Localization properties of two interacting particles in a quasiperiodic 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.

1. Introduction

The physics of a metal-insulator transition (MIT) in disordered electronic systems has been the subject of intense research activities over the last two decades and still receives much attention. The scaling hypothesis of localization [1] can successfully predict many of the universal features of the MIT for free electrons in disordered systems [2]. However, the influence of many-particle interactions on the MIT is much less understood [3] with recent investigations of an apparent MIT in two-dimensional (2D) systems even questioning 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]. In general, these investigations have shown that changes in the wave function interferences due to many-particle interactions [15, 16] can lead to a rather large enhancement of the localization lengths in 1D and 2D [17–19].

The standard approach for computing localization lengths in disordered, non-interacting systems is the transfer-matrix method (TMM) [20]. It has been used for investigations of the enhancement of the TIP localization length in a 1D random potential [12, 21] 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, 22], exact diagonalization [23] or Green function approaches [18, 24, 25].

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 μ [26]. 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 using the TMM approach and a careful finite-size-scaling analysis [14] following earlier analytical work [27, 28]. We showed that the model for TIP exhibits an MIT as a function of μ at $\mu_c = 1$

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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 ν of the correlation length, is also not affected by the interaction [14] and within the error margin $\nu = 1$. However, it has been demonstrated [12, 18] that a TMM approach applied to the TIP problem without finite-size scaling leads to unreliable localization lengths, i.e., it systematically overestimates the TIP localization length λ_2 in finite-sized samples in the case of vanishing interaction ($U = 0$). In addition, simple extrapolations to infinite sample size [12, 21] may lead to an underestimation of λ_2 [29]. An alternative approach, which does not suffer from the above problem, is based on the decimation method (DM) and has also been applied recently to TIP in a 1D random potential [18]. This encouraged us to reexamine the localization lengths for TIP in 1D quasiperiodic potentials with Hubbard interaction with the DM [30] We have found that the general conclusions of reference [14] remain valid, i.e., the MIT is not affected by the 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 $U = 10$.

In this paper we present the TIP localization lengths obtained via DM for different Hubbard interaction strengths. We compare the critical parameters estimated from different finite-scaling methods and extracted from the TMM results.

2. The TIP system

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

$$\begin{aligned}\mathbf{H} = \sum_{n,m} &|n,m\rangle\langle n+1,m| + |n,m\rangle\langle n,m+1| + \text{h. c.}\\ &+ |n,m\rangle\left[\mu_n + \mu_m + U(n,m)\right]\langle n,m| \,. \end{aligned} \tag{1}$$

Here $\mu_m \equiv 2\mu\cos(\alpha m + \beta)$ is the quasiperiodic potential of strength μ with $\alpha/2\pi$ being an irrational number which we choose as the inverse of the golden mean: $\alpha/2\pi = (\sqrt{5}-1)/2$. This value of $\alpha/2\pi$ may be approximated by the ratio of successive Fibonacci numbers — $F_n = F_{n-2} + F_{n-1} = 0, 1, 2, 3, 5, 8, 13, \ldots$ — as is customary in the context of quasiperiodic systems [31]. An arbitrary phase shift of the potential is denoted as β. 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.

We use the DM [18, 32] 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 [23, 29]. The quantity of our interest is the TIP localization length λ_2 defined by the TIP Green function $\mathbf{G_2}(E)$ [24]:

$$\frac{1}{\lambda_2} = -\frac{1}{|M-1|}\ln|\langle 1,1|\mathbf{G_2}|M,M\rangle|. \tag{2}$$

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 [18, 19].

The correlation length ξ_∞ for the infinite system may be obtained from the localization lengths $\lambda(M)$ for finite system sizes by using the one-parameter scaling hypothesis $\Lambda_M = f(M/\xi_\infty)$ [33] for the reduced localization lengths $\Lambda_M = \lambda(M)/M$. The MIT is characterized by a divergent correlation length $\xi_\infty(\mu) \propto |\mu - \mu_c|^{-\nu}$ [2]. In order to extract the critical parameters from the calculated values of $\lambda_2(M)$ one may apply a finite-size-scaling procedure [20] that numerically minimizes deviations of the data from the common scaling curve f. The critical exponent ν can then be calculated by fitting the ξ_∞ obtained from finite-size scaling. This method was used in [14] to find the critical parameters for the TIP in a quasiperiodic potential from the localization lengths calculated by means of TMM.

Higher accuracy can be achieved by a method applied recently [34, 35] 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 μ, i.e.,

$$\Lambda_M = \tilde{f}(\chi_{\rm r} M^{1/\nu}, \chi_{\rm i} M^y). \tag{3}$$

where $\chi_{\rm r}$ and $\chi_{\rm i}$ are the relevant and irrelevant scaling variables, respectively. $\tilde{f}$ is then Taylor expanded up to order $n_{\rm i}$ in terms of the second argument

$$\Lambda_M = \sum_{n=0}^{n_{\rm i}} \chi_{\rm i}^n M^{ny} \tilde{f}_n(\chi_{\rm r} M^{1/\nu}), \tag{4}$$

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

$$\tilde{f}_n = \sum_{i=0}^{n_{\rm r}} a_{ni} \chi_{\rm r}^i M^{i/\nu}. \tag{5}$$

Nonlinearities are taken into account by expanding $\chi_{\rm r}$ and $\chi_{\rm i}$ in terms of $u = (\mu_{\rm c} - \mu)/\mu_{\rm c}$ up to order $m_{\rm r}$ and $m_{\rm i}$, respectively,

$$\chi_{\rm r}(u) = \sum_{n=1}^{m_{\rm r}} b_n u^n, \quad \chi_{\rm i}(u) = \sum_{n=0}^{m_{\rm i}} c_n u^n, \tag{6}$$

with $b_1 = c_0 = 1$. The fit function is being adjusted to the data by choosing the orders $n_{\rm i}, n_{\rm r}, m_{\rm r}, m_{\rm i}$ 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 have calculated λ_2 at energy $E = 0$ for 20 values of the Hubbard interaction, i.e., $U = 0$ (the non-interacting single-particle case), 0.1, ..., 0.9, 1, 2, ..., 10 for 6 system sizes $M = 13$, 21, 34, 55, 89, 144. For $U = 0$ and 1, we also obtained the data for $M = 233$ and 377. The quasiperiodic potential strengths μ were chosen close to the single-particle transition at $\mu_{\rm c} \approx 1$ and ranged typically from 0.95 to 1.05. Following the reference [14] we averaged the results over different randomly chosen phase shifts β to reduce the fluctuations and improve the scaling. The number of β values used in this averaging ranged from 5000 for $M = 13$ to 1000 for $M = 377$.

In order to directly compare the results of the TMM and decimation method we applied to the data collected for $U = 0$ and $U = 1$ the same procedure as used in [14] to extract the critical parameters from the TMM results. The critical parameters estimated from the DM data are $\mu_{\rm c} = 0.99 \pm 0.03$, $\nu = 1.04 \pm 0.2$ for $U = 0$ and $\mu_{\rm c} = 1.00 \pm 0.02$, $\nu = 1.2 \pm 0.2$ for $U = 1$. In [14] we obtained from the TMM data $\mu_{\rm c} = 1.01 \pm 0.02$ for $U = 0$ and $\mu_{\rm c} = 1.04 \pm 0.04$ for $U = 1$; the critical exponent was $\nu = 0.8 \pm 0.2$ both for $U = 0$ and $U = 1$. Thus the critical parameters extracted from the TMM or DM data are the same within the estimated accuracy.

For all data collected from the DM calculations we applied the non-linear fit necessary for the finite-size-scaling procedure described in section 2; the Levenberg-Marquardt method [35, 36] was used. As the DM data — like the TMM results [14] — are still rather noisy we

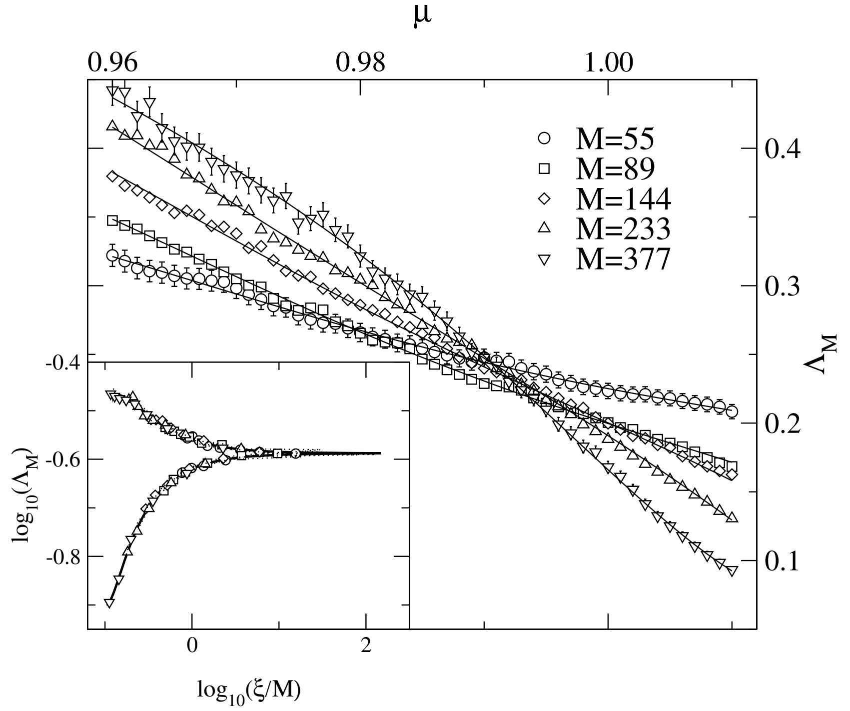

Figure 1. Reduced localization lengths Λ_M versus quasiperiodic disorder strength μ for $U = 0$. For clarity, only error bars for $M = 55$ and 377 are given. The lines are the fits to the data given by (3). Inset: scaling function (solid line) and scaled data points; only every 3rd data point is represented by a symbol.

had to suitably limit the ranges of the quasiperiodic potential strength μ and/or the system sizes M used for fitting the data.

For $U = 0$ and 1, which were examined by the TMM in detail [14], the best fit was obtained for $n_r = 3$, $n_i = 2$, $m_r = 2$ and $m_i = 1$. For $U = 0$ we used the data for μ ranging from 0.96 to 1.01 and $M = 55, 89, 144, 233$, and 377; for $U = 1$ we used all system sizes $M = 13, \ldots, 377$ and $0.97 \leq \mu \leq 1.05$.

Figure 1 and figure 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 (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 Λ_M with increasing M, is clearly seen.

The corresponding plots of the scaling curves are displayed in the insets of figures 1 and 2. The scaling curves are much better than reported previously [14] for the TMM data. The critical parameters can consequently be estimated to be $\mu_c = 0.989 \pm 0.001$, $\nu = 1.00 \pm 0.15$ 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 apriori 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 [35] to increase the error by one

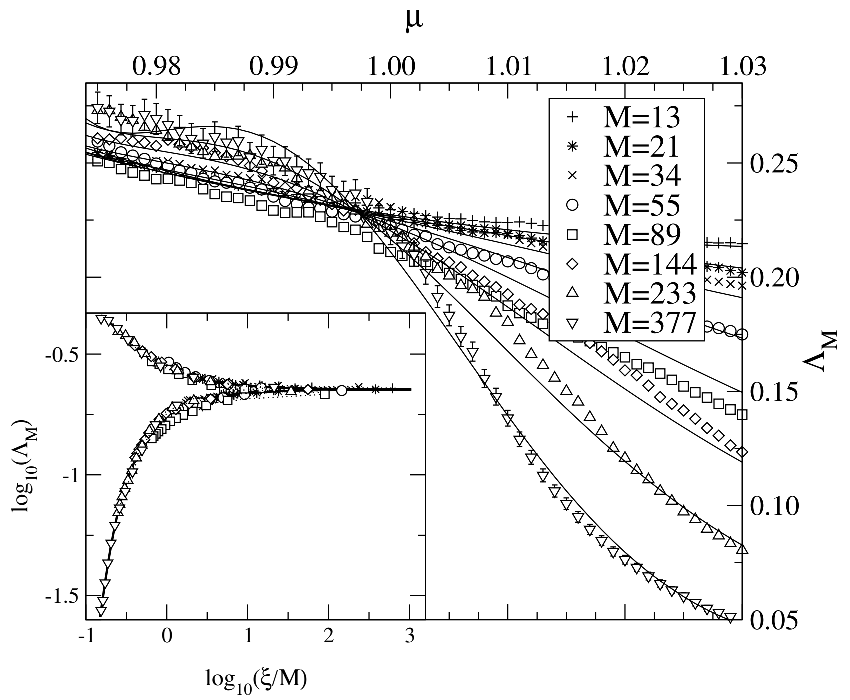

Figure 2. Reduced localization lengths Λ_M versus quasiperiodic disorder strength μ for $U = 1$. For clarity, only error bars for $M = 377$ are given. The lines are the fits to the data given by (3). Inset: scaling function (solid line) and scaled data points; only every 3rd data point is represented by a symbol

order of magnitude. Further results for other 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 χ^2 statistics and to get the most convincing scaling fit.

Figure 3 and figure 4 show the values of the critical quasiperiodic potential strength μ_c and the critical exponent ν. For almost all cases the critical quasiperiodic potential strength μ_c remains close to 1, the only exceptions are $U = 0, 0.1$ and 0.9, when $\mu_c = 0.99, 0.98$ and 1.015 respectively. However, since we know that the transition in the single-particle case is exactly at $\mu_c = 1$ [26], this observation can be used to estimate the true error of the estimate for μ_c. Thus comparing with the μ_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 μ_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 ν does not change with the Hubbard interaction strength and is close to 1. This is in agreement with the previous results obtained by the TMM and finite-size scaling [14]. We stress that the critical exponents can only be obtained with much less accuracy than the transition point μ_c as shown in table 1 and figure 4.

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 DM and extracted the critical parameters from the fit using the one-parameter scaling hypothesis. For both non-interacting particles as

Table 1. Values of the critical quasiperiodic disorder strength μ_c and the critical exponent ν obtained by the non-linear fit for various U values. The 4th and 5th columns for each U give 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 μ and M the range of the values which were used in the fit is given.

U	μ	M	n_i	m_i	μ_c	ν
0	0.96 − 1.01	55 − 377	2	1	0.989 ± 0.001	1.00 ± 0.15
0.1	0.97 − 1.01	55 − 144	0	0	0.978 ± 0.004	1.19 ± 0.40
0.2	0.97 − 1.05	13 − 144	1	1	0.999 ± 0.002	1.00 ± 0.10
0.3	0.95 − 1.05	13 − 144	1	1	0.996 ± 0.001	1.17 ± 0.04
0.4	0.97 − 1.05	13 − 144	1	1	1.000 ± 0.001	1.13 ± 0.06
0.5	0.95 − 1.05	55 − 144	0	0	1.000 ± 0.002	1.17 ± 0.07
0.6	0.95 − 1.05	55 − 144	0	0	1.000 ± 0.002	1.16 ± 0.08
0.7	0.97 − 1.05	13 − 144	2	1	0.998 ± 0.002	1.07 ± 0.06
0.8	0.97 − 1.05	13 − 144	2	1	0.994 ± 0.001	1.21 ± 0.07
0.9	0.98 − 1.02	55 − 144	1	1	1.015 ± 0.002	1.15 ± 0.16
1	0.97 − 1.05	13 − 377	2	1	0.997 ± 0.001	1.19 ± 0.16
2	0.97 − 1.05	55 − 144	0	0	1.001 ± 0.002	1.14 ± 0.11
3	0.95 − 1.05	13 − 144	2	1	1.000 ± 0.002	1.16 ± 0.08
4	0.97 − 1.05	55 − 144	0	0	1.000 ± 0.003	1.12 ± 0.10
5	0.95 − 1.05	13 − 144	1	1	1.002 ± 0.002	1.20 ± 0.09
6	0.95 − 1.05	55 − 144	0	0	0.999 ± 0.002	1.28 ± 0.08
7	0.95 − 1.05	55 − 144	0	0	0.997 ± 0.002	1.28 ± 0.07
8	0.97 − 1.05	55 − 144	0	0	1.001 ± 0.002	1.16 ± 0.08
9	0.97 − 1.05	13 − 144	1	1	1.000 ± 0.001	1.15 ± 0.05
10	0.97 − 1.05	55 − 144	0	0	1.000 ± 0.002	1.23 ± 0.08

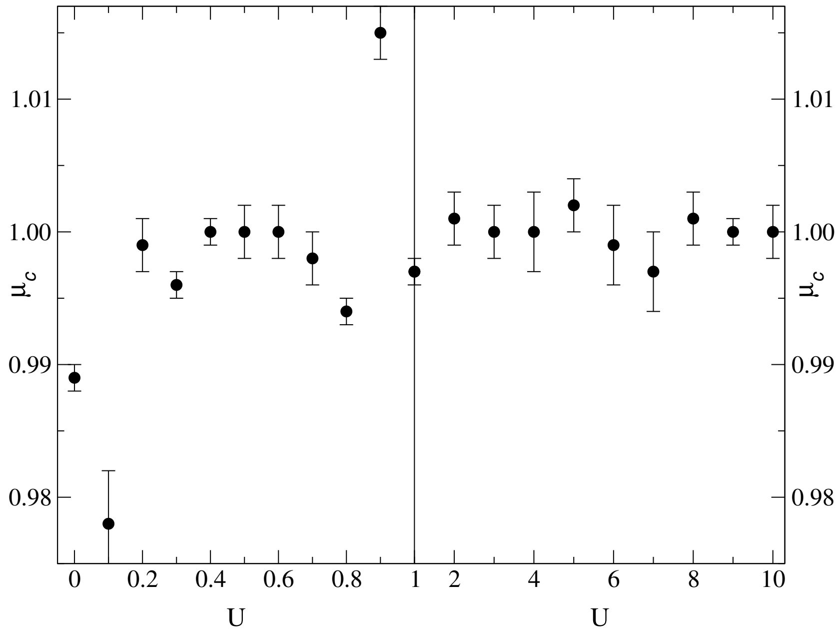

Figure 3. The critical quasiperiodic potential strength μ_c versus Hubbard interaction strength U. Error bars mark the errors resulting from the Levenberg-Marquardt method of the non-linear fit.

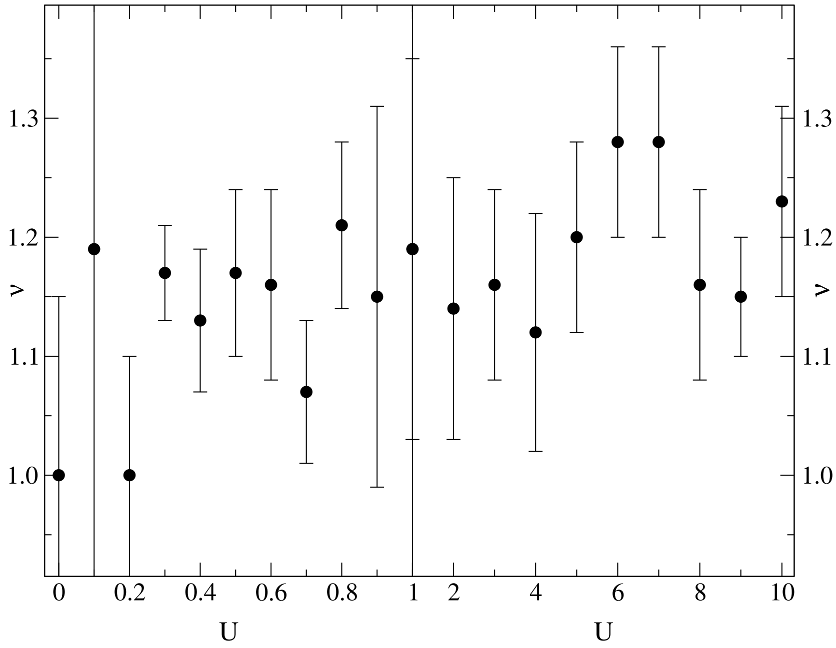

Figure 4. The critical exponent ν versus Hubbard interaction strength U. Error bars mark the errors resulting from the Levenberg-Marquardt method of the non-linear fit.

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 TMM calculations and finite-size scaling [14]. The results for $U > 1$ show that this conclusion remains valid also for much stronger interactions.

For the finite density case of N interacting spinless fermions on a 1D ring of circumference M with Aubry-André onsite potential μ and nearest-neighbour interaction V it is possible to treat system lengths up to about $M \approx 100 - 200$ using the DMRG. We refer the reader to reference [37] for a more detailed discussion of this case.

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