Extended Hubbard model at strong coupling

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The half-filled extended Hubbard model (containing nearest-neighbor interaction) is considered at strong coupling in fourth-order perturbation theory. The ground-state energies in the spin- and charge-density-wave phases and the resulting phase diagram are calculated in various dimensions: here $d=1$, $d=\infty$, high dimensions ($d\gg 1$), and $d=2,3$ are discussed separately. In $d=1$ it is shown that, for $U\gtrsim 6$, fourth-order perturbation theory leads to excellent agreement with existing Monte Carlo data. Second-order perturbation theory alone is valid only at unrealistically large values of U and V. In $d=\infty$, one needs fourth-order perturbation theory to obtain any nontrivial contribution to the phase diagram at all. As a consequence the fourth-order corrections to the ground-state energy and to the phase diagram are large also in $d=2,3$. The formalism used to obtain the perturbative expansion is discussed in an appendix.

I. INTRODUCTION

The Hubbard model, introduced independently in 1963 by Hubbard, Gutzwiller, and Kanamori[1] is perhaps the simplest model for the description of interacting electrons on a lattice. Its Hamiltonian describes itinerant electrons on a lattice with local (i.e., on-site) interaction. The importance of the Hubbard model is illustrated by the richness of its phase diagram. Its introduction[1] was motivated by the study of ferromagnetism.[2,3] Since then it has been used to describe widely different physical phenomena, such as antiferromagnetism,[4] paramagnetism,[5] incommensurate spin-density waves,[6] the metal-insulator transition,[7,8] and, more recently, high-T_c superconductivity.[9,10]

The Hubbard Hamiltonian as it stands can be derived only under rather drastic assumptions. This has been stressed already by Hubbard in his original derivation.[1] Many overlap matrix elements, some of which may appreciably change the phase diagram, are neglected. The largest of these is the matrix element for nearest-neighbor Coulomb repulsion. If the Hubbard model is generalized to include also this nearest-neighbor interaction one obtains the so-called *extended Hubbard model.*

The goal of this paper is to investigate the extended Hubbard model at *strong interaction* ($U,V\gg t$), using strong-coupling perturbation theory. Of particular interest will be the calculation of the ground-state energy and the $T=0$ phase diagram at half filling. It will be pointed out below that second-order perturbation theory alone is relevant only for unrealistically large values of the interaction. One therefore has to use at least *fourth-order* perturbation theory to obtain a quantitatively accurate description. In this paper we explain the method and present its results.

The Hamiltonian of the extended Hubbard model has the form

$$H=H_t+H_U+H_V+H_\mu\ , \tag{1.1}$$

where

$$H_t=-t\sum_{(ij),\sigma}c_{i\sigma}^\dagger c_{j\sigma};\quad H_\mu=-\mu\sum_i n_i$$

$$H_U=U\sum_i n_{i\uparrow}n_{i\downarrow}\ ;\quad H_V=\frac{V}{d}\sum_{\langle ij\rangle}n_i n_j\ .$$

Here $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (destroys) an electron with spin σ at site i, $n_{i\sigma}\equiv c_{i\sigma}^\dagger c_{i\sigma}$, $n_i\equiv n_{i\downarrow}+n_{i\uparrow}$, and d is the space dimension. The grand canonical Hamiltonian (1.1) describes hopping of electrons (H_t), interacting with each other through on-site (H_U) and nearest-neighbor (H_V) Coulomb repulsion. For simplicity we assume that the lattice has a (hyper-) cubical structure. The prefactor in H_V is chosen such that, if V is kept fixed, a meaningful result is obtained even for $d\to\infty$.[11] Similarly we use the scaling $t=t^*/\sqrt{2d}$ to obtain a meaningful result for H_t in all dimensions.[12] In this paper we consider only Coulomb *repulsion* ($U>0$ and $V\geq 0$). We investigate the extended Hubbard model as a function of U at the fixed ratio

$$v\equiv V/U\ .$$

In this notation the original Hubbard model corresponds to the special case $V=0$, or $v=0$, in (1.1). The half-filled band corresponds to a chemical potential $\mu=\frac{1}{2}U+2V$. In the sum over bonds $\langle ij\rangle$ it is understood that i and j are nearest neighbors and that every bond is counted only once. In contrast, the notation (ij), used in H_t, indicates that the bond directions $\langle ij\rangle$ and $\langle ji\rangle$ are counted as distinct.

On the basis of previous studies, both at weak and at strong coupling, the ground-state phase diagram of the half-filled extended Hubbard model is at least *qualitatively* clear. If the ratio $v=V/U$ is sufficiently large the system is in a charge-density-wave (CDW) phase, if v is small it is in the spin-density-wave (SDW) phase. The phase boundary $v_c(U)$ between these phases[13] is approximately located at $v\simeq\frac{1}{2}$. In fact this phase boundary is *precisely* located at $v=\frac{1}{2}$ both for $U\downarrow 0$ (i.e., at weak coupling,[14,15]) and for $U\to\infty$, if the kinetic energy H_t is sim-

ply neglected.[16] Deviations $\varepsilon_c \equiv v_c(U) - \frac{1}{2}$ from the line $v = \frac{1}{2}$ become apparent only if one calculates the corrections to the leading behavior. This can be done most easily at strong coupling, using strong-coupling perturbation theory up to second order in t/U. In this way it can be shown that the line $v_c = \frac{1}{2}$ is *not* exact in any dimension $d < \infty$.

However, at the level of second-order (strong-coupling) perturbation theory several issues remain unclear. For instance in high dimensions (i.e., $d = \infty$), there is *no* deviation from the line $v = \frac{1}{2}$ in second-order perturbation theory, either at strong or at weak coupling.[17] Thus second-order perturbation theory yields no information on the magnitude or even the sign of ε_c in $d = \infty$. Two questions to be answered in higher dimensions ($d \gtrsim 3$) are therefore: (i) What happens in $d = \infty$, where ε_c vanishes in second-order perturbation theory? Is in this case $\varepsilon_c > 0$, $\varepsilon_c < 0$, or perhaps exactly $\varepsilon_c(U) = 0$ for all U? And (ii) if ε_c is so small at large U in $d = \infty$, what does this imply for finite dimensions, such as $d = 3$?

There exist open problems, too, in low dimensions. For instance, in $d = 1$ the deviation of the exact phase boundary from $v = \frac{1}{2}$ has been investigated by Hirsch[18] in a Monte Carlo simulation. In this simulation Hirsch determined $\varepsilon_c(U)$ up to $U/t = 8$. He found that $\varepsilon_c > 0$ for all values of U/t considered, so that the actual phase boundary is slightly shifted upward relative to the line $v = \frac{1}{2}$. He also noticed that the simulation had not yet reached the asymptotic regime, i.e., that the data at $U/t = 8$ could not be explained quantitatively by second-order perturbation theory. Two of the questions left in the one-dimensional system are: (iii) Can one explain Hirsch's Monte Carlo data *quantitatively* if one goes to higher orders in perturbation theory? And (iv) actually how large is the asymptotic regime, where second-order perturbation theory alone is valid?

To answer these questions we calculate the ground-state energy of the extended Hubbard model at strong coupling in fourth-order perturbation theory. Special attention will then be paid to the phase boundary between the CDW and SDW phases, or rather to the deviation ε_c of the phase boundary from the line $v = \frac{1}{2}$. The deviation ε_c is physically more interesting than the leading term $v = \frac{1}{2}$, since ε_c contains information concerning the fluctuations in the CDW and SDW phases or, equivalently, concerning the ground-state energies of the Heisenberg antiferromagnet and more complicated quantum spin models.

It will become apparent below that the fourth-order corrections to the ground-state energy and to ε_c are important in any dimension. These corrections cannot be neglected if one seeks quantitative agreement with observed data at realistic values of U and V.

To substantiate these ideas we proceed as follows. First, in Sec. II, we present the effective Hamiltonian for the extended Hubbard model in the SDW phase up to fourth order in perturbation theory. We also give the explicit ground-state energy in the CDW phase up to fourth order. The ground-state energy for the SDW phase and the resulting phase diagram are discussed in Sec. III ($d = 1$), Sec. IV ($d = \infty$), Sec. V (the $1/d$ expansion), and Sec. VI ($d = 2, 3$). We end with a summary and a discussion. Technical calculations are deferred to the appendixes.

II. EFFECTIVE HAMILTONIAN AT STRONG COUPLING

To leading order in U and V the kinetic energy is negligible (of relative order U^{-1}) compared to the remaining terms in (1.1), so that the Hamiltonian can be approximated by $H_0 \equiv H_U + H_V + H_\mu$. In any dimension $d \geq 1$ it can easily be proved[16] that the ground state of this model at half filling has the CDW form (with all the electrons on either the A or the B sublattice) provided that $v > \frac{1}{2}$. Alternatively, if $v < \frac{1}{2}$, the ground state is highly degenerate, with all sites singly occupied. The corresponding ground-state energies are

$$E_0^{\mathrm{CDW}} = \tfrac{1}{2}\mathcal{N}U \quad (v > \tfrac{1}{2}) ,$$

$$E_0^{\mathrm{SDW}} = \mathcal{N}V \quad (v < \tfrac{1}{2}) ,$$

where $\mathcal{N}$ is the number of sites on the lattice. The corrections due to the hopping term H_t give rise to antiferromagnetic coupling in the phase without doubly occupied sites. This phase will therefore be referred to as the spin-density-wave phase throughout.

In order to study the corrections to the ground-state phase diagram due to hopping one can employ strong-coupling perturbation theory. The calculation proceeds in three steps. First one calculates an effective Hamiltonian that describes the dynamics at strong coupling. The effective Hamiltonian has a different form in the CDW and SDW phases. In the second step one then calculates the ground-state energy, assuming the system is in one of these two phases. Thirdly one compares both energies; the line in the phase diagram where they are equal then defines the phase boundary between the CDW and the SDW. In this section we concentrate on the first step. The calculation of ground-state energies and of the phase boundary will be presented in later sections for the various dimensions separately.

Strong-coupling perturbation theory for the Hubbard model ($v = 0$) has been developed and worked out to second order by Harris and Lange[19] and worked out to fourth order by Takahashi.[20] The basic idea of Harris and Lange is to transform from the $\{c_{i\sigma}^\dagger, c_{i\sigma}\}$ fermions to new particles $\{\bar{c}_{i\sigma}^\dagger, \bar{c}_{i\sigma}\}$, whose hopping leaves the number of doubly occupied sites invariant. The effective Hamiltonian at low temperatures is then obtained by restricting consideration to the subspace without doubly occupied sites.

Similarly one can apply this method to the extended Hubbard model by requiring that the hopping of the new particles leaves the extended Hubbard interaction H_0 invariant. This has been done by several authors in second-order perturbation theory[18,14,22] and will be extended here to higher order. The main difference between strong-coupling perturbation theory in the standard and the extended Hubbard model is that in the ex-

tended model the number of different excitation energies is larger, and that hopping processes with zero excitation energy (which play a special role in the standard model) do not occur. Technical details are presented in the appendixes. The method is presented in Appendix A, where it is shown that the effective Hamiltonian can be determined recursively to any desired order in perturbation theory. An explicit form for the effective Hamiltonian in the CDW or SDW phase is derived in Appendix B. In this section we present the results.

A. The CDW phase

In the CDW case the ground state of the Hamiltonian $H_0=H_U+H_V+H_\mu$ is unique (up to global symmetries). Consequently the "effective Hamiltonian" in this single state is simply a real number. In this case the effective Hamiltonian is therefore equal to the ground-state energy. From Appendix B it follows that to fourth order in perturbation theory the ground state energy $E_0^{\rm CDW}$ is given by

$$E_0^{\rm CDW}=\mathcal{N}\left[\tfrac{1}{2}U-\frac{(t^*)^2/U}{(4-1/d)v-1}+T_4\right], \tag{2.1}$$

where the fourth-order term T_4 is given by

$$T_4=\frac{(t^*)^4/U^3}{[v(4-1/d)-1]^2}\times\left[\frac{4-1/d}{v(4-1/d)-1}+\frac{1-1/d}{v(4-3/d)-1}-\frac{1}{4vd(2-1/d)}-\frac{4(1-1/2d)}{4v(2-1/d)-1}\right]. \tag{2.2}$$

This result is valid in all dimensions $d\geq 1$. Since all odd orders in perturbation theory vanish (as for the Hubbard model[20,23,24]) the expression (2.1) for $E_0^{\rm CDW}$ is accurate up to $O[(t^*)^5/U^4]$.

B. The SDW phase

In the SDW phase the ground state of H_0 is highly degenerate: any state without doubly occupied sites has the same energy $\mathcal{N}V$. In this subspace of states without double occupancy the effective Hamiltonian, found in Appendix B, works as a genuine operator. The result can most easily by expressed in terms of Hermitian operators Q_{ij}, which are in a simple way related to the Heisenberg interaction on the bond $\langle ij\rangle$, namely

$$Q_{ij}\equiv\sum_{\sigma\sigma'}c_{i\sigma}^\dagger c_{j\sigma}c_{j\sigma'}^\dagger c_{i\sigma'} \tag{2.3a}$$

$$=-2(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}), \tag{2.3b}$$

where $\mathbf{S}_i$ represents the standard Heisenberg spin at site i.

In terms of the operators Q_{ij} the effective Hamiltonian in the spin-density-wave phase takes a different form in $d=1$ and in dimensions $d>1$. The reason is that loop diagrams contribute in higher dimensions but not in the linear chain. In $d=1$ the effective Hamiltonian is

$$H_f=\mathcal{N}V-\tfrac{1}{2}J_0\sum_i Q_{i,i+1}-\tfrac{1}{2}J_1\sum_i Q_{i,i+2}, \tag{2.4}$$

where

$$J_0\equiv\frac{4t^2}{U(1-v)}-4J_1$$

$$J_1\equiv\frac{4t^4(1+v)}{U^3(1-v)^3}. \tag{2.5}$$

The pure Heisenberg interaction [second term in the right-hand side of Eq. (2.4)] has been obtained before[18,21,22] in second-order perturbation theory. From (2.4) and (2.5) it is clear that the fourth-order terms have two effects: they reduce the coupling constant obtained from second-order perturbation theory (first term in J_0) and they lead to frustration [the J_1 term in (2.4)]. It is intuitively clear that this tends to raise the ground-state energy of the SDW state.

In all higher dimensions ($d\geq 2$) the effective Hamiltonian takes the form

$$H_f=\mathcal{N}V-\tfrac{1}{4}J\sum_{(ij)}Q_{ij}+\frac{t^4A}{U^3}\sum_{\{\square\}}(Q_{12}Q_{34}+Q_{23}Q_{14}-Q_{13}Q_{24})+\frac{t^4C}{U^3}\sum_{i,\tau'\neq\pm\tau}Q_{i+\tau',i+\tau}-\frac{t^4D}{U^3}\sum_{i\tau}Q_{i+\tau,i-\tau}, \tag{2.6}$$

where

$$J\equiv\frac{4t^2}{U(1-v/d)}+\frac{4t^4B}{U^3} \tag{2.7}$$

and the constants A, B, C, and D have been defined in Appendix B [see below Eq. (B10)]. Here τ and τ' are lattice vectors connecting a site to one of its $2d$ neighbors, and "$\square$" represents a plaquette. Each plaquette is counted only once; the four sites $\{1,2,3,4\}$ represent its four corners in clockwise or anticlockwise order. Since A, B, C, and D are in general positive, we find that B and C tend to stabilize the SDW whereas A and D tend to destabilize it. The physical consequences of the fourth-order corrections will be investigated below, first for the linear chain ($d=1$), then in infinite ($d=\infty$) and in high ($d\gg 1$) dimensions, and finally for lower-dimensional lattices ($d=2,3$).

III. PHASE DIAGRAM FOR THE LINEAR CHAIN

In this section, we calculate the ground-state energies in the CDW and SDW phases. By comparing them we determine the phase diagram of the linear chain.

The ground-state energy in the CDW phase follows from (2.1) as

$$E_0^{\rm CDW}=\mathcal{N}\left[\tfrac{1}{2}U-\frac{2t^2}{(3v-1)U}+\frac{(12v^2+3v-1)t^4}{v(3v-1)^3(4v-1)U^3}\right], \tag{3.1}$$

which again is exact up to $O(t^5/U^4)$.

The effective Hamiltonian in the SDW phase is given

in (2.4). The J_1 term in (2.4) is small compared to the J_0 term and can therefore be treated in perturbation theory. In the absence of the J_1 term (2.4) has the form of the (exactly solved) antiferromagnetic (AFM) Heisenberg chain. From the exact solution by Bethe ansatz[25] we know that

$$\langle Q_{i,i+1}\rangle = 2\ln 2 \quad \text{or} \quad \langle \mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle = \tfrac{1}{4}-\ln 2 \ .$$

The correction due to the J_1 term is therefore known if one can determine the next-nearest-neighbor spin interaction $\langle Q_{i,i+2}\rangle$, or $\langle \mathbf{S}_i\cdot\mathbf{S}_{i+2}\rangle$, where the average is calculated in the ground state of the AFM Heisenberg chain. Fortunately this correlation function is known; it has been calculated by Takahashi[20] from the Lieb-Wu solution of the one-dimensional Hubbard model.[35] He finds that $\langle \mathbf{S}_i\cdot\mathbf{S}_{i+2}\rangle = \frac{1}{4}[1-16\ln 2+9\zeta(3)]$. We would like to add that this correlation function contains more physical information than just the nearest-neighbor spin interaction. For instance, it is easy to show that Takahashi's result is equivalent to the statement that the covariance of Heisenberg interactions $\mathbf{S}_i\cdot\mathbf{S}_j$ on neighboring bonds is given by

$$\langle\langle (\mathbf{S}_i\cdot\mathbf{S}_{i+1})(\mathbf{S}_{i+1}\cdot\mathbf{S}_{i+2})\rangle\rangle = \tfrac{9}{16}\zeta(3)-\tfrac{1}{2}\ln 2-(\ln 2)^2 \ .$$

Hence the correlation coefficient between $\mathbf{S}_i\cdot\mathbf{S}_{i+1}$ and $\mathbf{S}_{i+1}\cdot\mathbf{S}_{i+2}$ is approximately given by $-0.709\,33$, which reveals a strong coupling between neighboring bonds. In classical terms the negative correlation implies that if the "angle" between $\mathbf{S}_i$ and $\mathbf{S}_{i+1}$ is smaller than expected then most likely the "angle" between $\mathbf{S}_{i+1}$ and $\mathbf{S}_{i+2}$ is larger than expected.

Putting all the information together one obtains for the ground-state energy in the spin-density-wave phase:

$$E_0^{\mathrm{SDW}} = \mathcal{N}\left[V-\frac{4t^2\ln 2}{U(1-v)}+9\zeta(3)\frac{t^4(1+v)}{U^3(1-v)^3}\right], \tag{3.2}$$

again valid up to $O(t^5/U^4)$.

Equations (3.1) and (3.2) reduce near $v=\frac{1}{2}$ to

$$E_0^{\mathrm{CDW}} \sim \mathcal{N}\left[\tfrac{1}{2}U-\frac{4t^2}{(1+6\varepsilon)U}+56\frac{t^4}{U^3}\right] \tag{3.3a}$$

$$E_0^{\mathrm{SDW}} \sim \mathcal{N}\left[V-\frac{4t^2\ln 2}{(\frac{1}{2}-\varepsilon)U}+108\zeta(3)\frac{t^4}{U^3}\right], \tag{3.3b}$$

where we introduced a small parameter $\varepsilon \equiv v-\frac{1}{2}$. The phase boundary between the SDW and CDW phases is determined by the criterion that both energies in (3.3a) and (3.3b) are equal. One finds that the phase boundary is determined by

$$\begin{aligned}\varepsilon_c &= 4(2\ln 2-1)(t/U)^2 \\ &\quad -[108\zeta(3)+40-128\ln 2-128(\ln 2)^2](t/U)^4 \\ &\simeq 1.545(t/U)^2-19.60(t/U)^4 \ . \end{aligned} \tag{3.4}$$

It immediately catches the eye that the prefactor of the $(t/U)^4$ term is rather large.

Next we compare our result (3.4) to the Monte Carlo data of Hirsch,[18] first at $U/t=6$ and then at $U/t=8$. In either case the Monte Carlo (MC) data for ε_c lie below the value $\varepsilon_c(2)$ predicted by second-order perturbation theory, in agreement with Eq. (3.4).

For $U/t=6$ the MC data are in very good agreement with fourth-order perturbation theory: I find a value $\varepsilon_c(2+4)\simeq 0.0278$, which is approximately 7% higher than the Monte Carlo result[18] $\varepsilon_c(\mathrm{MC})=0.0260\pm 0.0010$. For comparison, the result $\varepsilon_c(2)$ of second-order perturbation theory turns out to be 65% larger than $\varepsilon_c(\mathrm{MC})$, so that the fourth-order terms lead to a significant improvement. However, this excellent agreement in fourth-order perturbation theory may be somewhat fortuitous since for $U/t\simeq 6$ the assumption that higher-order corrections are small may not be justified.

At $U/t=8$, Eq. (3.4) predicts a SDW-CDW transition for $\varepsilon_c(2+4)\simeq 0.019\,36$, which is about 20% lower than the result of second-order perturbation theory, $\varepsilon_c(2)\simeq 0.0241$. On the other hand in the Monte Carlo simulation[26] one finds that the system is clearly in the SDW phase for $V_c=4.10$ and clearly in the CDW phase for $V_c=4.20$, so that a SDW-CDW transition is expected to occur at $V_c=4.15\pm 0.05$, or $\varepsilon_c(\mathrm{MC})\simeq 0.019\pm 0.006$. As one can see, the expected location of the transition at $\varepsilon_c(\mathrm{MC})\simeq 0.019$ is in excellent agreement with the predictions of fourth-order perturbation theory, suggesting that the actual error bars in the MC data are *much* smaller than the estimate given above.[26] Obviously it would be desirable to redo the simulation at $U/t=8$ with greater accuracy, in order to determine numerically how good fourth-order perturbation theory really is at such physically interesting values of U/t.

In order to estimate the region of validity of fourth-order perturbation theory one needs to know the influence of higher-order perturbative corrections. Fortunately, in $d=1$, rough estimates are possible without calculating these corrections explicitly. For example, the influence of the sixth-order terms can be estimated from Takahashi's[27] asymptotic expansion for the ground-state energy of the (standard) Hubbard model ($v=0$). Here the sixth-order terms are smaller than the fourth-order terms by a factor of 10 for $U/t=8$. The relative size of the sixth-order term in the *extended* Hubbard model is probably larger since the excitation energies are smaller. As a consequence the uncertainty in $\varepsilon_c(2+4)$ could be as large as 10%. In view of this uncertainty one expects that a more accurate calculation of the transition at $U/t=8$ would yield a value for $\varepsilon_c(\mathrm{MC})$ between 0.0170 and 0.0210.

As a last remark I would like to point out that one has to go to *very* large values of U/t (probably unattainable in a Monte Carlo simulation) before second-order perturbation theory alone gives accurate predictions for V_c or ε_c. It follows from (3.4) that one has to go to $U/t\simeq 16$ before the second-order result is correct within 5% and to $U/t\simeq 36$ to obtain a precision of 1%. This shows that the asymptotic regime, where second-order perturbation theory alone is sufficient, corresponds to unrealistically large values of the interaction.

IV. PHASE DIAGRAM IN INFINITE DIMENSIONS

The case of infinite dimensions ($d=\infty$) is somewhat special since, as we shall see below, the leading term in ε_c

[which is in general proportional to $(t^*/U)^2$] vanishes. The phase boundary is therefore much closer to the line $V=\frac{1}{2}U$ in $d=\infty$ than in lower dimensions.

The ground-state energy in the CDW phase follows from (2.1) as

$$E_0^{\mathrm{CDW}}=\mathcal{N}\left[\tfrac{1}{2}U-\frac{(t^*)^2}{(4v-1)U}+\frac{(24v-1)(t^*)^4}{(4v-1)^3(8v-1)U^3}\right], \tag{4.1}$$

where we neglected all contributions of $O(1/d)$. The hopping amplitude has been scaled as $t=t^*/\sqrt{2d}$ as usual. Note that E_0^{CDW} is explicitly v dependent.

The corrections to the ground-state energy in the SDW phase are independent of v since the excitation energies contain v only to $O(1/d)$. Calculation of the expectation value $\langle H_f\rangle$, with H_f given by (2.6), is easy, since spin-flip processes contribute only to $O(1/d)$ and can be neglected. Hence only the Ising terms in (2.6) survive:

$$Q_{ij}\to Q_{ij}^N\equiv\sum_\sigma n_{i\sigma}(1-n_{j\sigma})\ .$$

Furthermore the term proportional to D in (2.6) is of $O(1/d)$ and can be neglected. The ground state of the remaining spin Hamiltonian is simply the Néel state since we assume $t^*/U\ll 1$. In the Néel state the expectation value of the C term is zero, so that only the J and A terms remain. To calculate the J term we note that each bond variable Q_{ij}^N equals unity in the Néel state; in total there are $\mathcal{N}d$ bonds, each of which is counted twice. Similarly, in the A term, there are $\frac{1}{2}\mathcal{N}d(d-1)$ plaquettes, each of which gives a contribution of 2 to the sum over "□". Consequently

$$\begin{aligned}E_0^{\mathrm{SDW}}&=\mathcal{N}(V-\tfrac{1}{2}Jd+t^4Ad(d-1)/U^3)\\&=\mathcal{N}\left[V-\frac{(t^*)^2}{U}+\frac{(t^*)^4}{U^3}\right],\end{aligned} \tag{4.2}$$

where we used the explicit form of J and A, see (2.7) and (B10). The ground-state energy of the standard Hubbard model ($v=0$) in $d=\infty$ (Ref. 28) is contained in (4.2) as a special case.

We can now compare the two energies (4.1) and (4.2). Near the mean-field line $v=\frac{1}{2}$ one obtains

$$E_0^{\mathrm{CDW}}=\mathcal{N}\left[\tfrac{1}{2}U-\frac{(t^*)^2}{(1+4\varepsilon)U}+\frac{11}{3}\frac{(t^*)^4}{U^3}\right], \tag{4.3}$$

where as usual $\varepsilon=v-\frac{1}{2}$. Comparison with (4.2) shows that the separation line is located at

$$\varepsilon_c=\frac{8}{3}\frac{(t^*)^4}{U^4}\ . \tag{4.4}$$

Hence the leading term, proportional to $(t^*)^2/U^2$, vanishes in $d=\infty$, thus yielding a much smaller deviation from the mean-field line than in lower dimensions. It is also noteworthy that the *direction* of the deviation is again towards larger V (as in $d=1$), so that in $d=\infty$, too, the SDW phase is stabilized by the hopping.

V. THE $1/d$ EXPANSION

In this section we investigate how the phase boundary, defined by ε_c, moves away from the infinite-dimensional result (4.4) as the dimension is lowered. This can be done systematically by calculating the ground-state energies E_0^{CDW} and E_0^{SDW} in a $1/d$ expansion. As we shall see, the $1/d$ corrections to the $d=\infty$ results are relatively large.

The ground-state energy for the CDW near $v=\frac{1}{2}$ follows from (2.1) as

$$\begin{aligned}E_0^{\mathrm{CDW}}/\mathcal{N}=&\tfrac{1}{2}U-\frac{(t^*)^2}{U}\left[1+\frac{1}{2d}+\frac{1}{4d^2}-\varepsilon\left[4+\frac{3}{d}\right]\right]\\&+\frac{(t^*)^4}{U^3}\left[\frac{11}{3}+\frac{169}{36d}+\frac{1027}{216d^2}\right],\end{aligned} \tag{5.1}$$

where we introduced the small parameter $\varepsilon=v-\frac{1}{2}$ and kept all relevant terms up to $O(1/d^2)$. Note that the convergence of E_0^{CDW} as a function of $1/d$ is rather slow, illustrating that fluctuations yield important contributions in physically interesting dimensions ($d=2,3$).

The $1/d$ expansion for the ground-state energy E_0^{SDW} in the SDW phase is obtained by expanding the effective Hamiltonian (2.6) around the Ising limit: the spin-flip terms in (2.6) are treated as a small perturbation. The $1/d$ expansion is formally very similar to the expansions in transverse coupling (see, e.g., Refs. 29,30,31,32) which have been developed for the Heisenberg antiferromagnet. We will carry out the $1/d$ expansion up to fourth order in perturbation theory (again using the methods of Appendix A), which yields values for E_0^{SDW} and ε_s, correct up to $O(1/d^2)$.

To perform the $1/d$ expansion we split up the Hamiltonian (2.6) into two parts, the Ising part H_f^N and the spin-flip part H_f^S:

$$H_f=H_f^N+H_f^S\ , \tag{5.2}$$

where

$$H_f^N=\mathcal{N}V-\tfrac{1}{4}J\sum_{(ij)}Q_{ij}^N+\frac{t^4A}{U^3}\sum_{\{\square\}}(Q_{12}^NQ_{34}^N+Q_{23}^NQ_{14}^N-Q_{13}^NQ_{24}^N)+\frac{t^4C}{U^3}\sum_{i,\tau'\neq\pm\tau}Q_{i+\tau',i+\tau}^N-\frac{t^4D}{U^3}\sum_{i\tau}Q_{i+\tau,i-\tau}^N \tag{5.3}$$

and

$$\begin{aligned}H_f^S=&-\tfrac{1}{4}J\sum_{(ij)}Q_{ij}^S+\frac{t^4C}{U^3}\sum_{i,\tau'\neq\pm\tau}Q_{i+\tau',i+\tau}^S-\frac{t^4D}{U^3}\sum_{i\tau}Q_{i+\tau,i-\tau}^S\\&+\frac{t^4A}{U^3}\sum_{\{\square\}}(Q_{12}^NQ_{34}^S+Q_{23}^NQ_{14}^S-Q_{13}^NQ_{24}^S+Q_{12}^SQ_{34}^N+Q_{23}^SQ_{14}^N-Q_{13}^SQ_{24}^N+Q_{12}^SQ_{34}^S+Q_{23}^SQ_{14}^S-Q_{13}^SQ_{24}^S)\ .\end{aligned} \tag{5.4}$$

The expectation value of the Ising part is again given by (4.2), where the constants J and A now have to be evaluated up to the $O(1/d^2)$ terms. The result is

$$\langle H_f^N\rangle/\mathcal{N}=V-\frac{(t^*)^2}{U}\left[1+\frac{v}{d}+\frac{v^2}{d^2}\right]+\frac{(t^*)^4}{U^3}\left[1+\frac{1+9v}{d}+\frac{30v^2-v}{d^2}\right]. \tag{5.5}$$

Evaluation of the spin-flip part $\langle H_f^S\rangle$ can be done in fourth-order perturbation theory, again using the methods of Appendix A. Technical details can be found in Appendix C. Here we give only the result:

$$\langle H_f^S\rangle/\mathcal{N}=-\frac{(t^*)^2}{4dU}\left[1+\frac{v+\frac{3}{8}}{d}-\frac{(t^*)^2}{U^2}\left[8+\frac{24v}{d}\right]\right]. \tag{5.6}$$

By combining (5.5) and (5.6) one finds the following result for the ground-state energy in the SDW phase:

$$E_0^{\mathrm{SDW}}/\mathcal{N}=V-\frac{(t^*)^2}{U}\left[1+\frac{v+\frac{1}{4}}{d}+\frac{v^2+v/4+\frac{3}{32}}{d^2}\right]+\frac{(t^*)^4}{U^3}\left[1+\frac{3+9v}{d}+\frac{30v^2+5v}{d^2}\right], \tag{5.7}$$

which is exact up to $O(1/d^2)$ and $O[(t^*)^5/U^4]$. Note that, as for E_0^{CDW}, the convergence of E_0^{SDW} as a function of $1/d$ is rather slow.

Comparison of (5.1) and (5.7) yields an expression for the deviation ε_c from the line $v=\frac{1}{2}$. The result, correct up to $O(1/d^2)$ and $O[(t^*)^5/U^5]$ is:

$$\varepsilon_c=\frac{(t^*)^2}{4dU^2}\left[1+\frac{7}{8d}\right]+\frac{8(t^*)^4}{3U^4}\left[1-\frac{65}{96d}-\frac{91}{72d^2}\right]. \tag{5.8}$$

Note that the $1/d$ corrections to the leading $(t^*/U)^2$ and $(t^*/U)^4$ terms are appreciable, showing that the stability of the SDW phase near $v=\frac{1}{2}$ depends sensitively on dimension. On the other hand, it should also be emphasized that the $1/d$ corrections are not so large as to make application of (5.8) in physical dimensions ($d=2,3$) meaningless. In fact the $1/d$ corrections in (5.8) are significantly smaller than those for E_0^{CDW} and E_0^{SDW} in Eqs. (5.1) and (5.7).

A comment on the ratio of the second- and fourth-order terms in (5.8) is in order. The fact that the second-order term *vanishes* in $d=\infty$ is reflected in its small prefactor in finite dimensions ($\propto 1/d$). As a consequence one has to go to rather large values of U/t^* in order that the second order dominates the fourth. We estimate on the basis of (5.8) that the crossover occurs in higher dimensions near $U/t^*\simeq\sqrt{10d}$, which diverges for $d\to\infty$. In $d=3$, the crossover occurs at $U/t^*\simeq 5.5$ (i.e., $U/t\simeq 13.5$); in $d=2$ it occurs at $U/t^*\simeq 2.3$ (i.e., $U/t\simeq 4.6$). This demonstrates clearly that in two- or three-dimensional systems, as in $d=1$, the fourth order in perturbation theory *must* be taken into account in order to calculate the CDW/SDW phase diagram quantitatively for physically reasonable values of U.

VI. QUALITY OF THE $1/d$ EXPANSION IN $d=2,3$

In the previous section we calculated the ground-state energy and the phase diagram in a $1/d$ expansion. In this section we will give a critical discussion of the relevance of these $1/d$ results for physically interesting dimensions ($d=2,3$).

The ground-state energy in the SDW phase follows from the $1/d$ expansion by inserting $d=2,3$ into (5.7). One finds that:

$d=2$:

$$E_0^{\mathrm{SDW}}/\mathcal{N}=V-\left[\frac{147}{128}+\frac{9v}{16}+\frac{v^2}{4}\right]\frac{(t^*)^2}{U}+\left[\frac{5}{2}+\frac{23v}{4}+\frac{15v^2}{2}\right]\frac{(t^*)^4}{U^3}, \tag{6.1a}$$

$d=3$:

$$E_0^{\mathrm{SDW}}/\mathcal{N}=V-\left[\frac{105}{96}+\frac{13v}{36}+\frac{v^2}{9}\right]\frac{(t^*)^2}{U}+\left[2+\frac{32v}{9}+\frac{10v^2}{3}\right]\frac{(t^*)^4}{U^3}. \tag{6.1b}$$

Similarly the position of the phase boundary can be obtained by inserting $d=2,3$ into (5.8). The result is

$$d=2:\ \varepsilon_c=\frac{23(t^*)^2}{128U^2}+\frac{199(t^*)^4}{216U^4} \tag{6.2a}$$

$$d=3:\ \varepsilon_c=\frac{31(t^*)^2}{288U^2}+\frac{1643(t^*)^4}{972U^4}. \tag{6.2b}$$

In the CDW phase the ground-state energy in $d=2,3$ can be obtained either from the $1/d$ expansion [see Eq. (5.1)] or from the exact expression for E_0^{CDW}, accurate to $O[(t^*)^5/U^4]$, which was given in (2.1).

Obviously the results from the $1/d$ expansion are accurate in higher dimensions, but it is not *a priori* clear whether they are also accurate in $d=2,3$. To obtain more insight into the validity of the $1/d$ results for ε_c and E_0^{SDW} it is helpful to perform a few checks.

First consider ε_c. The basic question is: how large is the error in ε_c due to the fact that we used the $1/d$ approximation for the ground-state energy instead of the exact expressions for E_0, accurate to $O[(t^*)^5/U^4]$, in $d=2,3$? To estimate this error we recall that ε_c in (6.2a) and (6.2b) was calculated using the $1/d$ approximation for E_0^{CDW}. Alternatively one can calculate the deviation ε_c' obtained by using the *exact* result (2.1) for E_0^{CDW} in $d=2,3$. The difference between ε_c and ε_c' then yields a measure for the error in ε_c, induced by the $1/d$ approximation. The calculation of ε_c' is straightforward. One finds in $d=2$ and $d=3$ respectively:

$$d=2:\ \frac{\varepsilon_c'}{\varepsilon_c}=0.884\frac{(t^*)^2}{U^2}+10.81\frac{(t^*)^4}{U^4}, \tag{6.3a}$$

$$d=3: \quad \frac{\varepsilon_c'}{\varepsilon_c}=0.948\frac{(t^*)^2}{U^2}+3.98\frac{(t^*)^4}{U^4} . \tag{6.3b}$$

This result shows that the error made in $d=2$ is significantly larger than in $d=3$: For $U/t^* \geq 6$ the estimated error due to the $1/d$ approximation is $\lesssim 18\%$ in $d=2$ and $\lesssim 6\%$ in $d=3$. For $U/t^* \geq 7$ the errors are $\lesssim 12\%$ in $d=2$ and $\lesssim 5\%$ in $d=3$.

Next we calculate the ground-state energy of the Heisenberg antiferromagnet in the $1/d$ approximation, and compare the outcome to known results in $d=2,3$. The ground-state energy of the Heisenberg model can be obtained from the first term, of $O[(t^*)^2/U]$, with $v=0$. In $d=2$ one obtains the estimate $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\tau} \rangle \simeq -0.324$, which is about 3.5% higher than the best estimates from series expansions or variational methods: $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\tau} \rangle \simeq -0.335(\pm 1)$.[33] From (5.7) one obtains in $d=3$ the estimate $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\tau} \rangle \simeq -0.297$, which agrees very well with results from $1/S$ expansions ($\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\tau} \rangle \simeq -0.301$).[34] These results show that the $1/d$ expansion is still reasonably accurate for calculating the ground-state energy of the Heisenberg model in $d=2,3$. Obviously the expansion is more accurate in $d=3$ than in $d=2$.

On the basis of these tests I conclude that the $1/d$ expansion, when applied in $d=3$, yields accurate predictions for ground-state properties. Furthermore, when applied in $d=2$, the $1/d$ expansion is definitely less accurate than in $d=3$, but the typical errors are still rather small (of the order of 10–15 % for ε_c). Thus the $1/d$ expansion appears to be very useful for the calculation of ground-state properties in both three- and two-dimensional systems.

VII. SUMMARY AND DISCUSSION

I start with the summary. I considered the extended Hubbard model (i.e., the one-band Hubbard model including nearest-neighbor interaction) at half filling on a d-dimensional (hyper-)cubical lattice. I determined the ground-state energy in the SDW and CDW phases at strong coupling up to fourth order in perturbation theory and used the results to calculate the boundary between the two phases in the ground-state phase diagram. Results were obtained for various dimensions; the special cases $d=1$, $d=\infty$, the $1/d$ expansion, and $d=2,3$ were discussed separately.

The location of the phase boundary in the ground-state phase diagram can be expressed most conveniently in terms of the deviation $\varepsilon_c \equiv v_c - \frac{1}{2}$ from the line $v=\frac{1}{2}$, as discussed in the Introduction. Generally speaking ε_c depends sensitively on the strength of the interaction and on dimension. Both in lower and in higher dimensions, second-order perturbation theory alone cannot explain ε_c at physically realistic values of the interaction.

The one-dimensional model is special since loop diagrams (which contribute in higher dimensions) do not occur. Moreover $d=1$ is the only dimension in which ε_c is *smaller* in fourth- than in second-order perturbation theory. In all other dimensions the fourth-order terms *enhance* ε_c. One can compare the results in $d=1$ with the Monte Carlo data of Hirsch.[18] If the fourth-order corrections are included excellent agreement with the Monte Carlo data is obtained even at moderately strong coupling ($U/t=6,8$). This is to be compared with the result from second-order perturbation theory, which is $\simeq 65\%$ larger than the data for $U/t=6$ and $\simeq 25\%$ larger for $U/t=8$. However, the error bars on the MC data at $U/t=8$ are too large to present definitive conclusions concerning the quality of fourth-order perturbation theory for such values of the interaction. More accurate MC data at $U/t \gtrsim 8$ would therefore be highly desirable.

In $d=\infty$ the most remarkable result is that the exact separation line at strong coupling is very close to the mean-field line, since the quadratic terms [proportional to $(t^*/U)^2$] in ε_c vanish. For example, ε_c at $U/t^*=6$ in $d=\infty$ is smaller than the corresponding value in $d=2$ or $d=3$ by an order of magnitude.

The transition from high to low dimensions has been studied in a systematic $1/d$ expansion. As a result one finds that lowering the dimension strongly *increases* the deviation ε_c from the mean-field line. The fact that ε_c depends sensitively on dimension also implies that a $1/d$ expansion up to $O(1/d^2)$ cannot be applied in too low dimensions, such as $d=1$. On the basis of several tests I argued that the $1/d$ expansion leads to reliable results in $d=3$ and is moderately accurate in $d=2$.

Next I discuss my results. I performed a perturbation expansion up to fourth order in t^*/U and, in the context of the $1/d$ expansion, up to fourth order in the transverse coupling. I argued repeatedly that the fourth order is indispensable for the calculation of physical quantities at realistic values of the interaction. In $d=1$ it is particularly clear that the fourth order is absolutely required to explain the Monte Carlo data at $U/t=6$ and $U/t=8$. In fact, I estimated that the regime where second-order perturbation theory alone can accurately describe ε_c starts only at $U/t \gtrsim 16$. In higher dimensions the situation is even clearer: the second-order result for ε_c is so small (it vanishes for $d \to \infty$) that the fourth order is necessary to obtain any nontrivial result at all.

Concerning the sign of the deviation ε_c: Throughout I found that ε_c is positive, as it is in the one-dimensional model. One might speculate whether ε_c might under suitable circumstances become negative, implying that the CDW (not the SDW) is stabilized by the hopping. This phenomenon could occur, e.g., at intermediate values of U and V. The most likely dimension for this to happen is $d=\infty$, because one knows already that ε_c is positive in low dimensions[18,36] and that ε_c is generally smaller for large U and V in high than in low dimensions. Probably the only way to find out whether $\varepsilon_c < 0$ can occur would be to perform a Monte Carlo simulation.

In this paper I could compare my results only to Monte Carlo simulations in $d=1$. In fact there exist also simulations carried out in two dimensions,[36] but here ε_c was estimated only for $U/t^*=2$, which is too small to be explained by the t/U expansion. An extension of the calculations of Ref. 36 to larger values of U/t would be valuable, but it is clear that such an extension may be difficult in $d=2$.

The work reported in this paper can be extended in

various directions. At half filling and $T=0$ other interesting quantities [like correlation functions and the $n(\mathbf{k})$ distribution] can be calculated. Furthermore one can apply the same methods to other fillings (like quarter filling) and to attractive U and/or V. Another extension would be to consider positive temperatures. For example, one could calculate the critical temperature of the fourth-order effective Hamiltonian in the SDW phase using a $1/d$ expansion, similar to the work by Fisher and Gaunt[37] on the Ising model.

In closing I would liked to attract attention to an interesting mathematical question concerning the large-U expansion, that was not addressed in this paper. In $d=1$ it is known[27] that the ground-state energy of the Hubbard model as a function of t/U is a Taylor series with a finite radius of convergence. To my knowledge no such statement has been proved for the extended Hubbard model in $d=1$ or in fact in any $d>1$. Still, it seems likely that the (extended) Hubbard model has a finite radius of convergence at strong coupling in all dimensions. It would be interesting if the analytical properties of the ground-state energy at large U and V could be clarified, possibly with the use of the recursion relations derived in Appendix A.

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APPENDIX A: DERIVATION OF THE EFFECTIVE HAMILTONIAN

In this Appendix we derive an effective Hamiltonian for the extended Hubbard model at strong coupling. The method used is a streamlined version of the method of Harris and Lange,[19] which is here considered to all orders of perturbation theory. It is shown that the various terms in the perturbation expansion of the effective Hamiltonian can be calculated *recursively*. Although we focus on the extended Hubbard model the formalism is more generally applicable.

The basic idea of the method of Harris and Lange is to apply a canonical transformation from the fermions $c_{i\sigma}$ to new particles $\bar{c}_{i\sigma}$:

$$c_{i\sigma}^{\dagger}=e^{S(\bar{c})}\bar{c}_{i\sigma}^{\dagger}e^{-S(\bar{c})}\ , \tag{A1}$$

where the operator $S(\bar{c})$ is anti-Hermitian. The transformation is chosen such that the hopping of the new particles leaves the interaction term $H_0(\bar{c})$ invariant. Here $H_0(\bar{c})$ is given by $H_0=H_U+H_V+H_\mu$ in (1.1) with $c_{i\sigma}$ replaced by $\bar{c}_{i\sigma}$. The basic idea is to split up the Hamiltonian into two parts,

$$\begin{aligned}H&=e^{S(\bar{c})}[H_t(\bar{c})+H_0(\bar{c})]e^{-S(\bar{c})}\\&\equiv H_t'(\bar{c})+H_0(\bar{c})\ .\end{aligned} \tag{A2}$$

The rationale behind this is that, at low temperatures ($T\ll U$), it suffices to take into account only the ground state of $H_0(\bar{c})$. The effective Hamiltonian at low temperatures is therefore simply given by $H_t'(\bar{c})$.

The requirement that $H_0(\bar{c})$ is a constant of the motion is formally expressed by

$$0=[H,H_0(\bar{c})]=[H_t'(\bar{c}),H_0(\bar{c})]\ . \tag{A3}$$

In order to solve this equation, which fixes $S(\bar{c})$, we expand $S(\bar{c})$ and $H_t'(\bar{c})$ in a power series in t/U:

$$S(\bar{c})=\sum_{n=1}^{\infty}\frac{1}{U^n}S_n(\bar{c})\ ;\quad H_t'(\bar{c})=\sum_{n=1}^{\infty}\frac{1}{U^{n-1}}H_{tn}'(\bar{c})\ , \tag{A4}$$

As we shall see below, both $S_n(\bar{c})$ and $H_{tn}'(\bar{c})$ are of order t^n. In this manner one obtains a systematic expansion of the operators $S(\bar{c})$ and $H_t'(\bar{c})$ in powers of t/U. The nth order contributions, $S_n(\bar{c})$ and $H_{tn}'(\bar{c})$, can be calculated successively from the equations

$$0=[H_{tn}'(\bar{c}),H_0(\bar{c})]\quad(n=1,2,\ldots)\ . \tag{A5}$$

Starting from these equations, Harris and Lange determined $H_{tn}'(\bar{c})$ for $n=1$ and 2. Below we shall see that $H_{tn}'(\bar{c})$ can in principle be calculated recursively to arbitrary order in perturbation theory.

In order to obtain an explicit expression for $H_{tn}'(\bar{c})$ in terms of the operators $S_n(\bar{c})$ we introduce the shorthand notation

$$[O_1O_2\cdots O_{n-1}O_n]\equiv[O_1,[O_2,\ldots[O_{n-1},O_n]\ldots]] \tag{A6}$$

for the nth order commutator of the operators $O_1,\ldots,O_n$. For $n=1$ we use the convention $[O_1]\equiv O_1$. With these definitions the general commutation relation

$$e^{S(\bar{c})}Xe^{-S(\bar{c})}=\sum_{m=0}^{\infty}\frac{1}{m!}[S^mX]$$

can be applied to $S(\bar{c})$ in (A4) to yield

$$e^{S(\bar{c})}Xe^{-S(\bar{c})}=\sum_{n=0}^{\infty}\frac{1}{U^n}C_n(X)\ , \tag{A7}$$

where $C_n(X)$ is for $n\geq 1$ defined by

$$C_n(X)\equiv\sum_{m=1}^{n}\frac{1}{m!}\sum_{\{n_1+\cdots+n_m=n\}}[S_{n_1}\cdots S_{n_m}X]\quad(n\geq 1) \tag{A8}$$

and $C_0(X)\equiv X$. As a consequence

$$\begin{aligned}H&=e^{S(\bar{c})}[H_t(\bar{c})+H_0(\bar{c})]e^{-S(\bar{c})}\\&=\sum_{n=0}^{\infty}\frac{1}{U^n}C_n(H_t+H_0)\\&=H_0+\sum_{n=1}^{\infty}\frac{1}{U^{n-1}}\{C_n(H_0/U)+C_{n-1}(H_t)\}\ .\end{aligned}$$

Comparison with (A2) shows that $H_{tn}'(\bar{c})$ is given by

$$H_{tn}'(\bar{c})=\frac{1}{U}C_n(H_0(\bar{c}))+C_{n-1}(H_t(\bar{c}))\ . \tag{A9}$$

This equation relates the nth-order hopping process $H'_{tn}(\bar{c})$ to the as yet unknown operators $S_1(\bar{c}),\ldots,S_n(\bar{c})$.

The operators $S_1(\bar{c}),\ldots,S_n(\bar{c})$ are determined by the requirement (A5) that the interaction is a constant of the motion. Insertion of (A9) into (A5) yields the following restriction on $S_n(\bar{c})$:

$$0=[H_0,C_n(H_0)+UC_{n-1}(H_t)]$$
$$=[H_0,[S_n,H_0]+\tilde{C}_n(H_0)+UC_{n-1}(H_t)]\ , \qquad \text{(A10)}$$

where we split up $C_n(X)$ into its $(m=1)$ component $[S_n,X]$ and the rest: $C_n(X)\equiv[S_n,X]+\tilde{C}_n(X)$. To solve (A10) we decompose $H_t(\bar{c})$ into hopping processes with the property that they change $H_0(\bar{c})$ by an amount λU:

$$H_t=\sum_{\lambda\in\Lambda} T_\lambda\ ;\ [T_\lambda H_0]=-\lambda U T_\lambda\ .$$

The summation variable λ takes values in the (finite) set Λ. Obviously such a decomposition is always possible, since the number of different hopping processes is finite. As a consequence a similar decomposition is possible for the operators $S_n(\bar{c})$:

$$S_n=\sum_{\lambda\in\Lambda_n} S_{n\lambda}\ ;\ [S_{n\lambda}H_0]=-\lambda U S_{n\lambda}\ ,$$

where λ now takes values in the (finite) set Λ_n. In general Λ_n will be different for different values of n. This decomposition allows us to solve (A10) for general n. The solution has the property $S_{n0}=0$ (so that effectively $0\notin\Lambda_n$ for all n) and for $\lambda\neq 0$:

$$S_{n\lambda}=\frac{1}{\lambda}P_\lambda\{\tilde{C}_n(H_0/U)+C_{n-1}(H_t)\}\ . \qquad \text{(A11)}$$

Here P_λ is the projection operator onto the subset of hopping processes that change H_0 by λU. If one inserts the explicit form of C_{n-1} and $\tilde{C}_n$ into (A11), one obtains the following recursion relation for the operators $S_{n\lambda}$ (with $\lambda\neq 0$):

$$\lambda S_{n\lambda}=\delta_{n1}T_\lambda-\sum_{m=2}^{n}\frac{1}{m!}\sum_{\substack{n_1+\cdots+n_m=n\\ \lambda_1+\cdots+\lambda_m=\lambda}}\lambda_m[S_{n_1\lambda_1}\ldots S_{n_m\lambda_m}]+\sum_{m=1}^{n-1}\frac{1}{m!}\sum_{\substack{n_1+\cdots+n_m=n-1\\ \lambda_1+\cdots+\lambda_{m+1}=\lambda}}[S_{n_1\lambda_1}\ldots S_{n_m\lambda_m}T_{\lambda_{m+1}}]\ . \qquad \text{(A12)}$$

Equation (A12) determines the canonical transformation $S(\bar{c})$ recursively to all orders in perturbation theory.

Once $S_{n\lambda}$ is known, one can proceed to calculate the effective Hamiltonian $H'_t(\bar{c})$ with the use of (A9). The result is

$$H'_{tn}(\bar{c})=\frac{1}{U}C_n(H_0)+C_{n-1}(H_t)=\frac{1}{U}\{[S_nH_0]+\tilde{C}_n(H_0)+UC_{n-1}(H_t)\}=\frac{1}{U}P_0\{\tilde{C}_n(H_0)+UC_{n-1}(H_t)\}\ . \qquad \text{(A13)}$$

With the use of the known form of C_{n-1} and $\tilde{C}_n$ one finds the following explicit expression for H'_{tn} in terms of the operators $S_{n\lambda}$:

$$H'_{tn}=\delta_{n1}T_0-\sum_{m=2}^{n}\frac{1}{m!}\sum_{\substack{n_1+\cdots+n_m=n\\ \lambda_1+\cdots+\lambda_m=0}}\lambda_m[S_{n_1\lambda_1}\ldots S_{n_m\lambda_m}]+\sum_{m=1}^{n-1}\frac{1}{m!}\sum_{\substack{n_1+\cdots+n_m=n-1\\ \lambda_1+\cdots+\lambda_{m+1}=0}}[S_{n_1\lambda_1}\ldots S_{n_m\lambda_m}T_{\lambda_{m+1}}]\ . \qquad \text{(A14)}$$

Thus $H'_{tn}(\bar{c})$ describes hopping of $\bar{c}$ fermions with a $(\lambda=0)$ component only; consequently $H_0(\bar{c})$ is a constant of the motion, as it should be. Equations (A14) and (A12) completely determine the effective Hamiltonian for the extended Hubbard model at strong coupling. The effective Hamiltonian consists of *connected* hopping processes, as is clear from the presence of multiple commutators in (A12) and (A14).

APPENDIX B: EXPLICIT FORM OF $H'_t(\bar{c})$

In this appendix we calculate the explicit form of the effective Hamiltonian $H'_t(\bar{c})$ for the CDW and SDW phases. The calculations for these phases are formally similar although the results are qualitatively very different: the "effective Hamiltonian" is a *number* for the CDW phase (since the ground state is unique, apart from global symmetries), whereas in the SDW phase the effective Hamiltonian is an operator.

Obviously all odd orders in perturbation theory vanish since one needs an even number of hopping processes to return to the subspace of allowed states. Below we consider first the second order and then the fourth order of perturbation theory.

The result in second-order perturbation theory is well known,[19]

$$H'_{t2}=\tfrac{1}{2}\sum_\lambda\lambda[S_{1,-\lambda}S_{1\lambda}]\ , \qquad \text{(B1a)}$$

$$S_{1\lambda}=\frac{1}{\lambda}T_\lambda\quad(\lambda\neq 0)\ . \qquad \text{(B1b)}$$

Within the subspace of allowed states only terms with $\lambda=\pm\lambda_1$ contribute, where λ_1 equals the excitation energy for jumps out of an allowed state. One finds that $\lambda_1=(4-1/d)v-1$ for the CDW phase and $\lambda_1=1-v/d$ for the SDW phase.

In fourth-order perturbation theory one finds that H'_{t4} has the form

$$H'_{t4}=\frac{1}{8}\sum_{\lambda_1+\lambda_2+\lambda_3+\lambda_4=0}[S_{1\lambda_1}S_{1\lambda_2}S_{1\lambda_3}T_{\lambda_4}]+\frac{1}{2}\sum_{\lambda}\lambda[S_{2,-\lambda}S_{2\lambda}]\ , \tag{B2}$$

where the operator $S_{2\lambda}$ is for $\lambda\neq 0$ given by

$$S_{2\lambda}=\frac{1}{2\lambda}\sum_{\lambda_1+\lambda_2=\lambda}[S_{1\lambda_1}T_{\lambda_2}]\ (\lambda\neq 0)\ , \tag{B3}$$

while $S_{20}\equiv 0$ as usual. Equation (B2) shows that H'_{t4} consists of four connected hopping processes; disconnected processes vanish due to the occurrence of commutators. The first (i.e., rightmost) and the last (i.e., leftmost) hopping process in a string of four always have the excitation energies $+\lambda_1$ and $-\lambda_1$ respectively. For the two processes in between there are two possibilities: (i) the second process can be connected to the first; such processes are labeled by c, and their excitation energies by λ_{2c}, or (ii) the second process can be disconnected from the first (i.e., the two are connected only by the third and fourth processes); such processes are labeled by d, and their excitation energies are λ_{2d}. With this notation Eq. (B2) can be simplified to

$$H'_{t4}=\frac{1}{\lambda_1^3}T_{-\lambda_1}T_{\lambda_1}T_{-\lambda_1}T_{\lambda_1}-\sum_{\{c\}}\frac{1}{\lambda_1^2(\lambda_1+\lambda_{2c})}T_{-\lambda_1}T_{-\lambda_{2c}}T_{\lambda_{2c}}T_{\lambda_1}-\sum_{\{d\}}\frac{1}{2\lambda_1^2\lambda_{2d}}T_{-\lambda_1}T_{-\lambda_{2d}}T_{\lambda_{2d}}T_{\lambda_1}\ , \tag{B4}$$

where it is understood that only connected graphs are to be taken into account. Equation (B4) holds for both the CDW and the SDW phase. The differences between the two phases arise in the evaluation of (B4). These differences will be pointed out below.

1. The CDW phase

The contribution in second-order perturbation theory follows from (B1a) as

$$H'_{t2}=-\frac{1}{\lambda_1}\langle T_{-\lambda_1}T_{\lambda_1}\rangle_0=-\frac{1}{(4-1/d)v-1}\mathcal{N}(t^*)^2\ . \tag{B5}$$

In the last step we evaluated H'_{t2} in the subspace of allowed states, which is simply the CDW ground state. The "effective Hamiltonian" thus reduces to a real number.

In fourth-order perturbation theory there are two relevant hopping processes of type c (denoted by c_1 and c_2) and one of type d. Diagrammatically, type c_1 corresponds to three-site processes, type c_2 to two-site processes, and type d to loop diagrams. The corresponding excitation energies are $\lambda_{2c_1}=v(4-3/d)$, $\lambda_{2c_2}=v(4-3/d)+1$, and $\lambda_{2d}=v(4-3/d)-1$. The first term in (B2) represents both three- and two-site processes. Evaluation of the various terms in the CDW ground state is straightforward. The result is

$$H'_{t4}=\mathcal{N}(t^*)^4\left[\frac{1}{\lambda_1^3}\left[4-\frac{1}{d}\right]-\frac{4}{\lambda_1^2(\lambda_1+\lambda_{2c_1})}\left[1-\frac{1}{2d}\right]-\frac{1}{\lambda_1^2(\lambda_1+\lambda_{2c_2})}\frac{1}{d}+\frac{1}{\lambda_1^2\lambda_{2d}}\left[1-\frac{1}{d}\right]\right]\ . \tag{B6}$$

This result is exact up to $O(x^5U)$, with $x=t^*/U$, for all dimensions $d\geq 1$.

The ground-state energy in the CDW phase thus follows as

$$E_0^{\mathrm{CDW}}=\mathcal{N}[\tfrac{1}{2}U+H'_{t2}/U+H'_{t4}/U^3]\ ,$$

where H'_{t2} and H'_{t4} are given in (B5) and (B6) respectively. The explicit result is given in Eq. (2.1).

2. The SDW phase

In the SDW phase the set of allowed states consists of all states without doubly occupied sites. Within this subspace, labeled by the subscript "0," the second order in perturbation theory yields

$$H'_{t2}=-\frac{1}{\lambda_1}\langle T_{-\lambda_1}T_{\lambda_1}\rangle_0=-\frac{(t^*)^2}{2d(1-v/d)}\sum_{(ij)}Q_{ij}\ , \tag{B7}$$

where we used the Q_{ij} operators defined in (2.3a).

In fourth-order perturbation theory there is just one possible hopping process of type c, corresponding to three-site processes with excitation energy $\lambda_c=v/d$, and there is one hopping process of type d, giving rise to loop diagrams and having excitation energy $\lambda_d=1-3v/d$. Since $\lambda_1+\lambda_c=1$, Eq. (B4) reduces to

$$H'_{t4}=\frac{1}{\lambda_1^3}T_{-\lambda_1}T_{\lambda_1}T_{-\lambda_1}T_{\lambda_1}-\frac{1}{\lambda_1^2}T_{-\lambda_1}T_{-\lambda_{2c}}T_{\lambda_{2c}}T_{\lambda_1}-\frac{1}{2\lambda_1^2\lambda_{2d}}T_{-\lambda_1}T_{-\lambda_{2d}}T_{\lambda_{2d}}T_{\lambda_1}\ . \tag{B8}$$

Diagrammatically the first two terms in (B8) represent diagrams without loops, and the last term corresponds to loops. Consequently one has to distinguish one-dimensional systems, where loops are impossible, and higher dimensions ($d\geq 2$). In $d=1$, Eq. (B8) can be rewritten in terms of Q_{ij} operators as

$$H'_{t4}=\frac{2(1+v)t^4}{(1-v)^3}\sum_{i\tau}(Q_{i,i+\tau}+Q_{i,i-\tau}Q_{i,i+\tau})\ , \tag{B9}$$

where $\tau=\pm 1$. For $d\geq 2$, Eq. (B8) can be written as

$$H'_{t4}=\frac{(t^*)^4}{4d^2}\left\{A\sum_{\{\square\}}(Q_{12}Q_{34}+Q_{23}Q_{14}-Q_{13}Q_{24})\right.$$
$$-B\sum_{(ij)}Q_{ij}+C\sum_{i,\tau'\neq\pm\tau}Q_{i+\tau',i+\tau}$$
$$\left.-D\sum_{i\tau}Q_{i+\tau,i-\tau}\right\}, \tag{B10}$$

where now τ is a lattice vector and the constants A, B, C, and D are defined as

$$A=\frac{8(4\lambda_d+1)}{2\lambda_1^2\lambda_d}\ ;\quad C=\frac{2(2\lambda_1-1)}{\lambda_1^3}\ ;$$
$$B=\frac{4}{\lambda_1^3}[\lambda_1(4d-3)-2d]\ ;\quad D=\frac{2-\lambda_1}{\lambda_1^3}\ .$$

In the derivation of (B9) and (B10) we used similar algebraic manipulations as have been used by Takahashi[20] for the special case of the Hubbard model ($v=0$). In the sum over plaquettes, denoted by boxes "□", each distinct plaquette is counted only once; the labels $\{1,2,3,4\}$ refer to the successive sites encountered as one goes around the plaquette.

The effective Hamiltonian in the SDW phase is now given by

$$H_f=\mathcal{N}[V+H'_{t2}/U+H'_{t4}/U^3]\ ,$$

where H'_{t2} and H'_{t4} are given in (B7) and (B9) (for $d=1$) or (B10) (for $d\geq 2$).

APPENDIX C: EXPANSION ABOUT THE ISING LIMIT

In this section the spin-flip part H_f^S of the effective Hamiltonian will be treated as a small perturbation. This is justified by the outcome, since these terms are of higher order in the small parameter $1/d$. Our results are also systematic in the small parameter t^*/U: we calculate all contributions up to $O[(t^*)^5/U^4]$ and neglect terms of higher order.

First consider the *second* order in perturbation theory. Since the excitation energy of a spin flip in the Néel state is of $O[(t^*)^2/U]$, all diagrams involving two spin flips from the A, C, or D terms in (5.4) can be neglected, since they are of $O[(t^*)^6/U^5]$. Hence the C and the D term can be discarded to start with. Non-negligible contributions are obtained only for two spin flips from the J term or possibly for one spin flip from each of the J and A terms. Consequently the factors Q^N in (5.4) simply yield factors of unity. Hence the contribution to the ground-state energy in second-order perturbation theory can be obtained from the effective Hamiltonian

$$H_f^S\triangleq-\tfrac{1}{4}J'\sum_{(ij)}Q_{ij}^S\ , \tag{C1}$$

where the new coupling constant J' is defined by

$$J'\equiv J-\frac{4(d-1)t^4A}{U^3} \tag{C2}$$

and J has been defined in (2.7). Consequently, if λ_0 is the excitation energy of a spin flip in the Néel state, there are to second order in perturbation theory only two possible processes: spin flips from the Néel state to an excited state, corresponding to the operator T_{λ_0}, and the reverse process, described by $T_{-\lambda_0}$. Thus one finds for the second-order contribution (which is a *real number*):

$$H'_{t2}=-\frac{1}{\lambda_0}\langle T_{-\lambda_0}T_{\lambda_0}\rangle_{\text{Néel}}$$
$$=-\frac{(J')^2}{8\lambda_0}\sum_{(ij)}\langle Q_{ij}^SQ_{ji}^S\rangle_{\text{Néel}} \tag{C3}$$
$$=-\frac{d(J')^2}{4\lambda_0}\mathcal{N}\ , \tag{C4}$$

which is of $O(1/d)$ since $J'\propto 1/d$. Therefore, to calculate H'_{t2} correct to $O(1/d^2)$ and to $O[(t^*)^4/U^3]$ it suffices to determine the excitation energy λ_0 to $O(1/d)$ and to $O[(t^*)^4/U^3]$. The energy of a single spin flip in the Néel state can easily be determined from (5.3). One finds that, up to the desired order,

$$\lambda_0=\frac{4(t^*)^2}{U^2}\left[1+\frac{2v-1}{2d}\right]-\frac{16(t^*)^4}{U^4}\left[1+\frac{5v-\frac{9}{8}}{d}\right],$$

so that (C4) gives a contribution of

$$\frac{1}{U}H'_{t2}=-\mathcal{N}\frac{(t^*)^2}{4dU}\left[1+\frac{v+\frac{1}{2}}{d}-\frac{8(t^*)^2}{U^2}\left[1+\frac{3v-\frac{3}{16}}{d}\right]\right] \tag{C5}$$

to the expectation value $\langle H_f^S\rangle$.

In third-order perturbation theory it suffices to take only the leading terms in t^*/U and $1/d$ into account, since third-order contributions are of $O[(t^*)^4/U^3d^2]$ or smaller. Hence the effective Hamiltonian H_f^S can be simplified in third order to

$$H_f^S=-\tfrac{1}{4}J\sum_{(ij)}Q_{ij}^S+\frac{2t^4}{U^3}\sum_{i,\tau'\neq\pm\tau}Q_{i+\tau',i+\tau}^S$$
$$+\frac{5t^4}{2U^3}\sum_{i,\tau'\neq\pm\tau}(Q_{12}^SQ_{34}^S+Q_{23}^SQ_{14}^S-Q_{13}^SQ_{24}^S)\ . \tag{C6}$$

From (A14) one finds that

$$H'_{t3}=\frac{1}{2}\sum_{\lambda_1+\lambda_2=0}\langle[S_{1\lambda_1}S_{1\lambda_2}T_0]\rangle_{\text{Néel}}$$
$$+\frac{1}{3}\sum_{\lambda_1+\lambda_2+\lambda_3=0}\lambda_3\langle[S_{1\lambda_1}S_{1\lambda_2}S_{1\lambda_3}]\rangle_{\text{Néel}}\ .$$

The first term gives rise to connected hopping processes of the form $T_{-\lambda}T_0T_\lambda$, with $\lambda>0$. The T_0 process cannot come from the J term in (C6), since nearest-neighbor spin flips have a nonvanishing excitation energy. Hence T_0 comes from one of the last two terms in (C6). This in turn implies that $T_{\pm\lambda}$ has to come from the J term in order to obtain diagrams of order $O[(t^*)^4/U^3]$. The only possibility is therefore $\lambda=\lambda_\infty$, with

$$\lambda_\infty \equiv \frac{4(t^*)^2}{U^2}\left[1-\frac{4(t^*)^2}{U^2}\right], \tag{C7}$$

and H'_{t3} reduces to

$$H'_{t3} = \frac{1}{(\lambda_\infty)^2}(\langle T_{-\lambda_\infty} T_0 T_{\lambda_\infty}\rangle_{\text{Néel}} + \langle T_{-\lambda_\infty} T_{-\lambda_\infty} T_{2\lambda_\infty}\rangle_{\text{Néel}}),$$

where only connected diagrams contribute. Finally one obtains the following result

$$\frac{1}{U^2}H'_{t3} = \frac{3(t^*)^4}{4d^2U^3}\mathcal{N} \tag{C8}$$

for the third-order contributions to $\langle H_f^S\rangle$.

The fourth-order contribution to $\langle H_f^S\rangle$ is again simple, since only single spin flips contribute and H_f^S is given by (C1), where now J' can be replaced by its leading term in $1/d$. Hence only excitations with energies $\lambda=\pm\lambda_\infty$ are possible and one finds, as in (B4), that

$$H'_{t4} = \frac{1}{\lambda_\infty^3}\langle T_{-\lambda_\infty} T_{\lambda_\infty} T_{-\lambda_\infty} T_{\lambda_\infty}\rangle_{\text{Néel}} - \frac{1}{2\lambda_\infty^3}\langle T_{-\lambda_\infty} T_{-\lambda_\infty} T_{\lambda_\infty} T_{\lambda_\infty}\rangle_{\text{Néel}}, \tag{C9}$$

where only connected diagrams are allowed. The first term in (C9) leads to three-site processes, the second to loop diagrams. Evaluation in the Néel state is easy. The result is

$$\frac{1}{U^3}H'_{t4} = \frac{(t^*)^2}{32d^2U}\left[1-\frac{12(t^*)^2}{U^2}\right]\mathcal{N}. \tag{C10}$$

Combination of (C5), (C8), and (C10) finally gives the result (5.6) for $\langle H_f^S\rangle$ quoted in the text.

[1] J. Hubbard, Proc. R. Soc. London Ser. A **276**, 238 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10**, 59 (1963); J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).
[2] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[3] H. Tasaki, Phys. Rev. B **40**, 9192 (1989).
[4] P. W. Anderson, Solid State Phys. **14**, 99 (1963); M. Cyrot, J. Phys. (Paris) **33**, 125 (1972); W. Langer, M. Plischke, and D. Mattis, Phys. Rev. Lett. **23**, 1448 (1969).
[5] M. Cyrot, Physica B & C **91B**, 141 (1977); for a recent numerical study of the paramagnetic small-U Hubbard model, see H. Schweitzer and G. Czycholl, Z. Phys. B **83**, 93 (1991).
[6] H. J. Schulz, Phys. Rev. Lett. **64**, 1445 (1990).
[7] N. F. Mott, Rev. Mod. Phys. **40**, 677 (1968); W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[8] J. Hubbard, Proc. R. Soc. London Ser. A **281**, 401 (1964).
[9] P. W. Anderson, Science **235**, 1196 (1987).
[10] A. E. Ruckenstein, P. J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).
[11] E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989).
[12] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[13] In $d=1$ the transition is known to be second order at weak and first order at strong interaction. In higher dimensions ($d\to\infty$) the transition is first order for all U and V.
[14] J. Solyom, Adv. Phys. **21**, 201 (1979); V. J. Emery, in *Highly Conducting One-Dimensional Solids,* edited by J. Devreese, R. Evrand, and V. van Doren (Plenum, New York, 1979).
[15] U. Wolff, Nucl. Phys. B **225**, 391 (1983).
[16] R. A. Bari, Phys. Rev. B **3**, 2662 (1971).
[17] P. G. J. van Dongen, Phys. Rev. Lett. **67**, 757 (1991).
[18] J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984).
[19] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).
[20] M. Takahashi, J. Phys. C **10**, 1289 (1977).
[21] V. J. Emery, Phys. Rev. B **14**, 2989 (1976).
[22] D. K. Campbell, J. Tinka Gammel, and E. Y. Loh, Jr., Phys. Rev. B **42**, 475 (1990).
[23] L. N. Bulaevskii, Zh. Eksp. Teor. Fiz. **51**, 230 (1967) [Sov. Phys.—JETP **24**, 154 (1966)].
[24] D. J. Klein and W. A. Seitz, Phys. Rev. B **8**, 2236 (1973).
[25] H. Bethe, Z. Phys. **71**, 205 (1931).
[26] I am grateful to Dr. Hirsch for making these data (not explicitly contained in Ref. 18) available to me. The actual error bars on the MC data were probably much smaller than the ones quoted.
[27] M. Takahashi, Prog. Theor. Phys. **45**, 756 (1971).
[28] W. Metzner, Ph.D. thesis, Rheinisch-Westfälische Technische Hochschule Aachen, 1990.
[29] H. L. Davis, Phys. Rev. **120**, 789 (1960).
[30] M. Parinello and T. Arai, Phys. Rev. B **10**, 265 (1974).
[31] D. A. Huse, Phys. Rev. B **37**, 2380 (1988).
[32] R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989).
[33] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).
[34] H. Nishimori and S. J. Miyake, Prog. Theor. Phys. **73**, 18 (1985).
[35] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[36] Y. Zhang and J. Callaway, Phys. Rev. B **39**, 9397 (1989).
[37] M. E. Fisher and D. S. Gaunt, Phys. Rev. **133**, A224 (1964).