Phase diagram and correlation functions of the half-filled extended Hubbard model in one dimension

Johannes Voit
Institut Laue-Langevin, Boîte Postale 156X, 38042 Grenoble, France
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The extended Hubbard model in one dimension is studied for half-filled bands using a continuum theory based on the Luttinger model. Interactions going beyond the Luttinger model are treated with a renormalization group. We compute correlation functions and use these to establish the phase diagram of the model. It compares favorably with earlier numerical work. Specifically, we identify additional interaction terms coupling charge and spin degrees of freedom; one of them is shown to mediate the crossover from a continuous to a first-order transition from spin- to charge-density waves at a finite value of $U=2V$. Our approach suggests viewing the model on this line as two weakly coupled interpenetrating systems of up-spin and down-spin electrons with strong backscattering interactions favoring charge-density waves separately in each of the subsystems. A first-order transition occurring for attractive interactions is interpreted as a characteristic instability of the Luttinger liquid towards phase separation. We finally discuss a possible equivalence to some recent studies of coupled two-dimensional XY models.

I. INTRODUCTION

Long-range Coulomb interactions have been recognized to play an important role in quasi-one-dimensional organic solids such as conjugated polymers[1] and charge-transfer crystals.[2] The extended Hubbard model (EHM) is the simplest one-dimensional (1D) lattice model including finite-range interactions. Its Hamiltonian is

$$H=-t\sum_{i,s}(c_{i,s}^{\dagger}c_{i+1,s}+\text{H.c.})+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}+V\sum_{i}n_{i}n_{i+1}\ , \tag{1.1}$$

where $c_{i,s}^{\dagger}$ creates an electron with spin s on the lattice site i. t is the nearest-neighbor hopping integral, U is the on-site, and V a nearest-neighbor interaction. While for the Coulomb interaction, $U \gg V$ are both repulsive, additional interactions present in a more realistic model (such as coupling to high-frequency phonons or excitons) can be modeled by more general U,V including attractive ones.

For half-filled bands, the EHM displays a surprising richness in its physical behavior although the results of several published studies show some disagreement. Fourcade and Spronken[3] studied the crossover from a spin-density-wave (SDW) to a charge-density-wave (CDW) ground state for repulsive interactions using real-space renormalization-group methods. They found a continuous transition close to the line $U=2V$ but slightly displaced towards larger V. This is interesting since both weak[4,5] and strong[6] coupling approximations predicted the transition to occur precisely at $U=2V$. Hirsch,[7] using Monte Carlo simulations, confirmed the deviations of the SDW-CDW transition line from $U=2V$ but surprisingly found a change from a continuous to a first-order transition at a finite critical interaction $U\approx 2V\approx 3t$. Evidence for the existence of a tricritical point at finite coupling has also been presented by Fourcade.[8] Later, Lin and Hirsch[9] discovered another first-order transition to a phase-separated "condensed" phase for negative V. In a further exact calculation on a four-site cluster Milans del Bosch and Falicov found a first-order transition exactly at $U=2V$.[10] These results have essentially been confirmed in an exact Lanczos diagonalization study.[11] In a refined continuum field theory, an umklapp scattering process involving parallel spins responsible for the crossover from a continuous to a first-order SDW-CDW transition has been identified by the present author.[12] Notice however that Hirsch[7] credits Haldane for predicting this crossover. More recently, Cannon and Fradkin[13] published a similar field theory combined with quantum Monte Carlo results that shows the tricritical point to occur at $U\approx 2V\approx 1.5t$. Both field theories[12,13] situate the SDW-CDW transition line at $U=2V$. In a very recent study Cannon, Scalettar, and Fradkin[14] extended their earlier study by including data obtained by Lanczos diagonalization. It was found that apparently the Monte Carlo method tends to underestimate the interaction where the tricritical point occurs and, although the clusters diagonalized were too small to accurately locate it, evidence was produced for a value $U\approx 2V\approx(4-5)t$.

In this paper, we present in more detail a continuum field theory for the extended Hubbard model yielding both the change from continuous to first order in the SDW-CDW transition for a repulsive interaction and the first-order condensation transition for an attractive interaction. Our calculation proceeds by solving exactly a Luttinger model including a subset of the interaction processes of the continuum field theory and by investigating perturbations around this "Luttinger liquid"[15] fixed point by renormalization-group (RG) methods; it therefore suggests interpreting the first-order transitions of the EHM as representative examples for two characteristic instabilities of a Luttinger liquid formed by spin-$\frac{1}{2}$ electrons in 1D—one with respect to strong charge-spin coupling, the other with respect to strong (bare) attractive interactions—in addition to its more usual instability against sine-Gordon-like current-nonconserving interactions yielding continuous transitions identified elsewhere in the phase diagram. In Sec. II, we formulate the continuum field theory and identify the interactions present in the bare theory; we further discuss additional new terms coupling charge and spin degrees of freedom generated by the RG method (Sec. II). In Sec. III we discuss the resulting phase diagram (in the U-V parameter space) of the model and its correlation functions. The calculation of the correlation function also reveals shortcomings of the present method, which will be discussed in Sec. IV, together with the relationship of the transitions found here to similar observations in classical 2D spin systems. While we also provide some results on the EHM, another aim of the present study is more pedagogical in nature: to demonstrate that the notion of a Luttinger liquid is not only an interesting concept in the physics of quasi-1D systems but also a useful device. We show that a continuum field theory based on the Luttinger model, when performed carefully, is capable of rendering a reasonably detailed picture of a model containing important perturbations, such as commensurability and charge-spin coupling leading to both continuous and discontinuous phase transitions and thus promises also to be a good starting point for the study of more delicate problems in 1D. Appendix A discusses details of the computation of the different correlation functions; Appendix B summarizes changes in the coupling constants necessary if one wishes to apply the present methods to more general problems including site-off-diagonal interactions.

II. CONTINUUM FIELD THEORY AND RG ANALYSIS

In order to derive a field theory, we perform the continuum limit (lattice constant $a \to 0$, number of lattice sites $N \to \infty$ such that $L = Na$ finite)

$$c_{i,s}^{\dagger} \to \sum_{r=\pm} \sqrt{a}\, \Psi_{r,s}^{\dagger}(x=ia) \ . \tag{2.1}$$

$\Psi_{r,s}^{\dagger}(x)$ creates a fermion of spin s on the branch $r=\pm$ of the linearized spectrum $E(k)=v_F(rk-k_F)$. The continuum limit is a good approximation for weak coupling and for asymptotic low-energy properties of the model. If the branches of this spectrum are extended to infinity and all negative-energy states filled (Luttinger model, cf. below), we can use the bosonization identity[15]

$$\Psi_{r,s}(x) = \lim_{\alpha\to 0} \frac{e^{irk_F x}}{\sqrt{2\pi\alpha}} U_{r,s}^{\dagger} \times \exp\left[-\frac{i}{\sqrt{2}} \{ r\Phi_\rho(x) - \Theta_\rho(x) + s[r\Phi_\sigma(x) - \Theta_\sigma(x)]\} \right] , \tag{2.2}$$

$$\Phi_\nu(x) = -\frac{i\pi}{L} \sum_{p\neq 0} \frac{1}{p} e^{-\alpha|p|/2 - ipx} [\nu_+(p) + \nu_-(p)] - (N_{+,\nu} + N_{-,\nu}) \frac{\pi x}{L} , \tag{2.3}$$

$$\Theta_\nu(x) = \frac{i\pi}{L} \sum_{p\neq 0} \frac{1}{p} e^{-\alpha|p|/2 - ipx} [\nu_+(p) - \nu_-(p)] + (N_{+,\nu} - N_{-,\nu}) \frac{\pi x}{L} , \tag{2.4}$$

$$\frac{\partial \Theta_\nu(x)}{\partial x} = \pi \Pi_\nu(x), \quad [\Pi_\nu(x), \Phi_{\nu'}(x')] = -i\delta_{\nu,\nu'}\delta(x-x') \ . \tag{2.5}$$

The fields $\Phi_\nu(x)$ and $\Theta_\nu(x)$ describe the collective charge and spin fluctuations ($\nu = \rho, \sigma$) in terms of boson operators $\nu_r(p)$ obeying the commutation relation $[\nu_r(p), \nu'_{r'}(-p')] = -\delta_{\nu,\nu'}\delta_{r,r'}\delta_{p,p'} rpL/2\pi$. $U_{r,s}$ is a fermion-raising operator necessary to make Eq. (2.2) an operator identity; its contributions in the thermodynamic limit vanish, however, and it will not be displayed in what follows (see, however, the discussion in Appendix A). In a language where the scattering processes are labelled by coupling constants g_i,[4] our Hamiltonian, Eq. (1.1), becomes the sum of the following terms:

$$H_0 = \frac{\pi v_F}{L} \sum_{\nu=\rho,\sigma} \sum_p [\nu_+(p)\nu_+(-p) + \nu_-(-p)\nu_-(p)] \tag{2.6}$$

which describe free charge- and spin-density fluctuations with the Fermi velocity $v_F = 2ta$ about the two Fermi points $\pm k_F$,

$$H_4 = \frac{1}{L} \sum_{\nu=\rho,\sigma} g_{4\nu} \sum_p [\nu_+(p)\nu_+(-p) + \nu_-(-p)\nu_-(p)] , \quad g_{4\rho} = \frac{Ua}{2} + 2Va, \quad g_{4\sigma} = -\frac{Ua}{2} \ . \tag{2.7}$$

Equations (2.7) are the forward scattering of fluctuations on the same branch of the spectrum. The effect is a trivial renormalization of the Fermi velocities $v_F \to v_F + g_{4\nu}/\pi$ of charge and spin fluctuations which, in general, now will differ. The interaction

$$H_2 = \frac{2}{L} \sum_{\nu=\rho,\sigma} g_{2\nu} \sum_p \nu_+(p)\nu_-(-p) , \quad g_{2\rho} = \frac{Ua}{2} + 2Va, \quad g_{2\sigma} = -\frac{Ua}{2} \tag{2.8}$$

represents the forward scattering between particles on different sides of the Fermi surface. $H_0 + H_2 + H_4$ is the Luttinger model for spin-$\frac{1}{2}$ fermions, which is exactly solvable.[16] The Hamiltonian for backscattering (momentum transfer $2k_F$) is

$$H_1 = H_{1\parallel} + H'_{1\perp} + H''_{1\perp} ,$$

$$H_{1\parallel} = -\frac{g_{1\parallel}}{L} \sum_{\nu=\rho,\sigma} \sum_p \nu_+(p)\nu_-(-p) , \tag{2.9}$$

$$H'_{1\perp} = \frac{2g'_{1\perp}}{(2\pi\alpha)^2} \int dx \cos[\sqrt{8}\Phi_\sigma(x)] , \tag{2.10}$$

$$H''_{1\perp}=\frac{2g''_{1\perp}}{(2\pi\alpha)^2}\int dx\,\cos[\sqrt{8}\Phi_\sigma(x)]\times\cos\{\sqrt{2}[\Phi_\rho(x)-\Phi_\rho(x+a)]\}\ , \quad (2.11)$$

$$g_{1\parallel}=-2Va,\ \ g'_{1\perp}=Ua,\ \ g''_{1\perp}=-2Va\ . \quad (2.12)$$

Parallel-spin scattering ($g_{1\parallel}$) has the same operator structure but opposite sign as forward scattering and simply renormalizes $g_{2\nu}\to g_{2\nu}-g_{1\parallel}/2$. Antiparallel-spin scattering involves two distinct terms $H'_{1\perp}$ and $H''_{1\perp}$, where the second one couples charge and spin fluctuations. Usually[4] when a local approximation on the interactions coming from the nearest-neighbor interaction is performed from the outset, $H''_{1\perp}$ reduces to the form of $H'_{1\perp}$ yielding a total backscattering Hamiltonian of type $H'_{1\perp}$ with a total coupling constant

$$g_{1\perp}=g'_{1\perp}+g''_{1\perp}=(U-2V)a\ . \quad (2.13)$$

Clearly, one can expand the second cosine factor in Eq. (2.11) as $\approx 1-(\partial\Phi_\rho/\partial x)^2$, making obvious that there is a backscattering contribution of the usual (local) form plus a correction, but keeping the cosine is computationally more practical. The reason for keeping explicitly the two terms is that in the RG treatment below, starting from the form $H'_{1\perp}$ with (2.13), the correction term in $H''_{1\perp}$ will be generated by the RG transformations so that consistency requires its presence from the outset. Commensurability effects are included through the following umklapp scattering processes:

$$H_3=H_{3\parallel}+H'_{3\perp}+H''_{3\perp}\ ,$$

$$H_{3\parallel}=\frac{2g_{3\parallel}}{(2\pi\alpha)^2}\int dx\,\cos[\sqrt{8}\Phi_\rho(x)]\cos[\sqrt{8}\Phi_\sigma(x)]\ , \quad (2.14)$$

$$H'_{3\perp}=\frac{2g'_{3\perp}}{(2\pi\alpha)^2}\int dx\,\cos[\sqrt{8}\Phi_\rho(x)]\ , \quad (2.15)$$

$$H''_{3\perp}=\frac{2g''_{3\perp}}{(2\pi\alpha)^2}\int dx\,\cos[\sqrt{8}\Phi_\rho(x)]\times\cos\{\sqrt{2}[\Phi_\sigma(x)-\Phi_\sigma(x+a)]\}\ , \quad (2.16)$$

$$g_{3\parallel}=-2Va,\ \ g'_{3\perp}=Ua,\ \ g''_{3\perp}=-2Va\ . \quad (2.17)$$

The familiar umklapp scattering process[4] would be $H'_{3\perp}$ with

$$g_{3\perp}=g'_{3\perp}+g''_{3\perp}=(U-2V)a\ . \quad (2.18)$$

For the splitting into two distinct processes, one of them coupling charge and spin fluctuations, the same remarks as those for (2.11) apply. The all-important new process is $H_{3\parallel}$, which also couples charge and spin degrees of freedom.[12,13] It arises from the fermion term

$$H_{3\parallel}=Va\sum_s\int dx[\Psi^\dagger_{+,s}(x)\Psi^\dagger_{+,s}(x+a)\Psi_{-,s}(x+a)\times\Psi_{-,s}(x)+\mathrm{H.c.}] \quad (2.19)$$

and would be missed (due to the Pauli exclusion principle) if the local approximation was performed before bosonizing. In fact, it is this term that generates the charge-spin coupling pieces $H''_{1\perp}$ and $H''_{3\perp}$ if not included from the outset, cf. below. $H_{3\parallel}$ is the spin-$\frac{1}{2}$ analog of a nonlocal umklapp scattering operator present also in spinless fermion systems generated through a Jordan-Wigner transformation of spin chains.[17,18] The interactions (2.10)–(2.16) change the total charge and/or spin on each of the two branches $r=\pm$ of the spectrum and therefore do not conserve the charge and/or spin currents.

In Eqs. (2.9)–(2.16) we have not exhibited the $U_{r,s}$ operators appearing in the bosonization formula (2.2). This emphasizes the similarity and differences with published versions of the interactions[4,19] and is sufficient in the incommensurate limit since the contributions of the $U_{r,s}$ operators to the asymptotic properties of the model vanish, and possible phase factors are compensated when contracting with the complex conjugate quantities to obtain a real partition or correlation function. This is so because the wave vectors $2k_F$ and $-2k_F$ are different (i.e., not related by a reciprocal lattice vector), and the associated particle-hole operators describe different physical processes. In the half-filled band, however, particle-hole fluctuations at $2k_F$ and $-2k_F$ are identical processes ($4k_F$ is a reciprocal lattice vector), the corresponding operators are real, and the $U_{r,s}$ operators do contribute important phase factors. These problems will be discussed in more detail in Appendix A where we also give the full form of $H_{1\perp}$, $H_{3\parallel}$, and $H_{3\perp}$.

Before proceeding with the solution of the model, let us emphasize that the interactions $H''_{1\perp}$, $H_{3\parallel}$, and $H''_{3\perp}$ arise solely from our particular way of taking the continuum limit (2.1): The lattice constant a in the arguments of the Fermi operators is kept finite until *after* bosonizing or, for calculational convenience, even for the computation of the perturbations to the correlation functions from the charge-spin coupling interactions. Another feature worth noting here is that one of these interactions $H''_{1\perp}$ is also present in the *incommensurate* extended Hubbard model. This is interesting since it appears from an analysis of the Bethe-Ansatz equations of the Hubbard model[20] that charge and spin degrees of freedom do couple, but that a theory separating them does give the correct critical exponents. We have not been able to identify such an (irrelevant) interaction, which would be present also in the incommensurate Hubbard model. Our bare charge-spin coupling interactions are a consequence of the finite range of the interaction V.

To make progress we treat this model in two steps: (i) We diagonalize the Luttinger model part, and (ii) we derive RG equations for extensions to the simple Luttinger Hamiltonian.

$H_0+H_4+H_2+H_{1\parallel}$ separates into two (spinless) Luttinger models for charge and spin fluctuations, each of which can be diagonalized by a Bogoliubov transformation.[16] The properties of each of these models are described by two nonuniversal parameters β_ν, exponents characterizing the power-law decay of various correlation functions, and v_ν, the renormalized velocities of the collective modes:

$$\beta_\nu = \left[\frac{\pi v_F + g_{4\nu} - g_{2\nu} + g_{1\parallel}/2}{\pi v_F + g_{4\nu} + g_{2\nu} - g_{1\parallel}/2} \right]^{1/2} ,$$
$$v_\nu = \left[\left[v_F + \frac{g_{4\nu}}{\pi} \right]^2 - \left[\frac{g_{2\nu}}{\pi} - \frac{g_{1\parallel}}{2\pi} \right]^2 \right]^{1/2} . \tag{2.20}$$

Under the Bogoliubov transformation, the phase fields transform as

$$\Phi_\nu(x) \to \sqrt{\beta_\nu}\Phi_\nu(x), \quad \Theta_\nu(x) \to \Theta_\nu(x)/\sqrt{\beta_\nu} . \tag{2.21}$$

The relations of β_ν and v_ν to the bare parameters are specific to the Luttinger model and universal only to lowest order in the g_i. More generally, the specific relation between β_ν and v_ν implied by Eq. (2.20) need not be fulfilled, but the concept of a Luttinger liquid requires relations between quantities depending on β_ν and v_ν to be universal for interacting 1D fermion systems. A remarkable feature of the Luttinger model is that all of its correlation functions

$$R_j(x-x',t-t') = -i\langle TO_j(x,t)O_j^\dagger(x',t')\rangle \tag{2.22}$$

can be computed exactly. Of interest below will be the operators for charge-density wave (CDW), bond-order wave (BOW), and spin-density wave (SDW) as well as singlet- and triplet-superconducting (SS, TS) fluctuations. We shall also consider $4k_F$ charge-density wave correlations. Since for a half-filled band, $4k_F$ equals a reciprocal lattice vector, they describe effectively long-wavelength ($q \approx 0$) density fluctuations. Within the present approach, this is not trivial since the $q \approx 0$ density correlations are marginal $\propto x^{-2}$ in the Luttinger model and formally not renormalized by the perturbations we consider. The $4k_F$ density correlations are affected, however, and therefore a convenient device to study changes in the long-wavelength charge order. The operators are given in Appendix A. The correlation functions decay as power laws

$$R_j(x-x') \sim |x-x'|^{-2+\alpha_j} \tag{2.23}$$

with exponents α_j, which depend in a universal way on the renormalized coupling constants β_ν of the model (their relation to the bare coupling constants is, however, universal only to lowest order for different models of interacting 1D electrons):

$$\alpha_{\rm CDW} = \alpha_{\rm BOW} = \alpha_{{\rm SDW},z} = 2 - \beta_\rho - \beta_\sigma , \tag{2.24}$$

$$\alpha_{{\rm SDW},x} = \alpha_{{\rm SDW},y} = 2 - \beta_\rho - \beta_\sigma^{-1} , \tag{2.25}$$

$$\alpha_{4k_F} = 2 - 4\beta_\rho , \tag{2.26}$$

$$\alpha_{\rm SS} = \alpha_{\rm TS,0} = 2 - \beta_\rho^{-1} - \beta_\sigma , \tag{2.27}$$

$$\alpha_{{\rm TS},+1} = \alpha_{{\rm TS},-1} = 2 - \beta_\rho^{-1} - \beta_\sigma^{-1} . \tag{2.28}$$

The single-particle Green's function can be computed in the same way; in many cases, this is not necessary since the many-particle correlation functions containing more direct information are available. An interesting quantity derived from the Green's function is the momentum distribution function $n(k)$ of the Fermi sea[21]

$$n(k_F - q) \approx \tfrac{1}{2} + C_1 {\rm sgn}(q)|q|^\alpha + C_2 q \tag{2.29}$$

with $\alpha = [\sum_\nu(\beta_\nu + \beta_\nu^{-1}) - 4]/4$ exhibiting, for weak interactions, a power-law variation around the Fermi surface and for stronger interaction a linear behavior (C_1 and C_2 are constants).

To include the remaining terms, at least for weak coupling, we derive RG equations following a procedure given by Chui and Lee.[22,23] We go over to the Matsubara formalism of imaginary times $\tau = it$, introduce a second spatial coordinate $y = v_\sigma \tau$ [i.e., $\mathbf{r} = (x, v_\sigma \tau)$], and compute the partition function of our model. In the absence of $H''_{1\perp}$, $H_{3\parallel}$, and $H''_{3\perp}$ (i.e., the case of the Hubbard model[19]), the model separates into a charge and a formally identical spin part whose partition functions can be shown to be equivalent to classical 2D Coulomb gases obeying the familiar Kosterlitz-Thouless scaling equations.[24] Their (inverse) temperatures (for unit charge) are $\beta_{\rm CG} = \beta_\nu$ and their fugacities $\propto g_{1(3)\perp}$. Adding the charge-spin coupling interactions $H''_{1\perp}$, $H_{3\parallel}$, and $H''_{3\perp}$ introduces corresponding couplings between the charges of these two gases with the coupling constants entering as new fugacities. We obtain the set of RG equations [with $l = \ln(\alpha/\alpha_0)$ being the change in length scale]

$$\frac{d\beta_\rho}{dl} = -\frac{1}{2\delta}\beta_\rho^2 (Y_\rho^2 + \tfrac{1}{2}Y_\parallel^2 + \tfrac{1}{2}Y_{\sigma\to\rho}) , \tag{2.30}$$

$$\frac{d\beta_\sigma}{dl} = -\tfrac{1}{2}\beta_\sigma^2 (Y_\sigma^2 + \tfrac{1}{2}Y_\parallel^2 + \tfrac{1}{2}Y_{\rho\to\sigma}) , \tag{2.31}$$

$$\frac{dY_\rho^2}{dl} = Y_\rho^2(4 - 4\beta_\rho) - Y_\rho Y_\sigma Y_\parallel , \tag{2.32}$$

$$\frac{dY_\sigma^2}{dl} = Y_\sigma^2(4 - 4\beta_\sigma) - Y_\rho Y_\sigma Y_\parallel , \tag{2.33}$$

$$\frac{dY_\parallel^2}{dl} = Y_\parallel^2(4 - 4\beta_\rho - 4\beta_\sigma) - 2Y_\rho Y_\sigma Y_\parallel , \tag{2.34}$$

$$\frac{dY_{\sigma\to\rho}}{dl} = Y_{\sigma\to\rho}(2 - 4\beta_\sigma) - 2Y_\rho Y_\sigma Y_\parallel , \tag{2.35}$$

$$\frac{dY_{\rho\to\sigma}}{dl} = Y_{\rho\to\sigma}(2 - 4\beta_\rho) - 2Y_\rho Y_\sigma Y_\parallel , \tag{2.36}$$

$$\frac{dv_\rho}{dl} = -\frac{\beta_\rho v_\sigma}{4}\left[Y_{\sigma\to\rho} - \beta_\sigma \frac{1-\delta^2}{2\delta} Y_\parallel^2 \right] , \tag{2.37}$$

$$\frac{dv_\sigma}{dl} = -\frac{v_\sigma \beta_\sigma}{4}\left[Y_{\rho\to\sigma} - \beta_\rho \frac{1-\delta^2}{2\delta} Y_\parallel^2 \right] , \tag{2.38}$$

where

$$Y_\rho = \frac{g_{3\perp}}{\pi v_\sigma}, \quad Y_\sigma = \frac{g_{1\perp}}{\pi v_\sigma}, \quad Y_\parallel = \frac{g_{3\parallel}}{\pi v_\sigma} ,$$
$$Y_{\sigma\to\rho} = Y_\sigma \frac{g''_{1\perp}}{\pi v_\sigma} , \quad Y_{\rho\to\sigma} = Y_\rho \frac{g''_{3\perp}}{\pi v_\sigma}, \quad \delta = \frac{v_\rho}{v_\sigma} . \tag{2.39}$$

Let us discuss these equations in some detail.

(i) Notice that in the RG equations, the contributions of $H'_{1\perp}$ and $H''_{1\perp}$ in the σ degrees of freedom and of $H'_{3\perp}$ and $H''_{3\perp}$ in the ρ degrees of freedom are such that they can be combined to yield the usual $g_{1\perp}$ and $g_{3\perp}$ terms in (2.30)–(2.33).

(ii) For $Y_{\parallel}=0$ and $Y_{\nu\to\bar{\nu}}=0$, Eqs. (2.30)–(2.33) decouple and are identical to the Kosterlitz-Thouless equations for the classical 2D Coulomb gas.[24] This situation applies to the Hubbard model at half-filling.[19]

(iii) The scaling dimensions of the actions corresponding to the operators (2.10)–(2.16) can be read off directly from the factors multiplying the respective coupling constant in the first members on the right-hand sides of Eqs. (2.32)–(2.36), e.g., the dimension of the action $\int d\tau H_{1\perp}(\tau)$ is $2-2\beta_\sigma$. They indicate the relevance (>0) or irrelevance (<0) of the operators with respect to the Luttinger-liquid fixed point and *in the absence of any other perturbing interaction.* The mutual influence of these additional perturbations is contained in the cross terms on the right-hand sides of Eqs. (2.32)–(2.38) and often leads to significant deviations from predictions based on the scaling dimensions alone.

Y_ν is marginal at $\beta_\nu=1$, i.e., effectively free fluctuations, and is relevant for effectively repulsive forward scattering $g_{2\nu}-g_{1\parallel}/2$. In the Hubbard model, Y_ρ (Y_σ) is relevant for $U>0$ ($U<0$).

$Y_{\parallel}$ is the only nonvanishing non-Luttinger-type interaction at $U=2V$. Its scaling dimension is

$$2-2\beta_\rho-2\beta_\sigma=-2\left[\frac{2\pi t-V}{2\pi t+7V}\right]^{1/2},$$

where the equality applies to $U=2V$ (here the bare $\beta_\sigma=1$). Since $\beta_\rho>0$ an analysis based on the scaling dimension of $Y_{\parallel}$ alone would predict that this term is never relevant. This conclusion is in striking contrast to results by Cannon and Fradkin[13] who find it relevant for $U=2V\geq U_{\text{crit}}=1.45t$. Actually, when solving the RG equation numerically, we do find the operator to be relevant for $U=2V\geq 4.76t$ with all the caveats in view of its derivation from a continuum approximation. That $Y_{\parallel}$ is relevant at all for $U=2V$ is uniquely due to the feedback of β_ν on $Y_{\parallel}$; here Eqs. (2.30)–(2.38) reduce to (corrections from $\delta\neq 1$ ignored)

$$\frac{d\beta_\nu}{dl}=-\frac{\beta_\nu^2}{4}Y_{\parallel}^2,\quad \frac{dY_{\parallel}}{dl}=Y_{\parallel}(2-2\beta_\rho-2\beta_\sigma)\ . \qquad (2.40)$$

The charge-spin coupling interactions $Y_{\nu\to\bar{\nu}}$ are generated under RG transformations even if zero initially as long as none of the Y_ν and $Y_{\parallel}$ vanish. Their scaling dimensions are $2-4\beta_\nu$ so that alone they would be relevant for $\beta_\nu<\frac{1}{2}$, i.e., quite a strong interaction. In that case, however, Y_ν is much more relevant and expected to dominate the physical behavior of the model except for small corrections. Our method (cf. below) does not allow a detailed study of the model in this regime at least if the bare couplings are restricted to the relations of the EHM.

(iv) Charge-spin coupling introduces a renormalization of the velocities v_ν of the collective charge and spin fluctuations, Eqs. (2.37) and (2.38), as is expected on physical grounds. Depending on the interactions, the ratio $\delta=v_\rho/v_\sigma$ may increase or decrease, and in general the complete solution of the RG equations is required for deciding which is the case. A straightforward discussion is possible, however, for $U=2V$, cf. Eq. (2.40), where $Y_{\nu\to\bar{\nu}}\equiv 0$. Here, for $V>0$, we have $\delta>1$ and $d\delta/dl<0$ while both of the velocities decrease; for $V<0$, the opposite conclusion is obtained. Technically, the renormalization of the velocities of the collective fluctuations come from the anisotropy in the 2D space generated from the contributions of $H_{3\parallel}$, $H''_{1\perp}$, and $H''_{3\perp}$ under RG transformations. The source of anisotropy from $H_{3\parallel}$ is the difference in velocity of charge and spin fluctuations; the source in $H''_{1(3)\perp}$ is the distinguished x direction in the $\cos\{\sqrt{2}[\Phi_\nu(x,\tau)-\Phi_\nu(x+a,\tau)]\}$ terms.[23] The corrections due to the factors δ on the right-hand side of Eq. (2.30) introduce additional powers of the interaction constants. Since these corrections are already second order in the interaction, they are neglected in what follows. The most important physical consequence of the velocity renormalization is a nontrivial dependence of thermodynamic properties (e.g., specific heat, compressibility, susceptibility) on the electronic interactions.[25]

III. CORRELATION FUNCTIONS AND PHASE DIAGRAM

In general, the full system of equations (2.30)–(2.38) has to be solved. There are several major difficulties in obtaining a physical interpretation of the solution.

(i) In many cases, there will be at least one relevant operator, i.e., driven towards strong coupling. The RG equations have been derived under the assumption that the different $Y\ll 1$.[22,23] This precludes integrating the equations to the upper integration limit $l=\infty$. Moreover scaling holds at a fixed point and is certainly violated when Y becomes large. Instead, we integrate up to some finite upper integration limit l^*, where $Y\sim 1$; then further information has to be obtained by a different approach. In many instances this is possible by making use of a remarkable solution of the original backscattering problem [all $Y\equiv 0$ except Y_σ in (2.30)–(2.38)] by Luther and Emery[26] (LE) who showed that this particular problem can be solved exactly for $\beta_\sigma=\frac{1}{2}$ in terms of spinless fermions and that there is a gap in their excitation spectrum. The size of the gap in the spin-fluctuation spectrum of the original model is then related to the Luther-Emery gap through $\Delta=\Delta_{\text{LE}}\exp(-l^*)$.

(ii) Through the cross terms in Eqs. (2.30)–(2.36) one relevant operator will often cause one or several other relevant operators. Fortunately, in most cases, integrating the RG equations up to some upper integration limit l^* so that the first $\beta_\nu(l^*)=\frac{1}{2}$ produces just one $Y\sim 1$ and all the other Y's, though formally relevant, i.e., $Y^{-1}dY/dl>0$, as well as their derivatives are significantly smaller there. If it is just the most relevant operator that determines the physics of the model, scaling the model up to the Luther-Emery line will allow at least a qualitative discussion. Moreover, the remaining (small) interactions will then yield perturbative corrections.

(iii) The Abelian bosonization identity, Eqs. (2.2)–(2.4), breaks the spin-rotation invariance of the model and works only with two $U(1)$ boson fields describing the charge and z component of the spin fluctuations. Usually, i.e., in simple cases such as the Hubbard model where charge and spin degrees of freedom separate, the spin symmetry is restored at the weak coupling fixed point of the RG if one is only interested in the fixed-point values of the effective coupling constants β_ν^* determining the power-law decay of correlations. Computing full spin-rotation invariant correlation functions including possible logarithmic corrections requires, however, integration of the whole RG trajectory.[19] The situation is more intricate if scaling goes towards strong coupling, although qualitative answers will be consistent with spin-rotation invariance (cf. below). In the present model, the situation is still more involved since there are fixed points (in particular $U=2V<U_{\rm crit}$) whose effective coupling constants are inconsistent with spin-rotation symmetry. We can show, however, that this symmetry is restored in the correlation functions, once the full RG trajectory has been integrated over. The necessity of integrating RG trajectories is, however, a serious limitation to our capability to obtain explicit solutions for general parameters U, V.

In order to discuss the ground state of our model, we now consider the various correlation functions introduced for the Luttinger model in Eqs. (2.22)–(2.28) in the presence of the additional non-Luttinger interactions. Details are discussed in Appendix A. In many but not all cases, it is sufficient to replace β_ν by its fixed-point value β_ν^*. In general, it is preferable to integrate over the RG trajectories; this restores the broken spin symmetry in Eqs. (2.24)–(2.28) if $\beta_\sigma^*\neq 1$, and one may also find logarithmic corrections to the power laws as well as renormalization effects on the amplitude (prefactor) of the correlation function lifting some of the degeneracies in (2.24) and (2.27) but introducing eventually others. These are qualitative deviations from the form of the Luttinger-liquid correlation functions and are necessarily missed if one simply takes effective Luttinger-liquid parameters obtained by the RG method. An explicit example for all of these statements is given below where we consider the Hubbard model. Except in such simple limiting cases, there is no analytical solution for the scaling equations; while a numerical integration of the correlation functions is formally possible, an operative way of distinguishing between logarithmic corrections and amplitude renormalization is not available, and in general we shall make only qualitative statements.

As one limiting case, consider now the Hubbard model. For $U>0$, umklapp scattering $Y_\rho>0$ is relevant. Y_ρ relevant implies a gap in the charge-fluctuation spectrum, and in the original lattice model localization of charges on neighboring sites. This interpretation is consistent with the correlation functions and will be discussed now. Y_σ is irrelevant yielding gapless spin fluctuations. The transition taking place as U is increased from zero is of Kosterlitz-Thouless type, and it has been shown earlier[19] that the three components of the SDW correlation functions decay as

$$R_{\rm SDW}(\mathbf{r})=A_{\rm SDW}r^{-1}\ln^{1/2}r\ , \tag{3.1}$$

while for BOW and CDW, one obtains

$$R_{\rm BOW,CDW}=A_{\rm BOW,CDW}r^{-1}\ln^{-3/2}r\ . \tag{3.2}$$

An interesting difference occurs in the prefactors, which vary as

$$\frac{dA_{\rm SDW,BOW}}{dl}=Y_\rho \quad\text{and}\quad \frac{dA_{\rm CDW}}{dl}=-Y_\rho,$$
$$A_i(l=0)\equiv 1\ . \tag{3.3}$$

Moreover, the $4k_F$ (≈ 0) function becomes a constant, independent of distance. This indicates long-range charge order consistent with localization of charges on all sites of the lattice. $Y_\rho(l)$ scales towards large *positive* values implying that SDW and BOW correlation functions have an additional enhancement of their prefactor with U compared to the noninteracting system, while the one for CDW correlations scales towards zero. Charge fluctuations, therefore, take place on the bonds between the sites where U is not active rather than on the sites where they are suppressed by U. Notice also that the SDW correlation function is the same as one of the Heisenberg chain[27] and, eventually up to the prefactor, independent of U.

To further clarify the significance of these results, let us digress to the case $U=0$, $V>0$. This is another simple case where umklapp scattering Y_ρ is relevant, although the ground state is very different. The bare coupling constants are $Y_\rho=Y_\sigma=Y_\parallel$, $Y_{\nu\to\bar\nu}=Y_\nu^2$, $\beta_\nu<1$. Both Y_ν are, therefore, relevant, and through the cross terms in the RG equations, the other Y's are relevant even for small V, and the solution of the RG equation shows that they are only a little smaller than Y_ν. We conclude (i) that due to the relevance of Y_ρ, umklapp scattering again leads to charge localization and a gap in the charge fluctuation spectrum. (ii) Since Y_ρ scales towards large *negative* values, the charge order must be of a different type from that in the Hubbard case, and in a strong coupling limit, in fact, charges are localized in pairs on alternating doubly occupied and empty sites. (iii) This is also indicated by the opening of a gap in the spin fluctuations caused by a relevant Y_σ indicating that the spins must be paired. (iv) That charges are localized on sites is easily seen by considering the above correlation functions. We have CDW long-range order formally characterized by $\beta_\rho^*=\beta_\sigma^*=0$, i.e., $\alpha_{\rm CDW}=2$. The same exponents also characterize the BOW and SDW_z correlation functions. The crucial difference is again found, however, in the behavior of the prefactor. For CDW, the prefactor increases under scaling, while for BOW and SDW_z correlation functions, it decreases towards zero. The picture of charge localization is again supported by the $4k_F$ (≈ 0) CDW function becoming constant, at the same time as the oscillating CDW function. (v) Observe a typical consequence of the breaking of spin-rotation invariance by our bosonization method. While the exponent $\alpha_{SDW,z} \rightarrow 0$ and only the suppression of the prefactor indicates the vanishing of the spin correlations, $\alpha_{SDW,x,y} \rightarrow \infty$, suggesting exponentially fast decay, and there are no prefactor corrections. While the general conclusion of the absence of divergent SDW correlations is the same for all three components, the formal outcome of the calculation is not manifestly spin-rotation invariant. (vi) Since $Y_\parallel$ and $Y_{\nu \rightarrow \bar{\nu}}$ are made relevant and not very small compared to Y_ν, charge-spin coupling is important. Consequently the transition is likely to be different from the Kosterlitz-Thouless behavior found for $V=0$, U finite, and also in the spinless $t-V$ model at $V=2t$, and in a yet undetermined universality class. (vii) For $V<0$, all perturbation operators are irrelevant; the Luttinger liquid is therefore a stable fixed point.

We return to the Hubbard model at $U<0$, where a very similar physical situation pertains. Here particles pair as a consequence of the on-site attraction. Now Y_σ is relevant, and there is a gap in the spin-fluctuation spectrum. However, Y_ρ is irrelevant and despite an on-site attraction, the pairs remain delocalized. We are again interested in the above correlation functions as well as in those for singlet and triplet pairing (the pairing correlation functions are not very interesting for $U>0$ since their exponents $\alpha_{SS,TS} \rightarrow \infty$ as a consequence of the scaling of $\beta_\rho \rightarrow 0$ implying exponential decay). We find

$$
\begin{aligned}
R_{CDW}(x) &= A_{CDW} r^{-1} \ln^{1/2} r \;, \\
R_{BOW}(x) &= A_{BOW} r^{-1} \ln^{-3/2} r \;, \\
R_{SS}(x) &= A_{SS} r^{-1} \ln^{1/2} r \;,
\end{aligned}
\tag{3.4}
$$

where the amplitudes of all three correlation functions increase under renormalization following $dA/dl = -Y_\sigma$. Notice the degeneracy of CDW and SS correlation in amplitude, correlation exponent, and logarithmic correction. Note further the symmetry of the BOW correlations and the exchange of the role of CDW and SDW under $U \leftrightarrow -U$; this is a consequence of the symmetry of the Hubbard model under a particle-hole transformation on the up-spin (*or* down-spin) fermions alone.[28] There are no SDW or TS correlations due to the gap in the spin-fluctuation spectrum; however as in the case of the $U=0$, $V>0$ model, the formal result looks different (exponential decay versus vanishing prefactor) for the XY and Z components of the SDW and for the $S_z=\pm 1$ and $S_z=0$ components of the TS correlations.

A last important special limit is $U=2V>0$. The only non-Luttinger operator is $Y_\parallel$; the bare $\beta_\rho<1$ while $\beta_\sigma=1$, and the scaling equations for this case are summarized in Eq. (2.40). The tremendous simplification is due to a very peculiar feature of this limit. We have $Y_\nu = Y_{\nu \rightarrow \bar{\nu}} \equiv 0$, and none of them is generated under renormalization, i.e., all non-Luttinger interactions involving antiparallel spins vanish identically. In fact, by linearizing the RG equations (2.40) for *small* interactions $\beta_\nu \approx 1$, they can further be reduced to

$$
d|g_{1\parallel}/\pi v_F|/dl = -\tfrac{1}{2}(g_{3\parallel}/\pi v_F)^2
$$

and there are no interactions between electrons with antiparallel spin. Our model can thus be visualized as being composed out of interacting up-spin particles and interacting down-spin particles, both with backscattering interactions implying density-wave correlations, which are completely decoupled from each other. We have checked that the spin-rotation invariance of the model on this special line is preserved despite the complete cancellation of antiparallel-spin interactions. The correlation functions for weak coupling on this line are given by

$$
\begin{aligned}
R_{CDW}(r) &= R_{SDW}(r) = R_{BOW}(r) = r^{-1-\beta_\rho^*} \;, \\
R_{SS} &= R_{TS} = r^{-1-\beta_\rho^{*-1}} \;.
\end{aligned}
\tag{3.5}
$$

Charge- and spin-density-wave correlations on the sites are degenerate and enhanced with respect to the noninteracting model, while pairing correlations are not divergent ($\beta_\rho^* \sim \beta_\rho < 1$ because of the irrelevance of $Y_\parallel$ here). For weak coupling $U=2V \le U_{crit}$, our picture of the EHM is consistent with a spin-$\frac{1}{2}$ Luttinger liquid.

When the interaction becomes stronger, we observe that $Y_\parallel$ is relevant for $U=2V=U_{crit} \approx 4.76t$, a much higher value than found by Cannon and Fradkin in their analytical calculations on a comparable theory. The transition along this line is apparently similar though within the present formalism not identical to a Kosterlitz-Thouless[24] one. Add and subtract the equations for $d\beta_\nu/dl$ in (2.40) to obtain

$$
\begin{aligned}
\frac{dK}{dl} &= -\tfrac{1}{2}(K^2+L^2)Y^2, \quad \frac{dY}{dl} = (2-2K)Y \;, \\
\frac{dL}{dl} &= -KLY^2 \;,
\end{aligned}
\tag{3.6}
$$

where $K=\beta_\rho+\beta_\sigma$, $L=\beta_\rho-\beta_\sigma$, and $Y=Y_\parallel/2$. $K>0$ by definition and $L<0$ on the line $U=2V$, implying that L is always irrelevant and scales to a fixed-point value L^*. Equations (3.6) have a line of stable fixed points ($K^* \ge 1$, $Y_\parallel^*=0$). As long as L can be replaced by its fixed-point value L^* in dK/dl and the equations can be linearized around the critical end point of the fixed line ($K^*=1$), the transition with increasing $U=2V$ will be of Kosterlitz-Thouless type. Then, at the tricritical point, all density-wave correlation functions decay as r^{-1} but acquire logarithmic corrections:

$$
\begin{aligned}
R_{CDW}(\mathbf{r}) &= R_{SDW,z}(\mathbf{r}) = r^{-1} \ln^{\gamma_1} r \;, \\
\gamma_1 &= 1/\sqrt{1+L^{*2}} - \tfrac{1}{2} \;,
\end{aligned}
\tag{3.7}
$$

$$
R_{BOW}(\mathbf{r}) = r^{-1} \ln^{\gamma_2} r, \quad \gamma_2 = -1/\sqrt{1+L^{*2}} - \tfrac{1}{2} \;. \tag{3.8}
$$

We have not been able to compute explicitly the x and y components of the SDW correlation functions since no simple approximation can be found for $\beta_\rho(l)$ and $\beta_\sigma(l)$

separately in the vicinity of the tricritical point; the approximations involved in reducing (3.6) to a Kosterlitz-Thouless problems break the spin-rotational invariance of the model. Moreover, a numerical evaluation of the exponent of the logarithmic corrections from the full system of equations is difficult.

The high value of the critical coupling is, in principle, not to be taken serious quantitatively since a continuum theory is not reliable at these coupling strengths. Accordingly, the quantitative disagreement with Monte Carlo simulations is serious: Hirsch finds a tricritical point at $U \approx 2V \approx 3t$ and Cannon and Fradkin, in their first study,[13] found it at $1.5t$. Therefore the quantitative agreement with the very recent work of Cannon, Scalettar, and Fradkin, yielding $4t \leq U_{\rm crit} \leq 5t$ (Ref. 14) is highly surprising. It is not clear to the author if this agreement is fortuitious or, in some sense, due to the structure of the theory (both on the level of the EHM and on that of the strategy, namely to solve exactly a nontrivial part of the model and then evaluate residual interactions). Presumably, only further comparative studies on numerical and field theoretical approaches to similar models will be able to clarify this issue. Notice, however, that $Y_\parallel$ is the most relevant operator left in a continuum theory on the line $U=2V$ and, in fact, the only one becoming relevant close to $U_{\rm crit}$. Despite (possibly only minor) quantitative shortcomings, we expect $Y_\parallel$ to contain the essential physics of the crossover from a continuous to a first-order CDW-SDW transition in the extended Hubbard model.

That $Y_\parallel$ in fact is capable of mediating such a crossover can be seen more formally by verifying three conditions on RG equations sufficient for the occurrence of a discontinuous phase transition established by Nienhuis and Nauenberg.[29] These conditions are formulated in terms of an order parameter and its associated ordering field. There are several possibilities in our model. In the CDW phase, charge fluctuations are localized on the sites of the lattice and $\langle \cos(\sqrt{2}\Phi_\rho)\rangle \neq 0$, while the associated field $Y_\rho < 0$. In the SDW phase for $Y_\rho > 0$, charge fluctuations are centered on the bonds, and $\langle \sin(\sqrt{2}\Phi_\rho)\rangle \neq 0$. A more convenient choice (yielding identical answers) is to consider the spin fluctuations. In the CDW phase for $U<2V$ ($Y_\sigma<0$) they are gapped implying $\langle \cos(\sqrt{2}\Phi_\sigma)\rangle \neq 0$, while in the SDW phase they are massless and $\langle \cos(\sqrt{2}\Phi_\sigma)\rangle = 0$. We now can check the following criteria. (a) Existence of a discontinuity fixed point: On the line $U=2V$, we have the usual weak-coupling fixed line $Y_\parallel^* = 0$, $\beta_\rho^* + \beta_\sigma^* \geq 1$. In addition, we have, for $U=2V>U_{\rm crit}$ a new fixed point $\beta_\nu^* = 0$, $Y_\parallel \to \infty$, i.e., scaling to strong coupling, which is the discontinuity fixed point (although outside the domain of validity of our approximations). (b) At the discontinuity fixed point, the eigenvalue associated with the ordering field equals the change in the scale of volume under RG transformations; the volume transforms as $V \to V' = V(1+dl)^2$. Taking Y_σ as the ordering field, we have from Eq. (2.33) evaluated at the discontinuity fixed point

$$Y_\sigma \to Y'_\sigma = Y_\sigma (1+dl)^{2-2\beta_\sigma^*} = Y_\sigma (1+dl)^2$$

so that both eigenvalues are equal to 2, i.e., the effective "spatial" dimension of the model. (c) The limit of the order-parameter discontinuity as the discontinuity fixed point is approached from both sides does not vanish. Following the RG equations as one approaches $U=2V$ from the CDW side we find that β_σ scales to zero in the whole CDW region *and* for $U=2V>U_{\rm crit}$, implying a finite spin gap and $\langle \cos(\sqrt{2}\Phi_\sigma)\rangle \neq 0$. On the SDW side, massless spin fluctuations together with spin-rotational invariance require an effective $\beta_\sigma^* = 1$ and $\langle \cos(\sqrt{2}\Phi_\sigma)\rangle = 0$. We reemphasize that the RG trajectories must be integrated over in order to obtain $\beta_\sigma^* = 1$ explicitly and that the fixed-point values of the RG equations alone are not sufficient. We have been able to perform this integration only for $V=0$ and $U=2V \ll t$; however since the sites remain singly occupied for $V<U/2$ and the spin degrees of freedom are unaffected by V [except for a change in the exchange integral $4t^2/U \to 4t^2/(U-V)$], this result is expected to carry over to the whole SDW phase. For comparison, notice that as the CDW-SDW boundary is approached from the CDW side for weak coupling, the spin gap vanishes in a Kosterlitz-Thouless manner so that the transition is continuous. (For weak coupling, the charge delocalization transition on approaching $U=2V$ from both sides is also of Kosterlitz-Thouless type.)

Our results are therefore consistent with a picture where, for $U=2V>U_{\rm crit}$ the system has long-range ordered CDW's both in the up-spin and in the down-spin degrees of freedom with only weak residual interactions between them. To see this more clearly, introduce new phase fields

$$\Phi_\uparrow = \Phi_\rho + \Phi_\sigma, \quad \Phi_\downarrow = \Phi_\rho - \Phi_\sigma ,$$

describing CDW's formed by up- (down-) spin electrons, and therefore accompanied by a SDW, and rewrite $H_{3\parallel}$ [Eq. (2.14)] as

$$H_{3\parallel} = \frac{g_{3\parallel}}{(2\pi\alpha)^2} \int dx \{\cos[\sqrt{8}\Phi_\uparrow(x)] + \cos[\sqrt{8}\Phi_\downarrow(x)]\} . \tag{3.9}$$

If the gap is sufficiently large and quantum fluctuations are frozen out, the fields $\Phi_{\uparrow,\downarrow}$ will take values $2\pi n/\sqrt{8}$ (n integer), which minimize the classical potential energy associated with $H_{3\parallel}$, i.e., charge and spin fluctuations are locked in such a way that $\langle \cos[\sqrt{8}\Phi_\uparrow(x)]\rangle = \langle \cos[\sqrt{8}\Phi_\downarrow(x)]\rangle \equiv 1$. If these up-spin and down-spin CDW's are taken as the fundamental objects and if one goes away from $U=2V$ towards larger V, the relevant attractive $g_{1\perp}$ and $g_{3\perp}$ interactions will correlate in phase canceling the spin degrees of freedom and leaving a pure CDW. Going towards larger U, the relevant repulsive $g_{3\perp}$ will correlate the two CDW's out of phase, thus cancel the charge degrees of freedom, and leave us with a SDW. The coexistence phase of CDW and SDW when the transition has become first order may then be viewed as a dilute gas of solitons in the relative phase of the up-spin and down-spin CDW's. At weak coupling, however, the CDW and the charge correlations of the SDW will disorder as the boundary line is approached and are described by Eqs. (3.5) [as well as (3.7) and (3.8) at criticality], characteristic of a spin-$\frac{1}{2}$ Luttinger liquid.

The occurrence of this tricritical point at finite coupling in a 1D theory both on a lattice and in the continuum is a nontrivial result since it contradicts the widely held belief that phase transitions, i.e., crossovers in 1D, can only occur at zero or infinite coupling.

We now allow for attractive interactions and first consider the case $V<0$, $U-2V>0$. In this range of parameters, charge-spin coupling is not relevant. Spin fluctuations are massless (as in the $U>0$ Hubbard model); for $U>-2V$ charges are localized and the correlation functions are the same as in the $U>0$ Hubbard model. Only the prefactors increase (decrease) less quickly due to the decreasing bare Y_ρ. As $U+2V\to 0^+$ (for weak coupling, i.e., for stronger interactions, corrections from the irrelevant $Y_\parallel$ could somewhat shift this line), a Kosterlitz-Thouless transition takes place towards a phase where charge fluctuations are massless, too, and which can be described in terms of a spin-$\frac{1}{2}$ Luttinger model. Here pairing correlations dominate and we obtain

$$R_{\rm TS}^{(\sigma)}=r^{-1-\beta_\rho^{*-1}}\ln^{1/2}r,\quad R_{\rm SS}=r^{-1-\beta_\rho^{*-1}}\ln^{-3/2}r\ , \tag{3.10}$$

where $\beta_\rho^*>1$ is the fixed-point value of β_ρ. Triplet-pairing correlations are thus most divergent, singlet pairing is logarithmically weaker, and density-wave correlations are not divergent [in fact, SDW (CDW, BOW) correlations can be obtained from TS (SS) by $\beta_\rho^{*-1}\to\beta_\rho^*$, respectively]. For $U=-2V$ both charges and spins are critical, the correlation functions all decay like r^{-2} for free particles but are distinguished by their logarithmic corrections

$$\begin{aligned}&R_{\rm TS}^{(\sigma)}=r^{-2}\ln r,\quad R_{\rm SS}=r^{-2}\ln^{-1}r\ ,\\&R_{\rm SDW}^{(\sigma)}=r^{-2},\quad R_{\rm BOW}=r^{-2}\ln^{-2}r,\quad R_{\rm CDW}=r^{-2}\ln^{-3}r\ .\end{aligned} \tag{3.11}$$

Crossing the line $U-2V=0$, a gap opens in the spin fluctuations indicating a transition into some nonmagnetic phase. We find the following correlation functions for $V\le 0$:

$$R_{\rm SS}=A_{\rm SS}r^{-\beta_\rho^{*-1}},\quad R_{\rm CDW}=R_{\rm BOW}=A_{\rm CDW}r^{-\beta_\rho^*}\ , \tag{3.12}$$

where the amplitudes increase under RG transformations as $dA/dl=-Y_\sigma$ as in the $U<0$ Hubbard model. TS and SDW correlations are frozen by the spin gap. As long as $V<0$, SS correlations dominate, although CDW ones may have a subdominant divergence for $\beta_\rho^*\le 2$. At $V=0$, SS and CDW are exactly degenerate and acquire logarithmic corrections due to Y_ρ becoming critical, cf. Eqs. (3.4). Notice that $Y_\parallel$ is completely irrelevant in this range and specifically does not introduce any new features in the phase diagram for attractive interactions. Here, the charge degrees of freedom are described by an effective Luttinger model.

When V becomes positive at $U<0$, there is another Kosterlitz-Thouless transition in the charge degrees of freedom, and one obtains a long-range-ordered CDW phase—a direct continuation of the one discussed for $2V>U>0$. At this transition, Y_ρ becomes relevant as a consequence of the bare β_ρ falling below 1. It is not a consequence of charge-spin coupling. In fact, solving our RG equations yields evidence that this is an important perturbation only at some finite though small V. The transition from a phase with dominant SS correlations to a CDW one has also been obtained within a strong-coupling picture ($-U\gg|t|$) by Emery and by Fowler by mapping a problem involving only doubly occupied and empty sites onto a ferromagnetic XXZ spin chain with $J_x=-2t^2/|U|$ and $J_z=-J_x+V$ (Ref. 30), which has a transition into an ordered antiferromagnetic state for $J_z/J_x<-1$ (Ref. 18), thereby extending our small-U picture towards strong coupling.

A very interesting transition occurs at stronger attractive interactions. Here all operators Y_i perturbing the Luttinger model(s) are irrelevant. However for $U+5V=-2\pi t$, the bare $\beta_\rho\to\infty$, indicating an intrinsic instability of the Luttinger liquid towards strong attractive interactions. The meaning of this instability can be seen more clearly by considering the compressibility

$$\kappa=\kappa_0\beta_\rho v_F/v_\rho\ , \tag{3.13}$$

where κ_0 is the compressibility of free fermions. A divergence in $\kappa=\partial n/\partial\mu$ indicates phase separation—this is a first-order transition. This is precisely the "condensation transition" to ground state consisting of a collection of doubly occupied sites clustered together found by Lin and Hirsch.[9] The numerical value of its location is, again, not reliable since β_ρ is universal only to lowest order in the g_i. However, around $U\approx 0$, our weak-coupling theory gives a remarkably accurate agreement with the results of Lin and Hirsch both regarding position and slope of the transition line. It is less accurate for larger U and in particular, the transition does not occur in the $U<0$ Hubbard model as is known from exact results.[31] However, putting together the work by Emery, Fowler, and den Nijs[18,30] for strongly attractive U, one finds that the condensation transition line asymptotically behaves like $V\sim 4t^2/U$ as $U\to-\infty$, again in good agreement with the Monte Carlo data.

A related charge separation transition has recently been found in the small-hopping limit of a model thought to describe the completely oxidized form of the polymer polyaniline[32]—interestingly an electron-phonon model not including Coulomb interactions but reducing *in the atomic limit* to the corresponding limit of an EHM with attractive interactions.

IV. CONCLUSIONS

We have calculated the correlation functions of the 1D extended Hubbard model with half-filled bands using familiar bosonization methods for the Luttinger model and renormalization-group techniques for determining the relevance of perturbations of the Luttinger-liquid fixed points. The phase diagram we have found is in good agreement with available numerical results,[7–11,14] and quantitative differences at stronger interactions are likely due to the weak-coupling approximation involved in our results. Moreover, the most recent numerical results[14] even yield impressive quantitative agreement concerning the location of the tricritical point, possibly suggesting that even these differences could be quite small. For weak coupling, the correlation function we have calculated provides significantly more detailed information on the physics of the EHM than the available numerical results (exponents describing power-law decay, logarithmic corrections, variations of prefactors, etc.) and, in many instances, are valid at or at least allow for, an extrapolation to stronger coupling. Where available, strong-coupling results are found to be consistent.

We have identified several continuous and discontinuous transitions in the EHM. Most of the continuous transitions are of Kosterlitz-Thouless type and caused by a relevant sine-Gordon-type operator that does not conserve charge or spin current. Examples are (i) localization of single charges on sites occurring in the region where SDW correlations are strongest, namely $U \geq 2V \geq 0$ and $U \geq -2V \geq 0$; (ii) opening of a spin gap when going from the line $U=2V$ towards larger V below the tricritical point; (iii) the opening of a charge gap associated with localization of charges on alternating doubly occupied and empty sites for $V>0$ at $U<0$ and $V>U/2$ at $U>0$ below the tricritical point with the possible exception of the neighborhood of $U=0$ where charge-spin coupling cannot be neglected (cf. below); (iv) the tricritical point $U=2V=U_{\rm crit}$ when approached on the $U=2V$ line where $Y_{\parallel}$ is relevant. $Y_{\parallel}$ is a product of two sine-Gordon operators coupling charge and spin fluctuations and violating simultaneously the conservation of charge and spin current of the Luttinger model. We have shown in detail that $Y_{\parallel}$, when relevant, is capable of mediating the crossover from a continuous to first-order SDW-CDW transition on $U=2V$. Another first-order transition to a charge-separated phase has been identified as the characteristic instability of the Luttinger liquid against strongly attractive forward-scattering interactions.

In the parameter range $2V>U>0$, the EHM is a CDW insulator, and both charge and spin fluctuations are massive. For $U>|2V|>0$, charges are localized and have a gap but spin fluctuations are gapless and reduce to a (spinless) Luttinger model. For $U<2V<0$, spin fluctuations have a gap but charges a free and can be described in terms of a (spinless) Luttinger model. Consequently, in all three cases, the momentum distribution of the electrons will vary linearly in the vicinity of the Fermi surface as is characteristic of insulators and superconductors, respectively, while those of the gapless pseudofermions would exhibit a power-law variation. The linear variation is a consequence of the multiplicative structure in ρ and σ of the correlation functions in real space, which are therefore dominated by the fastest decaying factor. The EHM reduces to a Luttinger liquid for $U=2V<U_{\rm crit}$ with divergent density-wave correlations (all types degenerate) and for $2V<U<-2V$, where TS fluctuations are most divergent and SS only logarithmically weaker. It is only in these two domains that the power-law variation of $n(k)$ could be observed. Notice however that there is apparently a finite strip in the U-V plane in this region, bounded on one side by the charge-separated phase, where the strong attractive interactions would lead to a linear decay of $n(k)$ not associated with the opening of a gap in one of the collective modes.

A drawback of the present theory is that the complexity of the system of RG equations often renders impossible explicit calculations for general parameters and requires interpolations from solved limiting cases. This is particularly regretable since we have shown that integrating over the RG trajectory both provides significantly more detailed information than just using fixed-point values for the effective couplings (which can be determined more easily numerically) and that in some cases this integration is required for providing results consistent with the symmetries of the model. We have, however, been able to demonstrate that these symmetries (in particular spin rotation) are respected in various relevant limits. The complexity of the RG equations is partly a consequence of the Abelian bosonization procedure we have used, and while we do not believe that qualitatively different results would arise from non-Abelian bosonization, the resulting equations will become simpler and presumably allow explicit calculations over a wider parameter range.

A central step in our solution was the mapping of the 1D quantum problem onto a classical 2D extended XY model. It is interesting that a crossover from continuous to first-order transitions also was observed in certain modified XY models,[33] and it has been speculated that it might be related to the one observed in the EHM for $U=2V$.[7] In the present theory, this speculation cannot be confirmed. In the EHM, the crossover to a first-order transition occurs as a consequence of the coupling ($Y_{\parallel}$ has the structure of a fugacity) between the vortices in two XY models becoming more relevant than the fugacities of the vortices in the individual XY models, resulting in the formation of hybrid vortices corresponding to the up-spin and down-spin CDW's discussed above. In the modified XY model studied by Van Himbergen,[33] the crossover occurs within a single XY model involving higher harmonics of the angle between two spins, which eventually prevents the formation of vortex-antivortex pairs at low temperatures. Translated into fermion language, this interaction would correspond to a kind of multiple-particle backscattering where pairs (and higher n-tuples) of fermions scatter across the Fermi surface. Such processes are inconsistent with two-particle interactions. Another way of realizing the important differences of the two models is to look at the symmetry under global rotations of the spins, which is obeyed by Van Himbergen's interactions. Such rotations correspond to change $\Phi_\nu(x) \rightarrow \Phi_\nu(x)+\varphi_\nu$. Even if one requires $\varphi_\rho=\varphi_\sigma$, Eq. (3.9) shows that $H_{3\parallel}$ is not compatible with such a transformation. This is a consequence of the half-filled band which reduced the U(1) symmetry of incommensurate charge density waves to a discrete Z_2 symmetry.

There have also been studies of the critical behavior of coupled XY models,[34] although these authors do not report the occurrence of first-order transitions. Here one considers two XY models which are coupled on the sites as $\cos\{p[\Theta(\mathbf{r})-\Phi(\mathbf{r})]\}$, where Θ and Φ are the angles the two spins make with an arbitrary axis and p describes its anisotropy. While some features of these studies are reminiscent of similar ones in the EHM, the above symmetry argument also rules out an equivalence of these models since the coupling of the two XY models is invariant under a global rotation of both $\Theta(\mathbf{r})$ and $\Phi(\mathbf{r})$ by the same angle φ, while the fermion model is not. The EHM apparently corresponds to a situation where two coupled XY models are placed in an external potential with twofold rotational symmetry in the case of a half-filled band. I am not aware of such studies for spin models, and it would certainly be interesting to see whether realistic spin models can be constructed that are in the same universality class as the extended Hubbard model or display at least part of the fascinating richness in physical behavior of this model.

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APPENDIX A: OPERATORS AND CORRELATION FUNCTIONS

In this appendix, we first discuss the exact boson form of the interaction terms not included in the Luttinger model including the fermion ladder operators $U_{r,s}$ necessary to make Eq. (2.2) an operator identity.[15] We then define the fluctuation operators for the types of order of interest in the main text and finally outline the calculation of their correlation functions in the extended Hubbard model.

The local backscattering process is described by

$$H'_{1\perp}=g'_{1\perp}\sum_s\int dx\,\Psi^\dagger_{+,s}(x)\Psi_{-,s}(x)\Psi^\dagger_{-,-s}(x)\Psi_{+,-s}(x)$$
$$=\frac{g'_{1\perp}}{(2\pi\alpha)^2}\sum_s U_{+,s}U^\dagger_{-,s}U_{-,-s}U^\dagger_{+,-s}\int dx\,\exp[\sqrt{8}is\Phi_\sigma(x)]\ . \tag{A1}$$

The nonlocal backscattering is

$$H''_{1\perp}=\frac{g''_{1\perp}}{2}\sum_s\int dx\,\Psi^\dagger_{+,s}(x)\Psi_{-,s}(x)\Psi^\dagger_{-,-s}(x+a)\Psi_{+,-s}(x+a)+\text{H.c.}$$
$$=\frac{g''_{1\perp}}{2(2\pi\alpha)^2}\sum_s U_{+,s}U^\dagger_{-,s}U_{-,-s}U^\dagger_{+,-s}\int dx\,\exp\{\sqrt{2i}\,[\Phi_\rho(x)-\Phi_\rho(x+a)+s\Phi_\sigma(x)+\Phi_\sigma(x+a)]\}+\text{H.c.} \tag{A2}$$

Here, the local limit can be safely performed for the Φ_σ fields but the charge-spin coupling effect would be missed if it were also performed in the Φ_ρ fields. Nonlocal corrections from Φ_σ are one power more irrelevant than those from Φ_ρ. Moreover, we have neglected corrections from the commutators of the $U_{r,s}$ operators with the phase fields, which are of order $1/L$, as well as any other corrections of this or higher order. The parallel-spin umklapp term is

$$H_{3\parallel}=\frac{g_{3\parallel}}{2}\sum_s\int dx\,\Psi^\dagger_{+,s}(x)\Psi^\dagger_{+,s}(x+a)\Psi_{-,s}(x+a)\Psi_{-,s}(x)+\text{H.c}$$
$$=\frac{g_{3\parallel}}{2(2\pi\alpha)^2}\sum_s(U_{+,s})^2(U^\dagger_{-,s})^2\int dx\exp\{\sqrt{2}i[\Phi_\rho(x)+\Phi_\rho(x+a)]\}\exp\{\sqrt{2}is[\Phi_\sigma(x)+\Phi_\sigma(x+a)]\}+\text{H.c.} \tag{A3}$$

For the local antiparallel-spin umklapp scattering, we have

$$H'_{3\perp}=\frac{g'_{3\perp}}{2}\sum_s\int dx\,\Psi^\dagger_{+,s}(x)\Psi^\dagger_{+,-s}(x)\Psi_{-,-s}(x)\Psi_{-,s}(x)+\text{H.c.}$$
$$=\frac{g'_{3\perp}}{2(2\pi\alpha)^2}\sum_s U_{+,s}U_{+,-s}U^\dagger_{-,-s}U^\dagger_{-,s}\int dx\,\exp[\sqrt{8}i\Phi_\rho(x)]+\text{H.c.} \tag{A4}$$

and for the nonlocal one

$$H''_{3\perp}=\frac{g''_{3\perp}}{2}\sum_s\int dx\,\Psi^\dagger_{+,s}(x)\Psi^\dagger_{+,-s}(x+a)\Psi_{-,-s}(x+a)\Psi_{-,s}(x)+\text{H.c.}$$
$$=\frac{g''_{3\perp}}{2(2\pi\alpha)^2}\sum_s U_{+,s}U_{+,-s}U^\dagger_{-,-s}U^\dagger_{-,s}$$
$$\times\int dx\,\exp\{\sqrt{2}i[\Phi_\rho(x)+\Phi_\rho(x+a)]\}\exp\{\sqrt{2}is[\Phi_\sigma(x)-\Phi_\sigma(x+a)]\}+\text{H.c.} \tag{A5}$$

We are interested in the following fluctuations. Charge-density waves

$$O_{\rm CDW}(n)=(-1)^n \sum_s c_{n,s}^\dagger c_{n,s} \rightarrow aO_{\rm CDW}(x),$$

$$\begin{aligned} O_{\rm CDW}(x) &= \sum_{r,s} \Psi_{r,s}^\dagger(x)\Psi_{-r,s}(x) \\ &= \frac{1}{2\pi\alpha}\sum_{r,s} U_{r,s}U_{-r,s}^\dagger \exp\{-2irk_Fx+\sqrt{2}ir[\Phi_\rho(x)+s\Phi_\sigma(x)]\} \\ &\approx \frac{2}{\pi\alpha}\cos(2k_Fx)\cos[\sqrt{2}\Phi_\rho(x)]\cos[\sqrt{2}\Phi_\sigma(x)] \ . \end{aligned} \tag{A6}$$

The approximate purely bosonic expression in the last line (as well as the corresponding ones appearing below) incorporates all phase factors coming from the $U_{r,s}$ operators and gives correct results when used with the expressions for the Hamiltonians involving only boson operators.

Bond order waves,

$$O_{\rm BOW}(n)=\frac{(-1)^n}{2}\sum_s (c_{n+1,s}^\dagger c_{n,s}+c_{n,s}^\dagger c_{n+1,s}) \rightarrow aO_{\rm BOW}(x) \ ,$$

$$O_{\rm BOW}(x)=\frac{1}{2}\sum_{r,s}[\Psi_{r,s}^\dagger(x+a)\Psi_{-r,s}(x)+\Psi_{r,s}^\dagger(x)\Psi_{-r,s}(x+a)]$$

$$\begin{aligned} &= \frac{1}{2\pi\alpha}\sum_{r,s} U_{r,s}U_{-r,s}^\dagger \exp(-2irk_Fx-irk_Fa)\exp\left[\frac{ir}{\sqrt{2}}\{\Phi_\rho(x)+\Phi_\rho(x+a)+s[\Phi_\sigma(x)+\Phi_\sigma(x+a)]\}\right] \\ &\quad\times\cos\left\{\frac{-i}{\sqrt{2}}\{\Theta_\rho(x)-\Theta_\rho(x+a)+s[\Theta_\sigma(x)-\Theta_\sigma(x+a)]\}\right\} \end{aligned} \tag{A7}$$

$$\approx \frac{2}{\pi\alpha}\cos(2k_Fx)\sin[\sqrt{2}\Phi_\rho(x)]\cos[\sqrt{2}\Phi_\sigma(x)] \ . \tag{A8}$$

Spin density waves,

$$\mathbf{O}_{\rm SDW}(n)=(-1)^n\sum_{s,s'} c_{n,s}^\dagger(\boldsymbol{\sigma})_{s,s'}c_{n,s'} \ .$$

Here $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ denotes the Pauli matrices. Components,

$$O_{{\rm SDW},x}(n)=(-1)^n\sum_s c_{n,s}^\dagger c_{n,-s} \rightarrow aO_{{\rm SDW},x}(x) \ ,$$

$$\begin{aligned} O_{{\rm SDW},x}(x) &= \sum_{r,s}\Psi_{r,s}^\dagger(x)\Psi_{-r,-s}(x) \\ &= \frac{1}{2\pi\alpha}\sum_{r,s} U_{r,s}U_{-r,-s}^\dagger \exp\{-2irk_Fx+\sqrt{2}ir[\Phi_\rho(x)-s\Theta_\sigma(x)]\} \\ &\approx \frac{-2}{2\pi\alpha}\cos(2k_Fx)\sin[\sqrt{2}\Phi_\rho(x)]\cos[\sqrt{2}\Theta_\sigma(x)] \ , \end{aligned} \tag{A9}$$

$$O_{{\rm SDW},y}(n)=-i(-1)^n\sum_s sc_{n,s}^\dagger c_{n,-s} \rightarrow aO_{{\rm SDW},y}(x) \ ,$$

$$\begin{aligned} O_{{\rm SDW},y}(x) &= -ia\sum_{r,s} s\Psi_{r,s}^\dagger(x)\Psi_{-r,-s}(x) \\ &= \frac{-i}{2\pi\alpha}\sum_{r,s} sU_{r,s}U_{-r,-s}^\dagger \exp\{-2irk_Fx+\sqrt{2}ir[\Phi_\rho(x)-s\Theta_\sigma(x)]\} \\ &\approx \frac{-2}{2\pi\alpha}\cos(2k_Fx)\sin[\sqrt{2}\Phi_\rho(x)]\sin[\sqrt{2}\Theta_\sigma(x)] \ , \end{aligned} \tag{A10}$$

$$O_{{\rm SDW},z}(n)=(-1)^n\sum_s sc_{n,s}^\dagger c_{n,s} \rightarrow O_{{\rm SDW},z}(x) \ ,$$

$$O_{\mathrm{SDW},z}(x)=\sum_{r,s} s\Psi^\dagger_{r,s}(x)\Psi_{-r,s}(x)$$

$$=\frac{1}{2\pi\alpha}\sum_{r,s} sU_{r,s}U^\dagger_{-r,s}\exp\{-2irk_Fx+\sqrt{2}ir[\Phi_\rho(x)+s\Phi_\sigma(x)]\} \qquad \text{(A11)}$$

$$\approx\frac{-2}{2\pi\alpha}\cos(2k_Fx)\sin[\sqrt{2}\Phi_\rho(x)]\sin[\sqrt{2}\phi_\sigma(x)]\ . \qquad \text{(A12)}$$

Singlet pairing,

$$O_{\mathrm{SS}}(x)=\frac{1}{\sqrt{2}}\sum_s s\Psi_{-,s}\Psi_{+,-s}=\frac{1}{\sqrt{2}2\pi\alpha}\sum_s sU^\dagger_{-,s}U^\dagger_{+,-s}\exp\{\sqrt{2}i[\Theta_\rho(x)+s\Phi_\sigma(x)]\}$$

$$\approx\frac{1}{\sqrt{2}\pi\alpha}\exp[\sqrt{2}i\Theta_\rho(x)]\cos[\sqrt{2}\Phi_\sigma(x)]\ . \qquad \text{(A13)}$$

Triplet pairing,

$$O_{\mathrm{TS}+1}(x)=\Psi_{-,\uparrow}\Psi_{+,\uparrow}=\frac{1}{2\pi\alpha}U^\dagger_{-,\uparrow}U^\dagger_{+,\uparrow}\exp\{\sqrt{2}i[\Theta_\rho(x)+\Theta_\sigma(x)]\}$$

$$\approx\frac{1}{2\pi\alpha}\exp\{\sqrt{2}i[\Theta_\rho(x)+\Theta_\sigma(x)]\}\ , \qquad \text{(A14)}$$

$$O_{\mathrm{TS},0}(x)=\frac{1}{\sqrt{2}}\sum_s \Psi_{-,s}\Psi_{+,-s}=\frac{1}{\sqrt{2}2\pi\alpha}\sum_s U^\dagger_{-,s}U^\dagger_{+,-s}\exp\{\sqrt{2}i[\Theta_\rho(x)+s\Phi_\sigma(x)]\}$$

$$\approx\frac{1}{\sqrt{2}\pi\alpha}\exp[\sqrt{2}i\Theta_\rho(x)]\sin[\sqrt{2}\Phi_\sigma(x)]\ . \qquad \text{(A15)}$$

$$O_{\mathrm{TS},-1}(x)=\Psi_{-,\downarrow}\Psi_{+,\downarrow}=\frac{1}{2\pi\alpha}U^\dagger_{-,\downarrow}U^\dagger_{+,\downarrow}\exp\{\sqrt{2}i[\Theta_\rho(x)-\Theta_\sigma(x)]\}$$

$$\approx\frac{1}{2\pi\alpha}\exp\{\sqrt{2}i[\Theta_\rho(x)-\Theta_\sigma(x)]\}\ . \qquad \text{(A16)}$$

$4k_F$ charge-density waves,

$$O_{\mathrm{4CDW}}(x)=\sum_{r,s}\Psi^\dagger_{r,s}(x)\Psi^\dagger_{r,-s}(x)\Psi_{-r,-s}(x)\Psi_{-r,s}(x)$$

$$=\frac{1}{(2\pi\alpha)^2}\sum_{r,s}U_{r,s}U_{r,-s}U^\dagger_{-r,-s}U^\dagger_{-r,s}\exp[-4irk_Fx+\sqrt{8}ir\Phi_\rho(x)]\approx\frac{1}{(\pi\alpha)^2}\cos[\sqrt{8}\Phi_\rho(x)]\ . \qquad \text{(A17)}$$

For the half-filled band, $4k_F$ equals a reciprocal-lattice vector, and the $4k_F$ function therefore describes effectively long-wavelength density fluctuations. The *approximate* forms of the fluctuation operators given in Eqs. (A6)–(A16) when used with the *approximate* expressions for the Hamiltonians, Eqs. (A1)–(A5), give identical expressions for the correlation functions to those obtained when the full expressions including the $U_{r,s}$ operators are used. Notice that they do not correspond to just dropping the $U_{r,s}$.

We then follow earlier work[19,22,23] to compute the correlation functions of type j in the Matsubara formalism $[\mathbf{r}=(x,v_\sigma\tau)]$

$$-R_j(\mathbf{r})=\langle T_\tau O_j(\mathbf{r})O_j^\dagger(0)\rangle=\frac{1}{Z}\mathrm{Tr}\left[T_\tau O_j(\mathbf{r})O_j^\dagger(0)\exp\left[\int_0^{\beta\to\infty}d\tau H(\tau)\right]\right]\ ,$$
$$H(\tau)=H_{\mathrm{Lutt}}(\tau)+H_{\mathrm{pert}}(\tau)\ , \qquad \text{(A18)}$$

where the trace (Tr) is performed over the charge and spin degrees of freedom, Z is the partition function, H_{Lutt} is the Luttinger part of the Hamiltonian, and H_{pert} subsumes the remaining interactions perturbing the Luttinger model. $\exp[-\int d\tau H_{\mathrm{pert}}(\tau)]$ is now expanded in a series, and the trace of the ensuing expression is evaluated using H_{Lutt} only[22] and then reexponentiated. Our correlation functions have the general form

$$-R_j(\mathbf{r})=\frac{\cos(2k_Fx)}{(\pi\alpha)^2}\mathcal{R}_j(\mathbf{r}) \qquad \text{(A19)}$$

for the density-wave functions ($j=$ CDW, BOW, SDW) and

$$-R_j(\mathbf{r})=\frac{1}{(2\pi\alpha)^2}\mathcal{R}_j(\mathbf{r}) \qquad \text{(A20)}$$

for the pairing functions ($j=$SS,TS). The difference in prefactor arises from the fact that the density-wave operators for the half-filled band are real. We obtain for the slowly varying part $\mathcal{R}_j(\mathbf{r})$ of the correlation functions of our model

$$\ln\mathcal{R}_{\rm CDW}(\mathbf{r})=-(\beta_\rho+\beta_\sigma)\ln\left[\frac{r}{\alpha}\right]-\int(Y_\rho+Y_\sigma+Y_\parallel/2)dl$$
$$+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{\beta_\rho^2Y_\rho^2+\beta_\sigma^2Y_\sigma^2+\tfrac{1}{2}[(\beta_\rho^2+\beta_\sigma^2)Y_\parallel^2+\beta_\rho^2Y_{\sigma\to\rho}+\beta_\sigma^2Y_{\rho\to\sigma}]\}\ , \quad \text{(A21)}$$

$$\ln\mathcal{R}_{\rm BOW}(\mathbf{r})=-(\beta_\rho+\beta_\sigma)\ln\left[\frac{r}{\alpha}\right]-\int(-Y_\rho+Y_\sigma-Y_\parallel/2)dl$$
$$+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{\beta_\rho^2Y_\rho^2+\beta_\sigma^2Y_\sigma^2+\tfrac{1}{2}[(\beta_\rho^2+\beta_\sigma^2)Y_\parallel^2+\beta_\rho^2Y_{\sigma\to\rho}+\beta_\sigma^2Y_{\rho\to\sigma}]\}\ , \quad \text{(A22)}$$

$$\ln\mathcal{R}_{{\rm SDW},z}(\mathbf{r})=-(\beta_\rho+\beta_\sigma)\ln\left[\frac{r}{\alpha}\right]-\int(-Y_\rho-Y_\sigma+Y_\parallel/2)dl$$
$$+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{\beta_\rho^2Y_\rho^2+\beta_\sigma^2Y_\sigma^2+\tfrac{1}{2}[(\beta_\rho^2+\beta_\sigma^2)Y_\parallel^2+\beta_\rho^2Y_{\sigma\to\rho}+\beta_\sigma^2Y_{\rho\to\sigma}]\}\ , \quad \text{(A23)}$$

$$\ln\mathcal{R}_{{\rm SDW},xy}(\mathbf{r})=-(\beta_\rho+\beta_\sigma^{-1})\ln\left[\frac{r}{\alpha}\right]+\int Y_\rho dl+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{\beta_\rho^2Y_\rho^2-Y_\sigma^2+\tfrac{1}{2}[(\beta_\rho^2-1)Y_\parallel^2+\beta_\rho^2Y_{\sigma\to\rho}-Y_{\rho\to\sigma}]\}\ , \quad \text{(A24)}$$

$$\ln\mathcal{R}_{\rm SS}(\mathbf{r})=-(\beta_\rho^{-1}+\beta_\sigma)\ln\left[\frac{r}{\alpha}\right]-\int Y_\sigma dl+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{-Y_\rho^2+\beta_\sigma^2Y_\sigma^2+\tfrac{1}{2}[(\beta_\sigma^2-1)Y_\parallel^2-Y_{\sigma\to\rho}+\beta_\sigma^2Y_{\rho\to\sigma}]\}\ , \quad \text{(A25)}$$

$$\ln\mathcal{R}_{{\rm TS},0}(\mathbf{r})=-(\beta_\rho^{-1}+\beta_\sigma)\ln\left[\frac{r}{\alpha}\right]+\int Y_\sigma dl+\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right]\{-Y_\rho^2+\beta_\sigma^2Y_\sigma^2+\tfrac{1}{2}[(\beta_\sigma^2-1)Y_\parallel^2-Y_{\sigma\to\rho}+\beta_\sigma^2Y_{\rho\to\sigma}]\}\ , \quad \text{(A26)}$$

$$\ln\mathcal{R}_{{\rm TS},\pm1}(\mathbf{r})=-(\beta_\rho^{-1}+\beta_\sigma^{-1})\ln\left[\frac{r}{\alpha}\right]-\tfrac{1}{2}\int\ln\left[\frac{r}{\alpha}\right][Y_\rho^2+Y_\sigma^2+Y_\parallel^2+\tfrac{1}{2}(Y_{\sigma\to\rho}+Y_{\rho\to\sigma})]\ , \quad \text{(A27)}$$

$$\ln\mathcal{R}_{\rm 4CDW}=-4\beta_\rho\ln\left[\frac{r}{\alpha}\right]+2\beta_\rho^2\int\ln\left[\frac{r}{\alpha}\right](Y_\rho^2+\tfrac{1}{2}Y_\parallel^2+\tfrac{1}{2}Y_{\sigma\to\rho})\ . \quad \text{(A28)}$$

The integrals have to be performed over the RG group trajectory for the interaction constants. The first terms on the right-hand sides of these equations are the bare functions of the Luttinger model. The last terms arise, in the expansion of $\exp[-\int H_{\rm pert}(\tau)d\tau]$ from the second-order terms. They are the direct generalization of the terms arising in the incommensurate limit and give the renormalization of the correlation exponents β_ν. The second terms on the right-hand sides of (A21)–(A26) are interesting in that they do not contain functions depending on $\mathbf{r}$ and, in principle, can be thought of as renormalizations to the amplitude (prefactor) of the correlation functions whose initial values are set to $A_j=1$. They come from the first order of the expansion of $\exp[-\int H_{\rm pert}(\tau)d\tau]$ and are nonvanishing whenever the perturbation Hamiltonian contains terms that roughly are squares of the correlation operators (or parts of them) in which one is interested, e.g., when one considers a correlation function containing $\cos[\sqrt{2}\Phi_\nu(x)]$ and a perturbation of type $\int\cos[\sqrt{8}\Phi_\nu(x)]dx$. They have been discussed in some detail for the Hubbard model earlier.[19] If the integrals are performed only over an infinitesimal path $(l\cdots l+dl)$ the expressions for the correlation functions can be converted to a set of differential equations yielding the RG equations for the coupling constants given in the main text, Eqs. (2.30)–(2.36), and the renormalization of the prefactors of the correlation functions also discussed in the text.

The further treatment now depends on the scaling behavior of the interactions. When they scale towards weak coupling, the integrals over the RG trajectories can be performed from zero up to infinity, in principle. Notice, however, that in practice an ultimate cutoff will be provided by the observation distance r of the correlations (if not by system size, temperature, frequency, etc.) so that the integrals over the RG trajectories are cut off at $l^*=\ln(r/\alpha)$. When performing the integrals, notice that the terms such as $\int Y_\nu dl$ independent of the distance will now become dependent on r due to the upper integration limit depending on r. They will thus contribute to the decay of the correlation function and not only yield a prefactor correction. Where an explicit solution to the scaling equations was available, the results of these integrations have been discussed in the main body of this paper. It is precisely these terms which are responsible for the appearance of logarithmic corrections. If scaling goes towards strong coupling, a consistent solution and integration of the RG equations to the upper integration limit $l^* = \ln(r/\alpha)$ is not possible since the condition $Y \ll 1$ under which they have been derived ceases to be valid. One possibility is then to integrate the equations up to some integration limit l_1 such that $Y(l_1) \sim 1$ if information on that model can then be obtained by different methods. As discussed in the text, we have repeatedly followed this procedure and made use of a solution for one degree of freedom ν in terms of spinless fermions provided by Luther and Emery.[26] As long as one is only interested in the qualitative features of the phase diagram, sufficient information is provided by using the differential equations for coupling constants and correlation function amplitudes generated by integrating only over an infinitesimal interval as discussed above. This is possible in particular since the integration limit now does not depend on distance (or any other external parameter) but on the coupling constants of the model and therefore will not convert prefactor corrections to contributions to correlation decay. Examples are also given in the text.

APPENDIX B: OFF-DIAGONAL INTERACTIONS

Models including more general interactions than the extended Hubbard model have been of some interest in recent literature. Specifically, the inclusion of site-off-diagonal interactions such as

$$\begin{aligned} H_{od} = \frac{W}{2} \sum_{n,s,s'} (c^\dagger_{n+1,s} c_{n,s} + \text{H.c.})(c_{n+1,s'} c_{n,s'} + \text{H.c.}) \\ + \frac{X}{4} \sum_{n,s} [\{(c^\dagger_{n+1,s} c_{n,s} + \text{H.c.}), c^\dagger_{n,-s} c_{n,-s}\}] \\ - \frac{X}{8} \sum_{n,s} (c^\dagger_{n+1,s} c_{n,s} + \text{H.c.}) \end{aligned} \qquad \text{(B1)}$$

(here, $\{\cdots,\cdots\}$ denotes the anticommutator) has been investigated in the context of electron-phonon models of conducting polymers,[35–37] where the W interaction also describes the effective electron-electron interaction generated by coupling to acoustic phonons in the antiadiabatic (phonon frequency $\to \infty$) limit;[36] they are also of interest in their own right[37–39] since these off-diagonal interactions are, *a priori,* required on a lattice from the translational invariance of the Coulomb interaction. One special limit even includes a model that is exactly solvable in arbitrary dimension.[39] The phase diagram of the purely electronic model, Eqs. (1.1) plus (B1), has been studied numerically, and one can apply the present methods to that problem, too. We do not elaborate in detail on this issue but only list here the coupling constants for the continuum field that which are modified in the presence of the off-diagonal interactions (B1):

$$g_{1\parallel} = g''_{1\perp} = (-2V + 4W)a \,, \qquad \text{(B2)}$$

$$g_{3\parallel} = g''_{3\perp} = (-2V - 4W)a \,. \qquad \text{(B3)}$$

At half-filling, the X interaction does not contribute to the interactions specified above but instead generates interactions of a slightly different form. There is a charge-spin coupling backscattering (we only give the approximate boson representation)

$$H^X_{1\perp} = \frac{4Xa}{(2\pi\alpha)^2} \int dx \cos[\sqrt{8}\Phi_\sigma(x)] \times \sin\left[\frac{\Phi_\rho(x+a) - \Phi_\rho(x)}{\sqrt{2}}\right] , \qquad \text{(B4)}$$

where we have omitted less relevant terms involving additional Θ_ν fields and which would be missed if the local limit was performed from the outset, and an umklapp term

$$H^X_{3\perp} = \frac{-2Xa}{(2\pi\alpha)^2} \sum_s \int dx \sin\left(\sqrt{8}\Phi_\rho(x) + \frac{s}{\sqrt{2}}[\Phi_\sigma(x+a) - \Phi_\sigma(x)]\right) \times \cos\left[\frac{1}{\sqrt{2}}\{\Theta_\rho(x+a) - \Theta_\rho(x) + s[\Theta_\sigma(x+a) - \Theta_\sigma(x)]\}\right] . \qquad \text{(B5)}$$

This term has a nonvanishing local limit

$$H^X_{3\perp} \approx \frac{-4Xa}{(2\pi\alpha)^2} \int dx \sin[\sqrt{8}\Phi_\rho(x)] \,, \qquad \text{(B6)}$$

but if charge-spin coupling is important, the full form must be used, and it is interesting that the Θ_ν fields will play a role then. All of these terms can be treated by the methods outlined in the main text and Appendix A.

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