Phase Diagram of strongly correlated one-dimensional fermions in incommensurate potentials

Juan Carlos Chaves and Indubala I. Satija
Department of Physics and Institute for Computational Sciences and Informatics, George Mason University, Fairfax, VA 22030

Mauro M. Doria
Department of Physics Institute de Fisica Universidade Federal Fluminense Campus da Praia Vermelha Niteroi, 24210-340, RJ, Brazil (April 20, 2001)

We study the interplay between strong correlations and incommensurability on fermions using mean field as well as exact many-body Lanczos diagonalization techniques. In a two-dimensional parameter space, mean field phase diagram of infinite system shows a critical phase with multifractal characteristics sandwiched between a Bloch-type extended and a localized phase. Exact numerical computation on finite size systems of the Kohn charge stiffness $D_c$, characterizing transport properties, and the charge exponent $K_p$, characterizing the superconducting pairing fluctuations, shows the existence of a phase with superconducting correlations. This phase may be characterized by a power law scaling of the charge stiffness constant in contrast to the Anderson localized phase where $D_c$ scales exponentially with the size of the system. We argue that this intermediate phase may be a dressed up analog of the critical phase of the noninteracting fermions in an incommensurate potential.

I. INTRODUCTION

The study of metal-insulator transition in strongly correlated one-dimensional (1D) disordered systems have been the subject of many recent studies. These studies have been motivated by various different viewpoints. A great deal of theoretical research in this area has been to account for the magnitude of persistent currents in mesoscopic rings. Another motivation for these studies has been the argument that 1D models in a staggered field may describe the physics of two-dimensional systems; the subject of great interest in high $T_c$ superconductivity.

In this paper, we describe our study of the phase diagram of many-body spinless fermion chain in presence of a sinusoidal potential with periodicity which introduces a new length scale in the problem. We approach the problem of understanding the phase diagram of this periodic system from a perspective very different from the previous studies. It has been known that noninteracting systems in incommensurate potentials exhibit metallic, insulating as well as an exotic fractal phase which is in-between metallic and insulating and is usually referred as critical. These systems which are in-between periodic and random have attracted a great deal of attention due to the possibility of exhibiting a novel type of transport as the multifractal wavefunctions are characterized by almost a power law decay. Technical complexities associated with studying strongly correlated systems make the study of the effect of strong correlations on incommensurate systems a rather difficult task. Hence, the natural questions like how the metal-insulator transition and the fractal characteristics of non-interacting fermions are affected when many-body fermion-fermion correlations are taken into account has remained an open theoretical challenge.

We recently published our preliminary results on this problem using Lanczos diagonalization method where we focussed on the transport studies of 1D spinless model in the presence of both repulsive as well as the attractive interaction. One of the intriguing results of our study for attractive interaction was the possibility of a new phase where the charge stiffness may scale as a power law. The purpose of this paper is three fold. Firstly, we present our simulation results for systems of bigger sizes than those reported in our earlier paper. This strengthens the possibility of a new type of phase in strongly correlated systems. Secondly, we compute the charge exponent $K_p$ which characterizes the long range correlations in the system. Our results show that the regime with superconducting fluctuations overlaps the regime where we see a new type of transport characteristics. Thirdly, we describe self-consistent mean field (MF) theory results where the mean field is assumed to be due to copper pairs. The self-consistent mean field theory shows the existence of a critical phase, sandwiched between an extended and localized phase. Interestingly, this critical phase exists in a finite parameter space of measure directly proportional...
to the strength of the cooper pair interactions. We correlate the MF and the exact diagonalization results and argue that the new type of behavior seen in numerical simulation may be a dressed up analog of the critical phase of noninteracting fermions.

In section II, we describe our model and two interesting limits where the model has been extensively studied. In section III, we discuss mean-field results for the spinless fermion case. In addition to the various remarks in the introduction, this section will further bring to focus our motivations for the proposed study. In section IV, we describe our results for the charge exponent $K_\rho$ and charge stiffness $D_c$. In section V we summarize our results.

**II. MODEL SYSTEM AND ITS TWO INTERESTING LIMITS**

Consider an interacting spinless fermion model on a 1D ring in a quasiperiodic potential,

$$H = - \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V \sum_{i=1}^{N} n_i n_{i+1} + \sum_{i=1}^{N} h_i n_i.$$  

(1)

The $c_i$ and $n_i$ are respectively the fermion and number operators at site $i$. The site dependent potential is chosen to be of the form, $h_i = \lambda \cos(2\pi \sigma_i)$. Here, $\lambda$ represents the strength of the potential and $\sigma$ is an irrational number which is chosen for convenience to be the Golden Mean ($\frac{\sqrt{5} - 1}{2}$). This parameter describes the two competing length scales in the system: namely, the fermion lattice space and the periodicity of the sinusoidal potential.

The above model has two interesting limits that have been studied extensively. For $\lambda = 0$, the interacting spinless fermion problem could be mapped to the Heisenberg-Ising XXZ spin problem \cite{15} for which a closed Bethe’s ansatz solution exists. \cite{11} For all densities, the model exhibits a Luttinger liquid phase. The Luttinger liquid phase differs from the conventional Fermi liquid which accounts for the conduction behavior in conventional metallic phase. In Fermi liquid phase the low energy excited states of the interacting electron gas can be described in terms of quasiparticle excitations which are analog to the single particle excitations of a free Fermi system. In contrast, the Luttinger phase is characterized by many-body collective excitations. For attractive interaction ($V < 0$), the model exhibit SC correlations that can be described in terms of the charge exponent $K_\rho$,

$$<O_i O_{i+r}> \propto r^{-1/K_\rho} \quad \text{(2)}$$

where $O_i$ is a (singlet) pairing operator,

$$O_i = \frac{1}{\sqrt{2}} (c_i c_{i+1} + h.c.) \quad \text{(3)}$$

Therefore, $K_\rho > 1$ signals the existence of SC fluctuations.

Other interesting limit of the model is the $V = 0$ case where the model describes the famous Harper equation \cite{23} which has also been studied both numerically as well as more recently by Bethe’s ansatz. \cite{11} The Harper equation is a paradigm in the study of low-dimensional incommensurate systems as it exhibits a metal-insulator transition in one dimension. \cite{23} At the onset of transition $\lambda_c = 2$, the quantum states are neither extended nor localized but instead exhibit fractal character and have been termed as critical. The spectrum contains an infinite number of gaps and is believed to be a Cantor set of zero measure. These interesting aspects of the wave function and the spectra have been shown to be reflected in the transport properties such as Launder resistance. \cite{14,17}

The possibility of a phase which is neither Anderson insulating nor metallic in strongly correlated systems is a fascinating theoretical problem. We explore this first using mean-field theory and then using exact many body Lanczos diagonalization on finite size systems. In correlated systems, we will focus directly on the transport properties characterized by the stiffness constant. This is in contrast to the mean-field case where the single particle wavefunctions can be used as the diagnostic tool for characterizing the nature of the phase in the system.

**III. MEAN FIELD THEORY**

For attractive interaction, we assume the existence of electron pairing resulting in a mean field $\Delta$

$$\Delta = \frac{1}{N} \sum_{i=1}^{N} < c_i c_{i+1} > \quad \text{(4)}$$

In terms of the mean field $\Delta$, the Hamiltonian becomes

$$H \approx -t \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) - V \Delta \sum_{i=1}^{N} (c_{i+1}^\dagger c_i^\dagger + c_i c_{i+1}) - \sum_{i=1}^{N} h_i n_i \quad \text{(5)}$$

The parameter $\Delta$ is a function of both $t$ and $V$ and has to be determined self-consistently.

The above mean-field Hamiltonian is the fermion representation of spin-$\frac{1}{2} XY$ chain in a transverse field. \cite{23} The fermion operators $c_i$ are related to spin operators $S_i$ by Jordan Wigner transformation,

$$S_i^+ = c_i^\dagger \exp(i\pi \sum_{m<n} c_m^\dagger c_m) \quad \text{(6)}$$

$$S_i^- = \exp(-i\pi \sum_{m<n} c_m^\dagger c_m) c_n \quad \text{(7)}$$
The parameters \( t \) and \( V\Delta \) are related to the exchange interactions in the spin model: \( t \) is proportional to the sum of the exchange interaction in the 2-dimensional spin space while the fermion non-conserving term \( V\Delta \) is proportional to spin space anisotropy. The \( V \) dependent term in the Hamiltonian breaks the \( O(2) \) symmetry of the spin chain and the spin model is in the universality class of the Ising model with anisotropy proportional to \( V\Delta \). The mean-field \( \Delta \) can be determined self-consistently by the methods described by Lieb et al (for example as the results shown in fig. 1). [10] In the absence of magnetic field \( (\lambda = 0) \), the \( \Delta \) can be determined analytically in the following two limits: For \( \frac{t}{V} = 0 \), \( \Delta = \frac{1}{2\pi} \) and for \( t = \Delta V \), \( \Delta = \frac{1}{8} \).

The anisotropic spin model in the presence of modulating magnetic field was studied recently as the perturbed Harper equation. [4] Numerical diagonalization as well as exact decimation scheme showed that the model exhibits extended (E), localized (L) as well as a critical (C) phase. A novel aspect of the model is the fact that unlike Harper, the C phase exists in a finite parameter interval. The term \( V\Delta \) results in fattening the critical point of Harper to a critical phase, sandwiched between the Bloch phase and the localized phase. The boundaries between the Bloch states and critical states as well as the boundaries between the critical and localized states were found numerically to be determined by simple relations:

- \( \lambda < 2(t + V\Delta) \), we have an E phase.
- If \( \lambda > 2(t - V\Delta) \), we have an L phase.
- If \( 2(t + V\Delta) \leq \lambda \leq 2(t + V\Delta) \), we have a C phase.

Therefore, by determining the parameter \( \Delta \) self-consistently, the phase boundaries of the model can be inferred. It should be noted that the mean-field theory can also be done in the absence of cooper pairs by writing mean field term as \( \langle c_j c_{j+1} \rangle \). In this case, the MF Hamiltonian belongs to the universality class of Harper equation which exhibit E-L transition. The critical phase in this case reduces to a critical line. Such a MF theory gives a self-consistent solution for both repulsive as well as attractive interaction \( V \).

Figure 1 shows the mean field \( \Delta \) obtained self-consistently. It should be noted that the strength of the aperiodic field \( \lambda \) determines a critical value of \( V \) below which the mean field \( \Delta \) is zero. For repulsive interaction, the self-consistent value of \( \Delta \) was always found to be zero.

Figure 2 shows the MF phase diagram in the two-dimensional parameter space of \( V - \lambda \). For attractive interaction, the model exhibits E, L as well as fat C phase beyond a critical value of \( \lambda \). Exact renormalization study of the C phase [10] has shown that the wave function exhibits self-similarity. The exponents characterizing the self-similar behavior at the onset of E-C and C-L transition are different from those of the fat critical phase sandwiched between these two phases. [10] Another interesting aspect of this diagram is the fact that C-L transition coincides with the magnetic transition to long range order which is in the universality class of Ising model in transverse field.

The MF model exhibits a gap in the energy spectrum (except at the conformal point which corresponds to the transition to magnetic long range order in the XY spin model). However, we argue that the transition under consideration in disordered systems is the Anderson transition and therefore the transport properties are determined by the nature of single particle wave function.

The Lanczos’s numerical results shown in the next section confirm the existence of superconducting pairing for attractive interaction. We would like to argue that this justifies our basic assumption about the existence of a mean field is derived from the cooper pairs. Reentrant nature of the MF diagram may be just the artifact of MF assumption. Therefore, the MF phase diagram may describe qualitatively the physics of strongly correlated systems in the regime where the superconducting fluctuations exist. In spite of the limitations of MFT in 1D, the interesting phase diagram provides a strong incentive for further exploration of phase diagram with a view to check the possibility of an exotic phase (with localization properties intermediate between metallic and insulating) in strongly correlated systems.

### IV. LANCZOS DIAGNOSTIC RESULTS

Motivated by the possibility of a new type of phase, we next use Lanczos exact diagonalization method to obtain the stiffness constant \( D_c \) which determines the transport properties of the system. In addition, we also compute the charge exponent to check the validity of MF theory based on the assumption that the MF derived from the fermion pairing. As explained below, both these quantities can be determined from the ground state properties of the system.

The first step in this computation is to determine the ground state energy \( E_0 \) of a one-dimensional ring with \( N \) lattice sites subjected to a transverse magnetic flux \( \Phi \). The the Kohn stiffness constant \( D_c \) is then given by

\[
D_c = \frac{N}{2} \frac{d^2 E_0(\Phi)}{d\Phi^2} |_{\Phi = \Phi_{\text{min}}}.
\]

The charge exponent \( K_{\rho} \) can also be determined in terms of ground state properties by first computing the compressibility \( \kappa \). As explained by P. Prelovsek et al [3] the
compressibility for finite systems can be calculated from values of ground state energies:

\[ \frac{1}{\rho^2 \kappa} = \frac{N}{4} \left[ E_0(N_e + 2) - 2E_0(N_e) + E_0(N_e - 2) \right] \] (10)

Here \( N_e \) are the number of fermions in the system with fermion density \( \rho = N_e/N \). Now the following two equations relate \( \kappa \) to the charge exponent via the renormalized Fermi velocity \( u_p \),

\[ K_p = \pi \frac{D_c}{u_p} \] (11)

\[ \frac{1}{\rho^2 \kappa} = \frac{\pi u_p}{2K_p} \] (12)

Our simulations are done for systems of various sizes \( N \) and electronic densities \( \rho = \frac{N_e}{N} \), in two-dimensional parameter space \( V \) and \( \lambda \). To simulate golden mean quasiperiodicity into the model, we used Lanczos methods for systems of various Fibonacci sizes. Furthermore, we worked with densities which are the rational approximants to the square of the golden mean \( \sigma^2 \). This procedure provides several possible sizes (5, 8, 13 and 21) for which the Lanczos diagonalization can be done keeping the density of the fermions almost constant. It should be noted that unlike the previous studies involving random disorder, we cannot work with arbitrary sizes. This limits not only the number of sizes that we can study, but also forces us to work with densities different from half-filling. Therefore, our studies are for systems away from half-filling where the umklapp processes become irrelevant and the system in absence of disorder is metallic. The next possible Fibonacci size 34 is rather hard to simulate using present day technology, and therefore, our results are in fact for the maximum possible exact diagonalization size (for simulating incommensurate effects) that can be done with current regular computers. To obtain additional data points, we also show some results for densities which are rational approximants of \( \frac{\sqrt{5}-1}{2} \) such as \( \rho = \frac{14}{18} \). However, the fermion density for this case is different from those of Fibonacci size systems.

Figures 3 and 4 respectively show our results for the charge exponent and the charge stiffness. Figures (a) and (b) correspond to two different densities and are included here to show the consistency of our results independent of the density. As shown in figure 3, comparison with the \( \lambda = 0 \) case show that the presence of a new competing length enhances the SC pairing fluctuations in the strongly correlated fermions. This effect becomes specially strong around \( V = -2 \) where the charge stiffness attains a maximum value as shown in figures 4 and 5. The existence of a characteristic peak in \( D_c \) was reported in our earlier paper for \( N \leq 13 \). Simulation results presented here confirms our earlier results for bigger size systems. What is new here is the fact that by computing the charge exponent \( K_p \), we are now able to correlate the regime characterized by a clear peak with the regime where the model exhibits SC fluctuations. This also provides a plausible argument to justify the use of an effective mean field approach (like the one use in section III) for the Copper like quasiparticles. Since the MF phase diagram exhibits a critical behavior with fractal self-similar wave function, we speculate that the phase diagram in the vicinity of the characteristic peak with strong SC fluctuations is a dressed up version of the critical phase in systems with strong fermion correlations. We would like to stress that we view our MF results as providing only qualitative predictions as the phase boundary (C-L) predicted by MF does not agree with the one obtain by the exact diagonalization method.

Unlike the MF case where the intermediate nature of the phase was due to the fractal nature of the single particle wave function, the many body phase diagram is characterized by its transport characteristics. Figures 4 and 5 indicate the possible existence of a region where \( D_c \) may take intermediate values: between those of a metallic and those corresponding to the Anderson localized insulating phase. Our simulations show that the height of the peak in \( D_c \) decreases rather slowly with the size of the system. This is in contrast to the Anderson localized phase where the \( D_c \) decays exponentially with the size of the system. We conjecture that in the regime near the peak, the charge stiffness decays as a power law. This conjecture was verified only at a at the special point \( V = 0 \). For arbitrary value of \( V \), it is rather difficult to verify this conjecture for large \( N \).

V. CONCLUSIONS AND DISCUSSION

Two central results of this paper are: the existence of SC fluctuations in the strongly correlated fermion model with competing length scales where the incommensurability enhances the SC fluctuation and a possibility of an intermediate phase (in-between metallic and Anderson localized) which may be related to the critical phase of noninteracting model which exhibits fractal characteristics. This is the first paper where the effects of two incommensurate lengths are studied in strongly correlated system. We hope that our results will stimulate further studies of this type of behavior in other models such as \( t-J \) and Hubbard models.

Our numerical calculation of the charge exponent parameter describing SC pairing coherence provides a justification of our mean field ideas where fermion-fermion correlations were explicitly assumed. We want to emphasize that in aperiodic case, one cannot disregard the mean field results in 1D as one does in the pure models. This is because, in the pure model, the metal-insulator transition is the Mott transition where a conducting phase becomes insulating due to the opening of a gap. Previous studies have shown that mean field theory contra-
dicts the exact results as far as the existence of a gap is concerned. In the aperiodic cases, the metal-insulator transition is the Anderson transition. In the noninteracting model, this transition is characterized by the localization of the single-particle wave function and a point spectrum. Therefore, we would like to argue that even though mean field results are incorrect regarding the existence or nonexistence of a gap, it may still be of some validity in describing the Anderson transition.

Recently, there have been density matrix renormalization group (DMRG) studies of spinless fermion models that show the existence of a delocalized phase for Anderson disordered potentials.\[25\] The range of the parameter $V$ for which this phase seems to exist coincides with the values of $V$ for which we postulated the possibility of an intermediate phase. We think that these findings further support our argument that an intermediate phase may exist for the case of quasiperiodic potentials.

Our previous results, hinting a new mechanism involving some sort of competition other than the known screening of the disorder due to SC fluctuations, are strengthened by our studies with bigger size systems. Furthermore, the study, involving mean field and exact diagonalization, provides a more convincing argument that this new phase may be related to the critical phase of non-interacting systems.

ACKNOWLEDGMENTS

The research of I.I.S. is supported by a grant from National Science Foundation DMR 097535. We also acknowledge the support of the Pittsburgh Supercomputing Center where part of our numerical results were obtained. J.C.C. would like to thank the people at CIF (International Physics Center) in Bogotá for their constant help and encouragement during his career and acknowledge the support obtained through COLCIENCIAS-IDB-ICETEX from Colombia.

[1] e-mail: jchaves@gmu.edu.
[2] e-mail: isatija@sitar.gmu.edu.

FIG. 1. Self-consistent mean-field $\Delta$ vs $V$ for several values of $\lambda$. Namely, solid line $\lambda = 0.5$, dotted line $\lambda = 1$, short-dashed line $\lambda = 1.5$ and long-dashed line $\lambda = 2.1$.

FIG. 2. Mean-field phase diagram in $V - \lambda$ plane showing the E, the C and the L phases. Along the dashed line describing the C-L transition, the model is conformally invariant.
FIG. 3. The Charge exponent $K_p$ vs $V$ for $\lambda = 0.0$ (dashed curve) and $\lambda = 1.0$ (un-dashed curve). Part (a) for $\rho = \frac{5}{13}$ and part (b) for $\rho = \frac{13}{18}$ showing that incommensurability enhances the SC pairing.

FIG. 4. Charge stiffness $D_c$ versus $V$ for $\lambda = 1.0$. Part (a) shows $\rho = \frac{5}{13}$ part (b) $\rho = \frac{13}{18}$. Shaded parts indicate the regime where SC fluctuations exist.

FIG. 5. Charge stiffness versus $V$ for $\rho = \frac{13}{21}$ and $\lambda = 1.0$. The points obtained for this case are indicated by crosses. The interpolated dashed curved is mean to be used as a guide to the eye.