

# Localization properties of two interacting particles in a quasi-periodic potential with a metal-insulator transition

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**Abstract.** We study the influence of many-particle interactions on a metal-insulator transition. We consider the two-interacting-particle problem for onsite interacting particles on a one-dimensional quasiperiodic chain, the so-called Aubry-André model. We show numerically by the decimation method and finite-size scaling that the interaction does not modify the critical parameters such as the transition point and the localization-length exponent. We compare our results to the case of finite density systems studied by means of the density-matrix renormalization scheme.

**PACS.** 71.30.+h Metal-insulator transitions and other electronic transitions – 71.27.+a Strongly correlated electron systems; heavy fermions

## 1 Introduction

The metal-insulator transition (MIT) in disordered electronic systems has been the subject of intense research activities over the last two decades and still continues to attract much attention. For free electrons in disordered systems [1] the scaling hypothesis of localization [2] can successfully predict many of the universal features of the MIT. However, the influence of many-particle interactions on the MIT is not equally well understood [3] and recent investigations of an apparent MIT in two-dimensional (2D) systems even question the main assumptions of the scaling hypothesis [4–9]. A simple theoretical approach to the interplay of interactions and disorder is based on the two-interacting-particles (TIP) problem in 1D random [10–12] or quasiperiodic potentials [13,14]. Furthermore, numerical results for spinless fermions at finite particle density have given additional insight [15–17]. In general, these investigations have shown that changes in the wave function interferences due to many-particle interactions [18,19] can lead to a rather large enhancement of the localization lengths in 1D and 2D [16,20,21].

The standard approach for computing localization lengths in disordered, non-interacting systems is the transfer-matrix method [22]. It has been used for investigations of the enhancement of the TIP localization length in a 1D random potential [12,23] where there is no MIT as all wave functions are always localized. Other numerical approaches to the TIP problem have been based on the time evolution of wave packets [10,24], exact diagonalization [25] or Green function approaches [20,26,27].

In the single-particle case, the 1D quasiperiodic Aubry-André model is known rigorously to exhibit an MIT for all states in the spectrum as a function of the quasiperiodic potential strength  $\mu$  [28]. The ground state wave function is extended for  $\mu < 1$  and localized for  $\mu > 1$ . The system at  $\mu_c = 1$  is critical: there the wave functions decrease algebraically, not exponentially as in the localized case. Recently, we examined this model for TIP by means of the transfer-matrix method together with a careful finite-size-scaling analysis [14] following earlier analytical work of references [29,30]. We showed that the model for TIP exhibits an MIT as a function of  $\mu$  at  $\mu_c = 1$  as in the single-particle case. Our finite-size-scaling results for onsite (Hubbard) interaction suggest that the critical behavior, *i.e.*, the value for the critical exponent  $\nu$  of the correlation length, is also not affected by the interaction [14]. However, it has been demonstrated [12,20] that a transfer-matrix-method approach applied to the TIP problem without finite-size scaling leads to unreliable localization lengths, *i.e.*, it systematically overestimates the TIP localization length  $\lambda_2$  in finite-sized samples in the case of vanishing interaction ( $U = 0$ ). In addition, simple extrapolations to infinite sample size [12,23] may lead to an underestimation of  $\lambda_2$  [31]. An alternative approach, which does not suffer from the above problem, is based on the decimation method and has also been applied recently to TIP in a 1D random potential [20]. This encouraged us to reexamine the localization lengths for TIP in 1D quasiperiodic potentials with Hubbard interaction with the decimation method. As we shall show in the following, we find that the general conclusions of reference [14] remain valid, *i.e.*, the MIT is not affected by the

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interaction. The critical properties of the single-particle transition at  $\mu_c = 1$  are not altered within the accuracy of our calculation. One-parameter scaling is obeyed for onsite interaction strengths up to  $U = 10$ .

As an independent extension of these low-density results, Chaves and Satija [32] have studied a model of nearest-neighbor interacting spinless fermions [33] at finite particle density in the same quasiperiodic potential by means of Lanczos diagonalization for small systems up to chain size  $M = 13$ . They have found evidence for a critical region. In order to reach much larger system sizes for interacting systems, one can employ the numerical density-matrix renormalization group (DMRG) [34]. With the DMRG the ground state properties in 1D can be obtained very accurately [35,36]. In a recent paper [37], we studied the quasiperiodic model of reference [32] at various densities and interaction strengths  $V$  by DMRG. We compare the results with the present TIP data at the end of the paper.

The paper is organized as follows. In Section 2 we describe the Hamiltonian of our TIP system and explain how to obtain the TIP localization lengths *via* the decimation method. In Section 3, we comment on the particular finite-size-scaling method employed and present the estimated critical parameters. We summarize and conclude in Section 4.

## 2 The TIP system and the numerical approach

The Hamiltonian for TIP in the 1D quasiperiodic potential of the Aubry-André model is given as

$$\mathbf{H} = \sum_{n,m} |n, m\rangle \langle n+1, m| + |n, m\rangle \langle n, m+1| + \text{h.c.} \\ + |n, m\rangle [\mu_n + \mu_m + U(n, m)] \langle n, m|. \quad (1)$$

Here  $\mu_m \equiv 2\mu \cos(\alpha m + \beta)$  is the quasiperiodic potential of strength  $\mu$  with  $\alpha/2\pi$  being an irrational number.  $\beta$  is an arbitrary phase shift and we choose  $\alpha/2\pi = (\sqrt{5}-1)/2$ , *i.e.*, the inverse of the golden mean. This value of  $\alpha/2\pi$  may be approximated by the ratio of successive Fibonacci numbers —  $F_n = F_{n-2} + F_{n-1} = 0, 1, 2, 3, 5, 8, 13, \dots$  — as is customary in the context of quasiperiodic systems [38]. The Hubbard onsite interaction matrix  $U(n, m)$  is diagonal, *i.e.*,  $U(n, m) = U\delta_{nm}$ . The indices  $n$  and  $m$  correspond to the positions of each particle on a chain of length  $M$ . Now we use the decimation method [20,39] to construct an effective Hamiltonian for the diagonal of the  $M \times M$  lattice along which the cigar-shaped TIP wave function has its largest extent [25,31]. The quantity of interest is the TIP localization length  $\lambda_2$  defined by the TIP Green function  $\mathbf{G}_2(E)$  [26]:

$$\frac{1}{\lambda_2} = -\frac{1}{|M-1|} \ln |\langle 1, 1 | \mathbf{G}_2 | M, M \rangle|. \quad (2)$$

For TIP in 1D and 2D random potentials, this approach has led to high precision results supporting the proposed

increase of the TIP localization lengths due to the repulsive interaction [20,21]. We remark that similar data have also been obtained for nearest-neighbor [26] and long-ranged interactions [24].

The correlation length  $\xi_\infty$  for the infinite system may be obtained from the localization lengths  $\lambda(M)$  for finite system sizes by the using one-parameter scaling hypothesis  $\Lambda_M = f(M/\xi_\infty)$  [40] for the reduced localization lengths  $\Lambda_M = \lambda(M)/M$ . The MIT is characterized by a divergent correlation length  $\xi_\infty(\mu) \propto |\mu - \mu_c|^{-\nu}$  [1]. In order to reliably extract the critical parameters from the calculated values of  $\lambda_2(M)$  one may apply a finite-size-scaling procedure [22] that numerically minimizes deviations of the data from the common scaling curve  $f$ . The critical exponent  $\nu$  can then be extracted by fitting the  $\xi_\infty$  obtained from finite-size scaling [41,42]. This method was used previously [14] for finding the critical parameters of the present model.

Higher accuracy can be achieved by a method applied recently [41–44] to the MIT in the Anderson model of localization. We construct a family of fit functions which include corrections to scaling such as (i) nonlinearities of the dependence of the scaling variable on the quasiperiodic potential strength and (ii) an irrelevant scaling variable which accounts for a shift of the crossing point of the  $\Lambda_M(\mu)$  curves as a function of  $\mu$ , *i.e.*,

$$\Lambda_M = \tilde{f}(\chi_r M^{1/\nu}, \chi_i M^y), \quad (3)$$

where  $\chi_r$  and  $\chi_i$  are the relevant and irrelevant scaling variables, respectively.  $\tilde{f}$  is then Taylor expanded up to order  $n_i$  in terms of the second argument

$$\Lambda_M = \sum_{n=0}^{n_i} \chi_i^n M^{ny} \tilde{f}_n(\chi_r M^{1/\nu}), \quad (4)$$

and each  $\tilde{f}_n$  is Taylor expanded up to order  $n_r$ :

$$\tilde{f}_n = \sum_{i=0}^{n_r} a_{ni} \chi_r^i M^{i/\nu}. \quad (5)$$

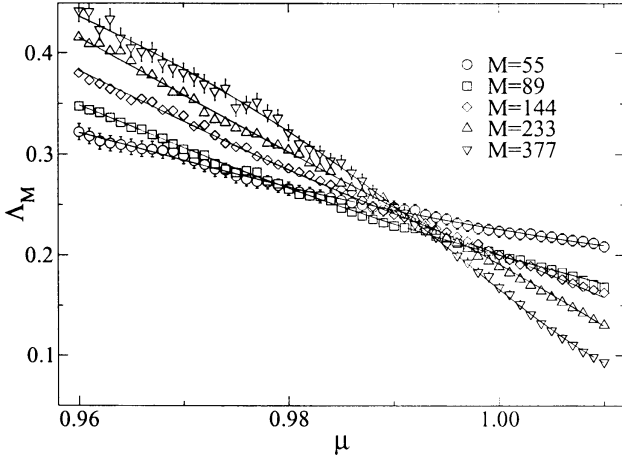
Nonlinearities are taken into account by expanding  $\chi_r$  and  $\chi_i$  in terms of  $u = (\mu_c - \mu)/\mu_c$  up to order  $m_r$  and  $m_i$ , respectively,

$$\chi_r(u) = \sum_{n=1}^{m_r} b_n u^n, \quad \chi_i(u) = \sum_{n=0}^{m_i} c_n u^n, \quad (6)$$

with  $b_1 = c_0 = 1$ . The fit function is being adjusted to the data by choosing the orders  $n_i, n_r, m_r, m_i$  up to which the expansions are carried out. Of course, the orders have to be taken not too large to keep the number of fit parameters  $a_{ni}, b_n$ , and  $c_n$  reasonably small.

## 3 Numerical results for TIP

We calculate  $\lambda_2$  at energy  $E = 0$  for 20 values of the Hubbard interaction, *i.e.*,  $U = 0$  (the non-interacting single-particle case), 0.1,  $\dots$ , 0.9, 1, 2,  $\dots$ , 10 for 6 system sizes  $M = 13, 21, 34, 55, 89, 144$ . For  $U = 0$  and 1,

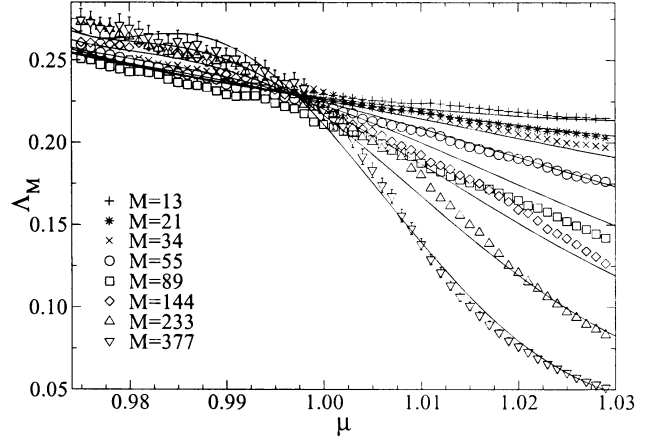


**Fig. 1.** Reduced localization lengths  $\Lambda_M$  versus quasiperiodic disorder strength  $\mu$  for  $U = 0$ . For clarity, only error bars for  $M = 55$  and  $377$  are given. The lines are the fits to the data given by equation (3).

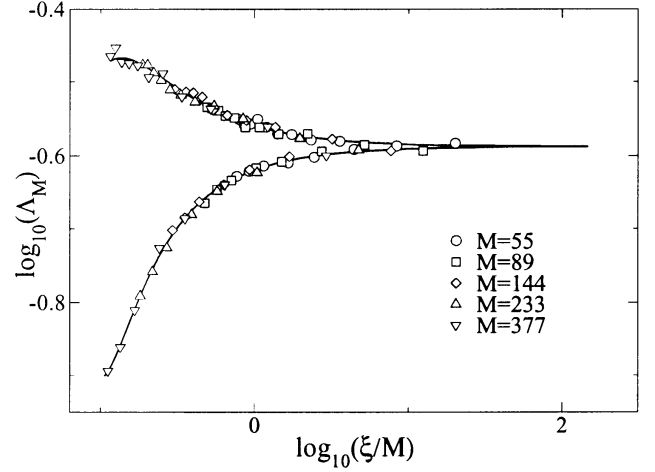
we also have data for  $M = 233$  and  $377$ . The quasiperiodic potential strengths  $\mu$  is chosen close to the single-particle transition at  $\mu_c \approx 1$  and ranges typically from 0.95 to 1.05. As in reference [14] we average the results over different randomly chosen phase shifts  $\beta$  in order to reduce the fluctuations. The number of  $\beta$  values used in this averaging ranges from 5000 for  $M = 13$  to 1000 for  $M = 377$ . In order to perform the non-linear fit necessary for the finite-size-scaling procedure as outlined in Section 2, we use the Levenberg-Marquardt method [44,45]. As the decimation-method data — like the transfer-matrix-method results [14] — are still rather noisy we have to suitably limit the ranges of the quasiperiodic potential strength  $\mu$  and/or the system sizes  $M$  used for fitting the data.

For  $U = 0$  and 1, which were examined by the transfer-matrix method in detail [14], the best fit is obtained for  $n_r = 3$ ,  $n_i = 2$ ,  $m_r = 2$  and  $m_i = 1$ . For  $U = 0$  we use the data for  $\mu$  ranging from 0.96 to 1.01 and  $M = 55, 89, 144, 233$ , and  $377$ ; for  $U = 1$  we use all system sizes  $M = 13, \dots, 377$  and  $0.97 \leq \mu \leq 1.05$ . Figures 1 and 2 show the resulting TIP localization lengths for  $U = 0$  and 1. Also shown are the fits of the finite-size-scaling curves to the data as given by equation (3) for  $U = 0$  and 1, respectively. We find that for both  $U$  values, there is an apparent transition close to  $\mu_c = 1$ . For the case  $U = 0$ , we also observe a systematic shift of the crossing point with increasing system sizes necessitating the inclusion of an irrelevant scaling variable as discussed in Section 2. The transition point is not so clearly distinguished for  $U = 1$ , albeit the different behavior for  $\mu \leq 1$  and  $\mu \geq 1$ , namely the increase and decrease, respectively, of  $\Lambda_M$  with increasing  $M$ , is clearly seen.

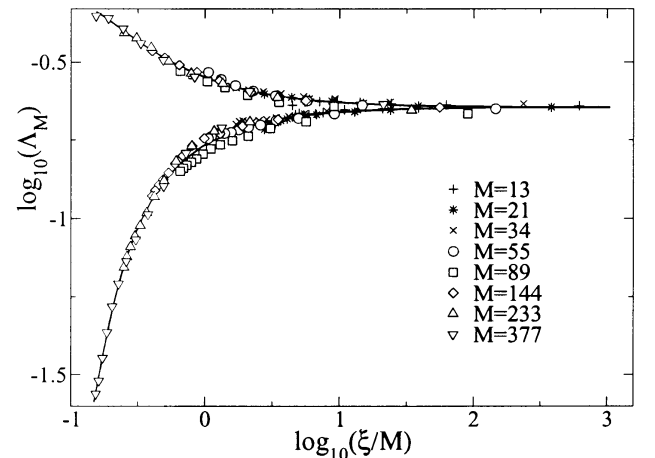
The corresponding plots of the scaling curves are displayed in the Figures 3 and 4. The scaling curves are much better than reported previously [14] for the transfer-matrix-method data. The critical parameters can consequently be estimated to be  $\mu_c = 0.989 \pm 0.001$ ,



**Fig. 2.** Reduced localization lengths  $\Lambda_M$  versus quasiperiodic disorder strength  $\mu$  for  $U = 1$ . For clarity, only error bars for  $M = 377$  are given. The lines are the fits to the data given by equation (3).



**Fig. 3.** Scaling function (solid line) and scaled data points for  $U = 0$ . For clarity only every 3rd data point is represented by a symbol.



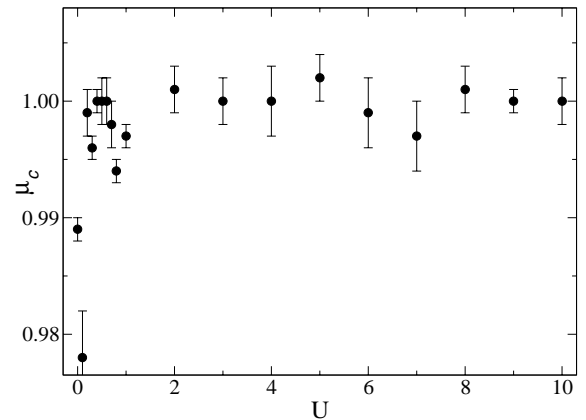
**Fig. 4.** Scaling function (solid line) and scaled data points for  $U = 1$ . For clarity only every 3rd data point is represented by a symbol.

**Table 1.** Values of the critical quasiperiodic disorder strength  $\mu_c$  and the critical exponent  $\nu$  obtained by the non-linear fit for various  $U$  values. The first row for each  $U$  gives values and the orders  $n_i$ ,  $m_i$ , used in the expansion (4–6), for which the best fits have been obtained. In all cases we find  $n_r = 3$  and  $m_r = 2$ . For  $\mu$  and  $M$  the range of the values which were used in the fit is given. The second row contains values of the critical parameters obtained from a weighted average of fits for various choices of  $n_i$  and  $m_i$ .

$U$	$\mu$	$M$	$n_i$	$m_i$	$\mu_c$	$\nu$
0	0.96 – 1.01	55 – 377	2	1	$0.989 \pm 0.001$	$1.00 \pm 0.15$
	0.95 – 1.05	13 – 377	0 – 2	0 – 1	$0.99 \pm 0.02$	$1.3 \pm 0.5$
1	0.97 – 1.05	13 – 377	2	1	$0.997 \pm 0.001$	$1.19 \pm 0.16$
	0.95 – 1.05	13 – 377	0 – 2	0 – 1	$0.99 \pm 0.01$	$1.3 \pm 0.4$
2	0.97 – 1.05	55 – 144	0	0	$1.001 \pm 0.002$	$1.14 \pm 0.11$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$0.99 \pm 0.02$	$1.5 \pm 1$
3	0.95 – 1.05	13 – 144	2	1	$1.000 \pm 0.002$	$1.16 \pm 0.08$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.02$	$1.8 \pm 1$
4	0.97 – 1.05	55 – 144	0	0	$1.000 \pm 0.003$	$1.12 \pm 0.10$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.01$	$1.5 \pm 0.8$
5	0.95 – 1.05	13 – 144	1	1	$1.002 \pm 0.002$	$1.20 \pm 0.09$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.01$	$1.2 \pm 0.3$
6	0.95 – 1.05	55 – 144	0	0	$0.999 \pm 0.002$	$1.28 \pm 0.08$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.02$	$1.3 \pm 0.1$
7	0.95 – 1.05	55 – 144	0	0	$0.997 \pm 0.002$	$1.28 \pm 0.07$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.01$	$1.5 \pm 0.6$
8	0.97 – 1.05	55 – 144	0	0	$1.001 \pm 0.002$	$1.16 \pm 0.08$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$0.99 \pm 0.02$	$1.4 \pm 0.4$
9	0.97 – 1.05	13 – 144	1	1	$1.000 \pm 0.001$	$1.15 \pm 0.05$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.01$	$1.4 \pm 0.5$
10	0.97 – 1.05	55 – 144	0	0	$1.000 \pm 0.002$	$1.23 \pm 0.08$
	0.95 – 1.05	13 – 144	0 – 2	0 – 1	$1.00 \pm 0.01$	$1.4 \pm 0.4$

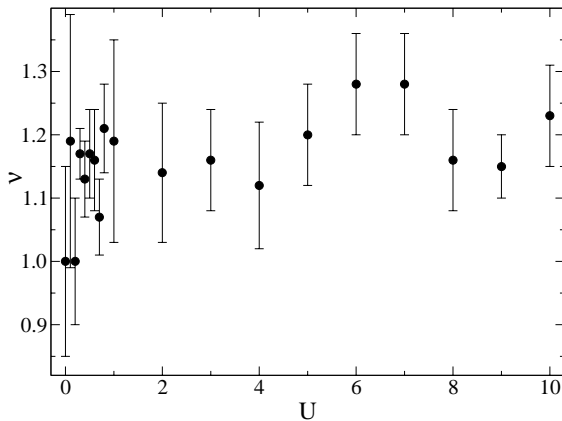
$\nu = 1.00 \pm 0.15$  for  $U = 0$  and  $\mu_c = 0.997 \pm 0.001$ ,  $\nu = 1.19 \pm 0.16$  for  $U = 1$ . The irrelevant scaling exponents are close to  $y = 1.8 \pm 0.2$  and  $y = 0.15 \pm 0.1$  for  $U = 0$  and 1, respectively. Note that the quoted errors correspond to the standard deviations estimated from the non-linear fit procedure. In this way the accuracy is significantly overestimated. Since it is *a priori* not clear, which values  $n_i, n_r, m_r, m_i$  to use, we estimate the true errors from a comparison of various fits with different  $n_i, n_r, m_r, m_i$ . Even in the case of extremely high precision data close to the MIT in the Anderson model of localization, this has been shown [44] to increase the error by one order of magnitude. Therefore we conclude that the interaction strength  $U$  for TIP does not influence the MIT in the quasiperiodic potential within the accuracy of the present calculation.

Further results for larger  $U$  values are collected in Table 1. The expansion orders  $n_i, n_r, m_r, m_i$ , the system sizes and ranges of the quasiperiodic potential strength have been chosen in order to minimize the  $\chi^2$  statistics and to get the most convincing scaling fit. Furthermore, one has to check that various initial parameters ( $a_n, b_n, c_n$ ) converge to the same values of the critical quasiperiodic potential strength  $\mu_c$  and the critical exponent  $\nu$ . Figures 5 and 6 show the values obtained in this way. For almost



**Fig. 5.** The critical quasiperiodic potential strength  $\mu_c$  versus Hubbard interaction strength  $U$ . Error bars mark the errors resulting from the Levenberg-Marquardt method of the non-linear fit.

all cases the critical quasiperiodic potential strength  $\mu_c$  remains close to 1, the only exceptions are  $U = 0$  and 0.1, when  $\mu_c = 0.99$  and 0.98, respectively. However, since we know that the transition in the single-particle case is



**Fig. 6.** The critical exponent  $\nu$  versus Hubbard interaction strength  $U$ . Error bars mark the errors resulting from the Levenberg-Marquardt method of the non-linear fit.

exactly at  $\mu_c = 1$  [28], this observation can be used to estimate the true error of the estimate for  $\mu_c$ . Thus comparing with the  $\mu_c$  estimates for  $U \neq 0$ , we find that the errors calculated within the non-linear fitting procedure are significantly underestimated as discussed above. We therefore conclude that within the accuracy of our calculation there is no change of the critical quasiperiodic potential strength  $\mu_c$  for the Hubbard interaction in the range  $0 \leq U \leq 10$ . The same argument leads to the conclusion that within the error bars the critical exponent  $\nu$  does not change with the Hubbard interaction strength and is close to 1. This is in agreement with the previous results obtained by the transfer-matrix method and finite-size scaling [14]. We stress that the critical exponents can only be obtained with much less accuracy than the transition point  $\mu_c$  as shown in Table 1.

## 4 Conclusions

In this work, we have studied the interplay of disorder and interactions for a quantum system at very low density (TIP). We calculated the pair localization lengths for a quasiperiodic potential and Hubbard interaction by means of the decimation method and extracted the critical parameters from the fit using the one-parameter scaling hypothesis. For both non-interacting particles as well as onsite interaction we obtain the value of the critical quasiperiodic potential strength  $\mu_c = 1$  and the critical exponent  $\nu \approx 1$  in agreement with the previous results of transfer-matrix-method calculations and finite-size scaling [14]. The results for  $U > 1$  show that this conclusion remains valid also for much stronger interactions.

Let us briefly compare these results to the finite density situation. For  $N$  interacting spinless fermions on a 1D ring of circumference  $M$  with Aubry-André onsite potential  $\mu$  and nearest-neighbour interaction  $V$  it is possible to treat system lengths up to about  $M \approx 100$ –200 using the DMRG. We applied [37] the finite lattice algorithm for non-reflectionsymmetric models as described in [46]. For

a system of free fermions at finite density like  $\rho = 1/2$  (incommensurate compared to the wave vector of the quasiperiodic potential — an irrational multiple of  $\pi$ ), we reproduced [37] the expected transition at  $\mu_c = 1$  in agreement with references [14, 32]. For attractive and repulsive interactions at  $\rho = 1/2$  the numerical results are available for only two system sizes ( $M = 34$  and 144), therefore conclusions about these regimes appear rather speculative. At commensurate densities  $\rho_i \approx \lim_{n \rightarrow \infty} F_{n-i}/F_n \approx 0.618, 0.382, 0.236,$  and  $0.146$  — corresponding to  $i = 1, \dots, 4$  — and in the repulsive regime (nearest-neighbour interaction  $V > 0$ ), the ground state is localized for  $\mu > 0$  [37] in agreement with previous studies for disordered and periodically disturbed systems [15, 36]. The above increase of the localization lengths as predicted by the arguments for TIP [10] is most likely too small [16] to be detected by the present accuracy. For attractive interactions  $V$ , all densities  $\rho_i$  and  $\mu \rightarrow 0$ , the system shows a *Peierls-like* transition from insulating to metallic phase at  $V \approx -1.4$  [37] in agreement with the weak-coupling renormalization group treatment [47] of spinless fermions on a Fibonacci lattice.

In conclusion, we have studied the influence of interactions on an MIT in a quasiperiodic model in 1D. Our results suggest that the delocalization found for low density TIP in the localized phase cannot simply be extrapolated to the finite-density situation. At finite densities, other effects such as a Peierls-like commensurability become important and dominate the transport properties.

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