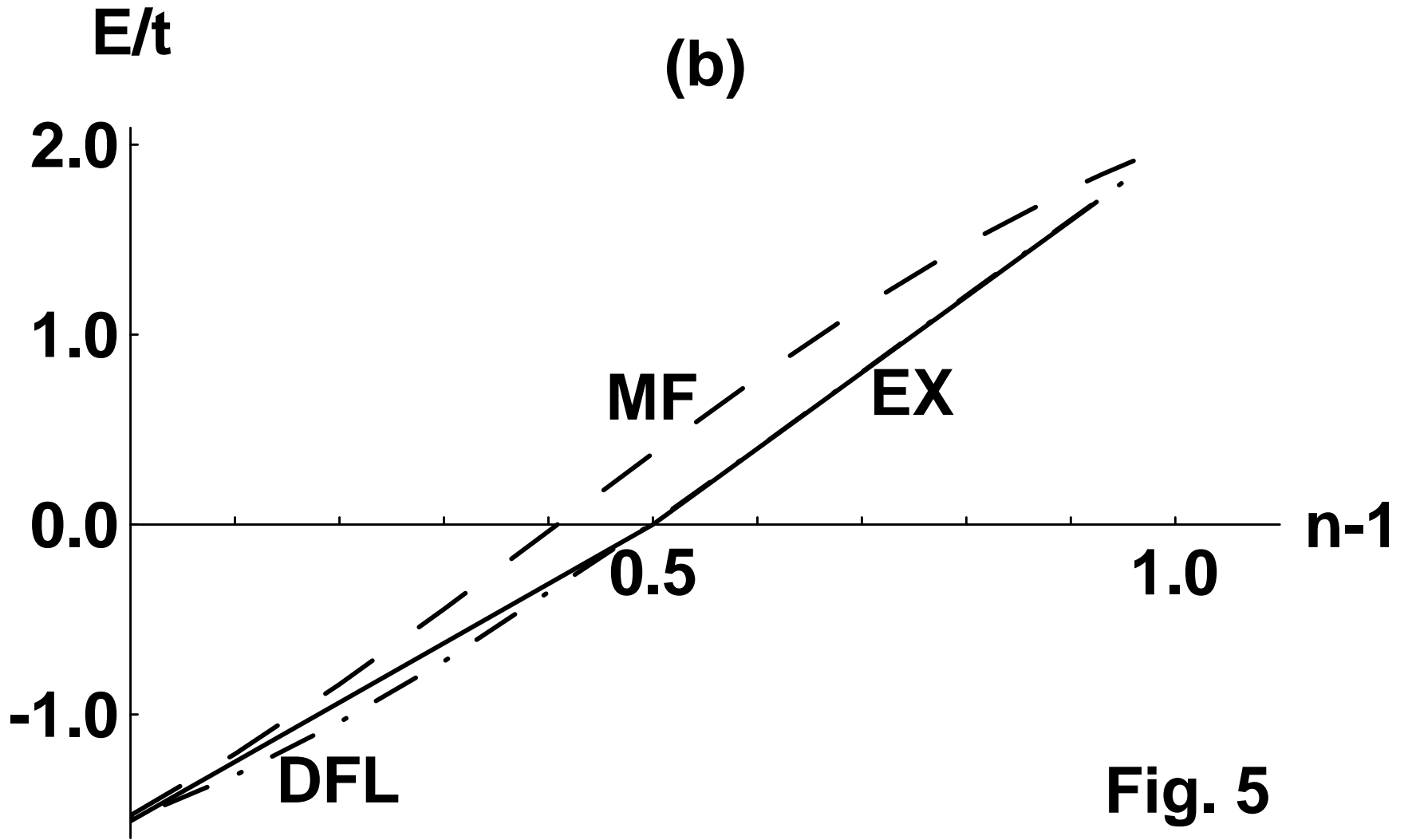


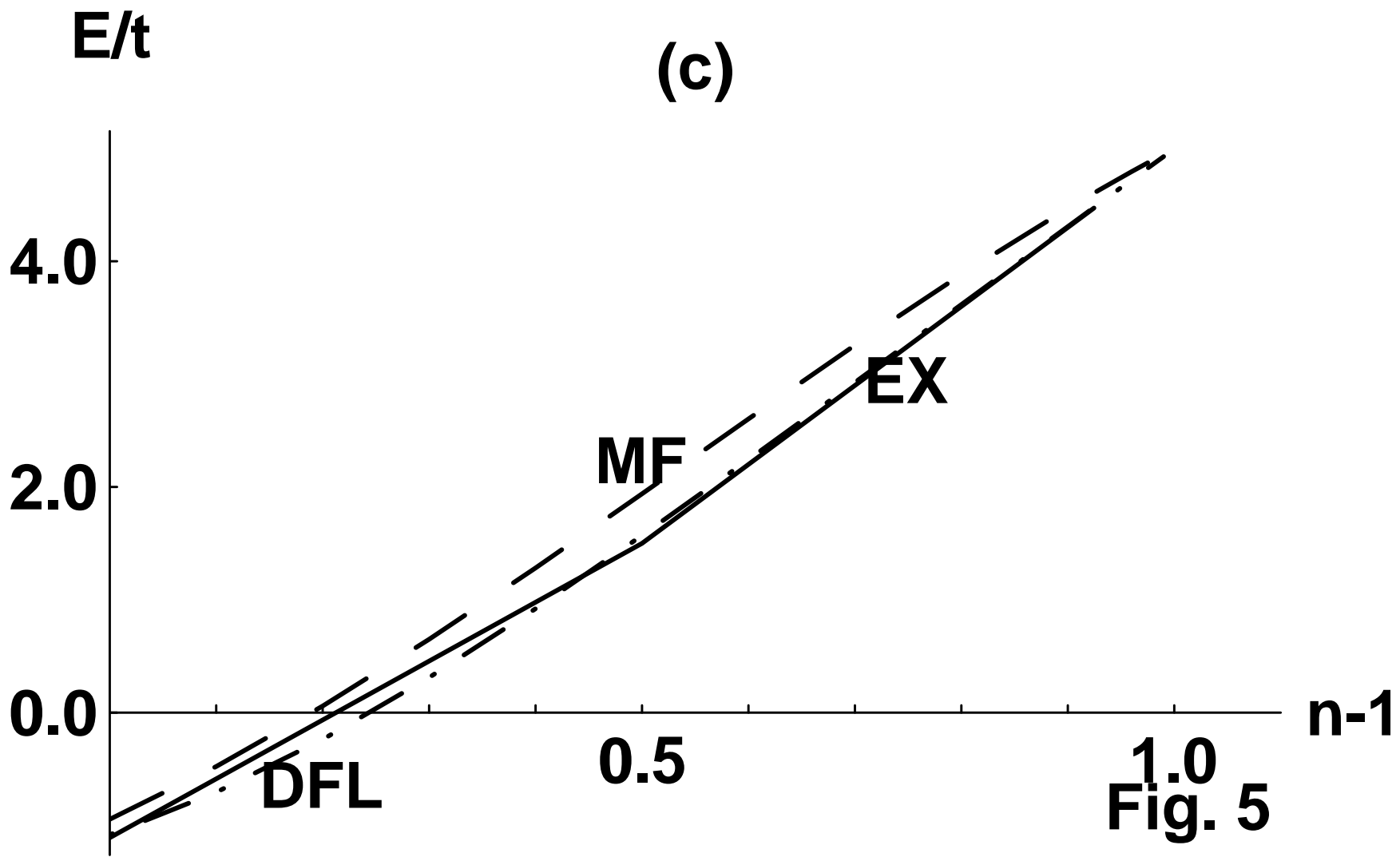


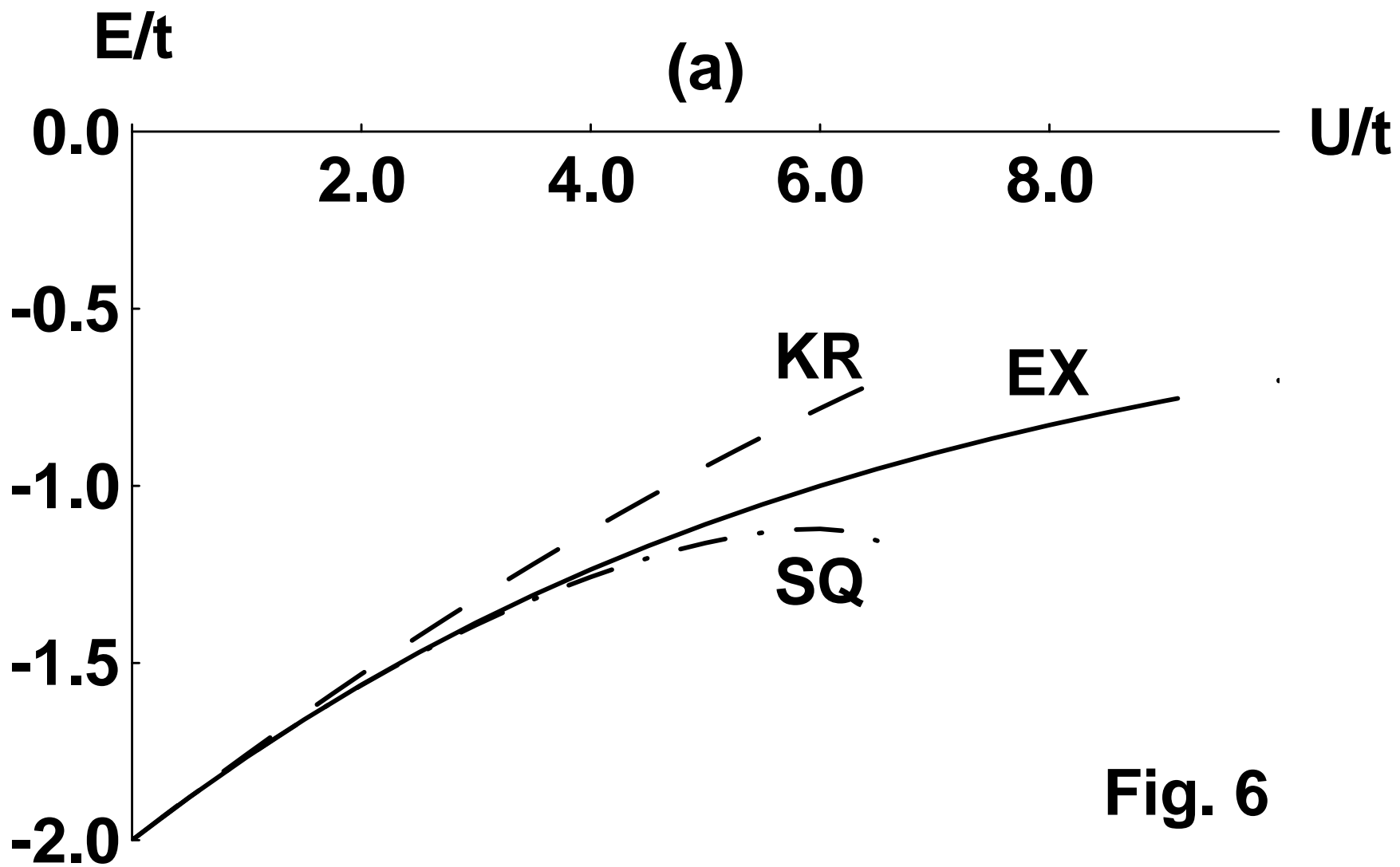


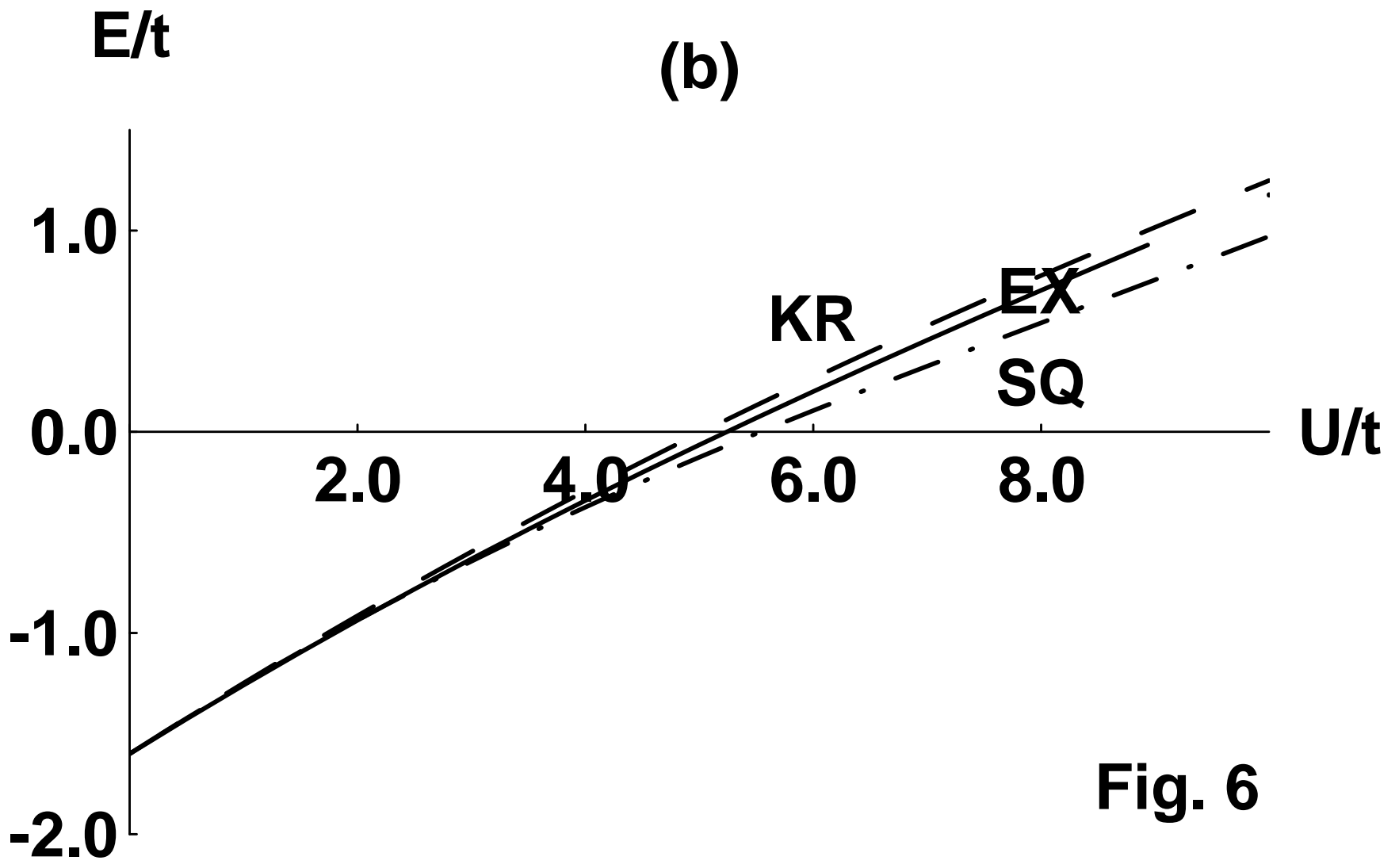
(a)

Fig. 5









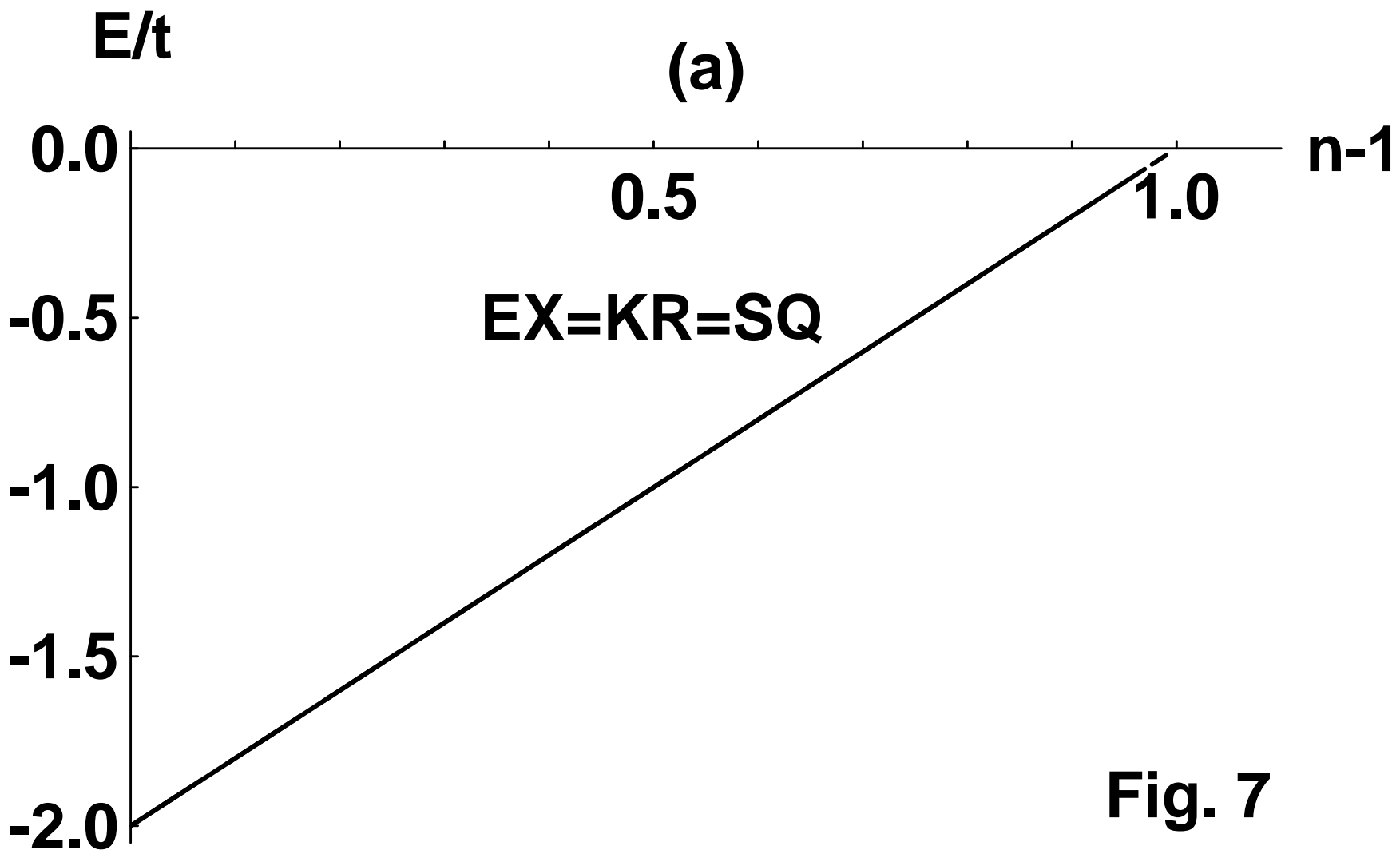
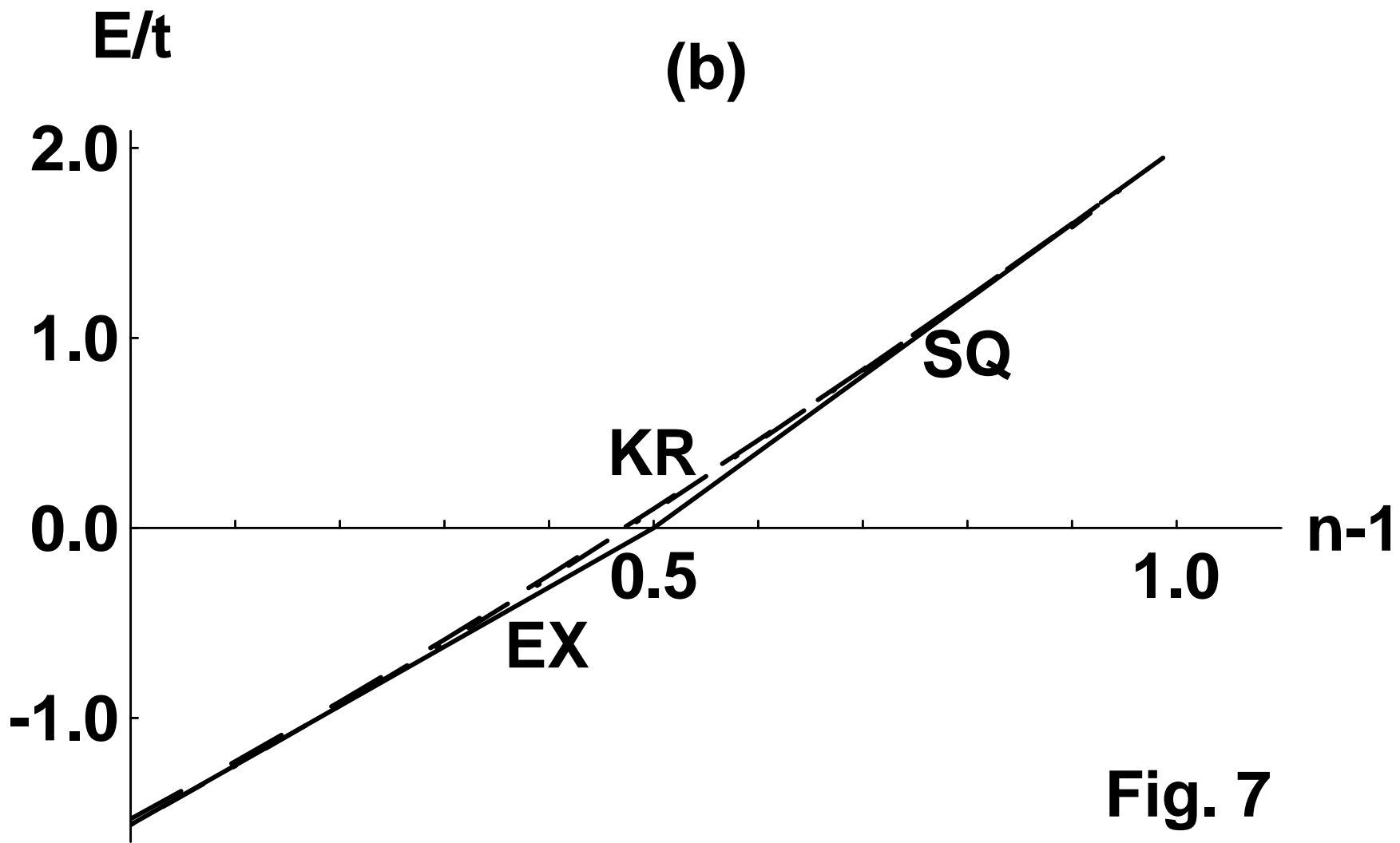
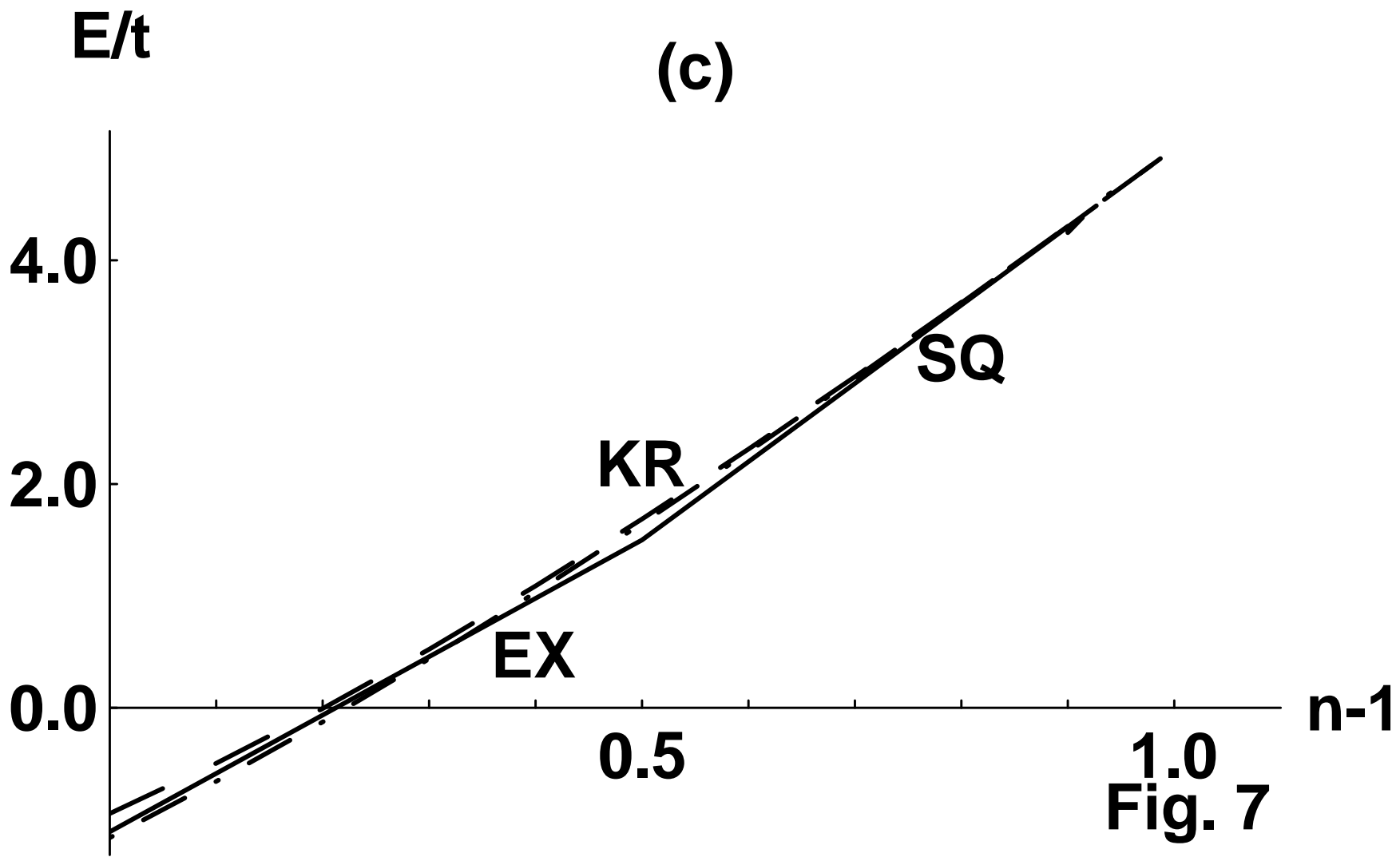


Fig. 7





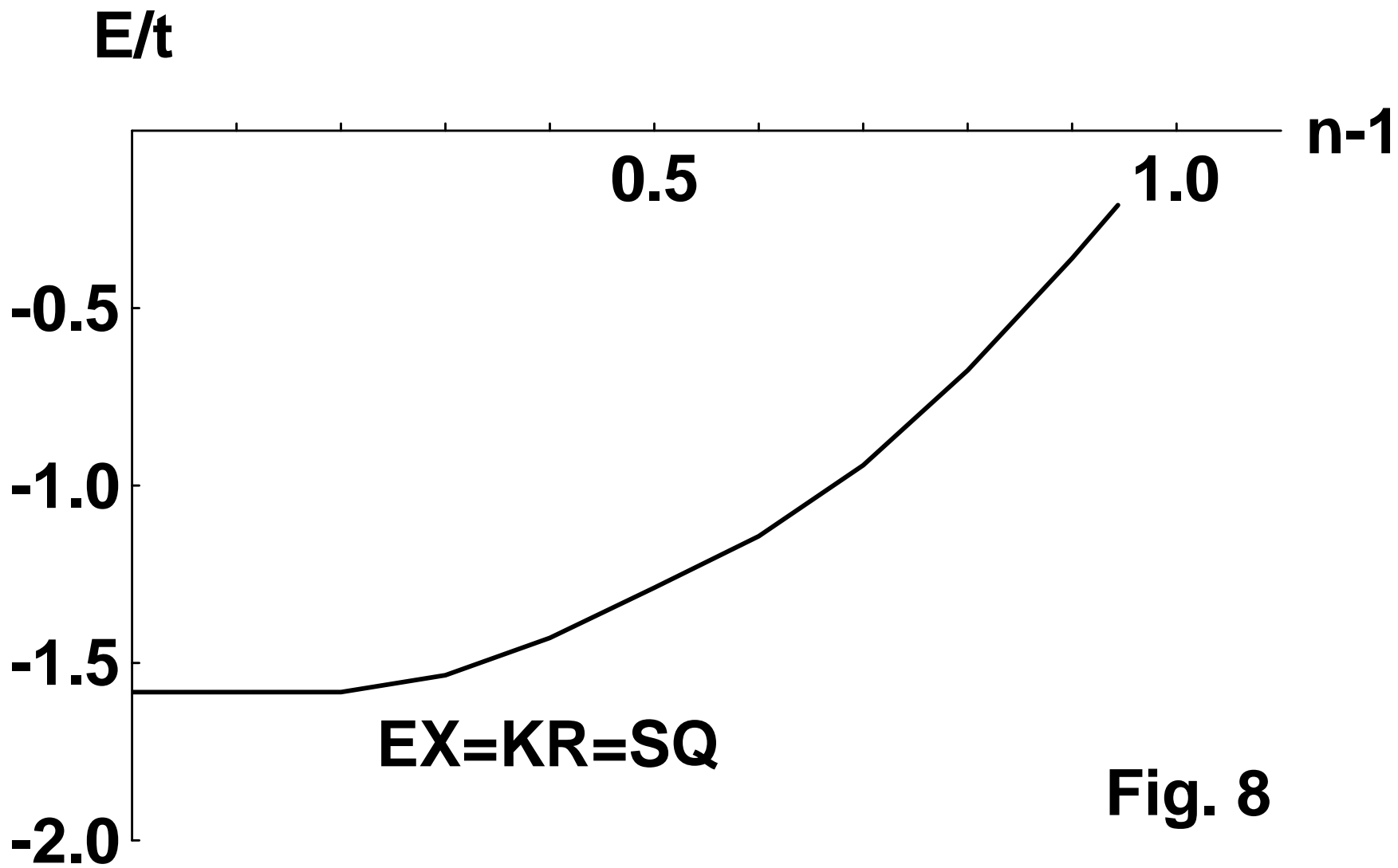


Fig. 8