

Enhanced compressibility due to repulsive interaction in the Harper model

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We study the interplay between a repulsive interaction and an almost staggered on-site potential in one dimension. Specifically, we address the Harper model for spinless fermions with nearest-neighbor repulsion, close to half filling. Using the density matrix renormalization group, we find that, in contrast to standard behavior, the system becomes more compressible as the repulsive interaction is increased. By deriving a low-energy effective model, we unveil the effect of interactions using mean-field analysis: The density of a narrow band around half filling is anticorrelated with the on-site potential, whereas the density of lower occupied bands follows the potential and strengthens it. As a result, the states around half filling are squeezed by the background density, their band becomes flatter, and the compressibility increases.

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There has been much interest in the influence of electron-electron (e - e) interactions on the compressibility of electronic systems. This interest is motivated by the intricate many-body physics revealed by the behavior of the compressibility, as well as by the technological challenge of building field effect transistors with a larger capacitance, essential for lower power consumption and quicker clock rates [1,2].

The compressibility of an electronic system, i.e., the change in the number of electrons residing in a system as the chemical potential is varied, can be measured via capacitive coupling to another metallic system. Alternatively, the system can be weakly coupled to a plunger gate and leads. Jumps in the current that passes through the leads as a function of the gate voltage count the number of electrons in the system as a function of the chemical potential. In the context of quantum dots, this is known as the addition spectrum [3].

Compressibility is measurable also in highly controlled many-body systems such as molecular manipulation on metal surfaces [4] and ultracold atoms and ions in optical lattices [5–8]. In optical lattices, transport measurements are challenging. Nevertheless, squeezing the trapping potential acts on the density as a variation of the chemical potential, revealing the bulk compressibility [9].

Usually, the influence of repulsive interactions on the ground state of disordered metallic systems is well described by a mean-field theory, which may be reduced to the classical capacitance of the system. Increasing the repulsive interaction then corresponds to reduced capacitance, i.e., the system becomes less compressible, and eventually localizes [10]. This is true even beyond the mean-field treatment, as shown for one-dimensional (1D) Luttinger liquids with $K < 1$ [11], and in zero-dimensional (0D) quantum dots [3]. There are some cases, in clean systems near a Mott transition, where the opposite occurs [12–14]. Interestingly, there are several unexplained counter examples measured in disordered semiconducting dots [15,16].

In this Rapid Communication, we present a simple 1D nonhomogeneous metallic system for which the compressibility *increases* with a weak e - e interaction, i.e., we report on a flow from a metal to localization, driven by a repulsive interaction, that is outside the standard paradigm. Specifically,

we study the Harper (or Aubry-André) model [17,18] of spinless fermions close to half filling with a nearest-neighbor repulsive interaction. The on-site potential is spatially modulated with a frequency of an almost two lattice-sites period, corresponding to a fast modulation with a slow envelope. Using the density matrix renormalization group (DMRG), we numerically extract the inverse compressibility as a function of the density, and find it decreasing with the interaction strength. We analytically show that this effect results from the presence of a flat band at half filling, which is composed of a superlattice of states that reside at the valleys of the potential envelope. The repulsive interaction from occupied lower bands squeezes these valley states, and accordingly, the central band flattens and its compressibility increases. Our approach can be extended to numerous other models, such as disordered systems with fast and slow spatial components of disorder, and Harper models with spin.

The tight-binding Harper model for spinless fermions with nearest-neighbor repulsive interaction is

$$H = \sum_{j=1}^L [t c_j^\dagger c_{j+1} + \text{H.c.} + \lambda \cos(2\pi b j + \phi) n_j + U n_j n_{j+1}], \quad (1)$$

where c_j is the single-particle annihilation operator at site j , $n_j = c_j^\dagger c_j$ is the density, t is a real hopping amplitude, $\lambda > 0$ controls the amplitude of the on-site potential, and $U > 0$ is the strength of the repulsive interaction. The potential is cosine modulated in space with frequency b , and ϕ is an arbitrary phase factor.

The Harper model is a wellspring of physical phenomena, and is therefore under continuous study. For example, when the modulation frequency b is an irrational number, and in the absence of an interaction, a metal-insulator transition takes place as a function of the potential strength at $\lambda = 2t$ [6,18–23]. Much effort has gone into understanding the influence of interactions on this transition [24–27]. Recently, it was also found that for an irrational b , the Harper model is topologically nontrivial, and may have topological boundary states [28–31].

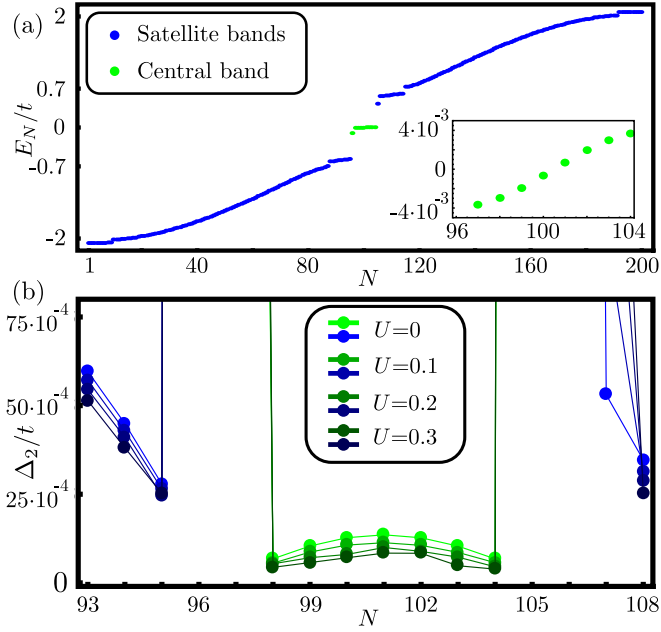


FIG. 1. (Color online) The effect of interactions: (a) The single-particle spectrum of the Harper model [cf. Eq. (1)] with $U = 0$ with an open boundary condition, for $L = 200$, $t = 1$, $\lambda = 0.7$, $\phi = 0.7\pi$, and $b = \sqrt{30}$, which corresponds to $\epsilon \approx -0.023$. The central band (bright green) is almost flat, as seen in the zoom-in inset [35]. (b) The inverse compressibility as a function of the number of particles [cf. Eq. (2)], obtained by DMRG, for various values of interaction strength U . Surprisingly, the central band becomes more compressible as a function of interaction strength U .

Here, we take a different approach, and study the effect of the interplay between the inhomogeneous potential and the interaction on compressibility. Therefore, in the following, we assume that we are in the metallic phase, i.e., $\lambda < 2t$. Moreover, we consider the cases of $b \bmod 1 = 1/2 + \epsilon$ with $|\epsilon| \ll 1/2$, be it rational or irrational. The striking property of such b is that in the vicinity of half filling, the energy spectrum is composed of an almost flat central band separated from the other bands by large gaps, as depicted in Fig. 1(a). Therefore, even a weak interaction may generate interesting phenomena.

The inverse compressibility of a system with N particles $\Delta_2(N)$ is defined as the change in the chemical potential due to the insertion of the N th particle. For many-body systems, it is given by

$$\Delta_2(N) = \mathcal{E}(N) - 2\mathcal{E}(N-1) + \mathcal{E}(N-2), \quad (2)$$

where $\mathcal{E}(N)$ is the system's many-body ground-state energy with N particles. For noninteracting systems at zero temperature, $\Delta_2(N; U = 0) = E_N - E_{N-1}$, where E_N is the N th single-particle eigenenergy.

A finite sized Harper model can be thought of as a quasidisordered 1D quantum (anti)dot. At low temperatures, the inverse compressibility of a disordered quantum dot is usually described by the constant-interaction (CI) model, which has been shown to fit experimental measurements very well [3]. According to this model, $\Delta_2(N) = \Delta_2(N; U = 0) + e^2/C$, where $C \approx L$ is the total capacitance, and $e^2 \approx U$. Thus, an increase in U increases Δ_2 .

We extract $\Delta_2(N)$ of our interacting system using DMRG [32,33]. We choose $b = \sqrt{30}$ and $\phi = 0.7\pi$. The former corresponds to $\epsilon \approx -0.023$ [34]. The system is of length $L = 200$, with $N = 91, 92, \dots, 108$ electrons. For $t = 1$, the potential amplitude is $\lambda = 0.7$, which creates a central band that is very flat, but keeps Δ_2 greater than the numerical accuracy. Interaction strengths of $U = 0.1, 0.2, 0.3$ are considered. The boundary condition is open, since it significantly improves accuracy [32,33]. Keeping 384 target states, we extract the ground-state energy $\mathcal{E}(N)$ for each N . The numerically obtained $\Delta_2(N)$, using Eq. (2), is depicted in Fig. 1(b). The accuracy of Δ_2 drops as U increases, and is about $\pm 3 \times 10^{-4}t$ for $U = 0.3$. Strikingly, the inverse compressibility decreases with increasing U . This implies that the underlying physics is very different than the one of the CI model.

Remarkably, we can reproduce this behavior analytically. First we study the noninteracting case, i.e., $U = 0$. The on-site cosine modulation can be rewritten as $\lambda \cos(2\pi bj + \phi) = \lambda \cos(2\pi \epsilon j + \phi)(-1)^j$. Since $\epsilon \ll 1$, the potential is locally oscillating with modulation frequency $b = 1/2$, while being subject to an amplitude envelope $\lambda(j)$ varying slowly in space with wavelength $1/\epsilon$ [see Fig. 2(a)].

We postulate that the low-energy physics around $E = 0$, and in particular that of the central flat band, is governed by states that minimize both the kinetic and potential energies. The potential energy is minimized by states that reside

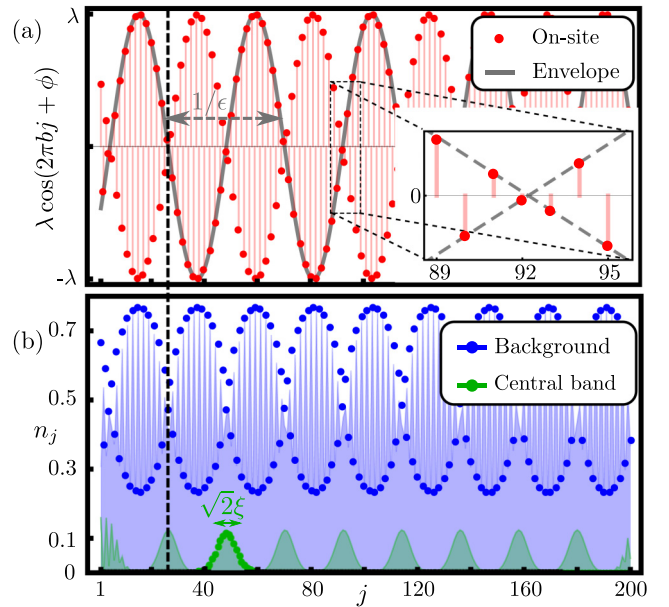


FIG. 2. (Color online) Modulated potential: (a) The on-site potential (red dots) is a product of a fast alternating part and a slow envelope (solid gray line), corresponding to $\cos(2\pi \epsilon j + \phi)$. Inset: At its valleys, the potential is linearly approximated. (b) The density of the central band (green), and the background density of the occupied states below it (blue). The filling corresponds to numerical results, whereas the dots correspond to the analytical expressions [cf. Eqs. (5) and (9), respectively]. The central band is composed of waves of hybridized Gaussians that form a superlattice. Remarkably, the states of the central band reside in the potential valleys, whereas the background density follows the potential peaks.

within the valleys of the potential, where the envelope vanishes, i.e., in the vicinity of $j \approx l_z$, where $2\pi\epsilon l_z + \phi \approx (\mathbb{Z} + 1/2)\pi$. Within the z th valley of the potential, we can linearly approximate the envelope, $\cos(2\pi\epsilon j + \phi) \approx 2\pi|\epsilon|(j - l_z)s_z$, where $s_z = -\text{sgn}[\sin(2\pi\epsilon l_z + \phi)] = \pm 1$. The effective Hamiltonian for a particle confined to the valley is therefore

$$H^{\text{valley}} = \sum_{j=1}^L [t c_j^\dagger c_{j+1} + \text{H.c.} + s_z 2\pi|\epsilon|\lambda(-1)^j(j - l_z)c_j^\dagger c_j] \\ = \int_0^\pi \frac{dk}{2\pi/L} \psi_k^\dagger [2t \cos(k)\sigma_x + s_z 2\pi|\epsilon|\lambda(\hat{p}_k - l_z)\sigma_z] \psi_k, \quad (3)$$

where $\hat{p}_k = i\partial_k$, σ_i are Pauli matrices, and $\psi_k = (c_{ek}, c_{ok})^T$ is the sublattice pseudospinor that splits the lattice into even and odd sites, according to $c_{ek} = \sqrt{2/L} \sum_{j=1}^{L/2} e^{ik2j} c_{2j}$ and $c_{ok} = \sqrt{2/L} \sum_{j=1}^{L/2} e^{ik(2j-1)} c_{2j-1}$.

Around zero kinetic energy, we linearize $\cos(k) \approx -(k - \pi/2)$. Now, using the rotation $\hat{T} = (1 + is_z\sigma_x)/\sqrt{2}$, we rewrite the Hamiltonian in a supersymmetric form,

$$H^{\text{valley}} = \sqrt{8} \frac{t}{\xi} \int_0^\pi \frac{dk}{2\pi/L} (\hat{T} \psi_k)^\dagger \begin{pmatrix} 0 & a_k^\dagger \\ a_k & 0 \end{pmatrix} (\hat{T} \psi_k), \quad (4)$$

where $a_k = -(k - \pi/2)\xi/\sqrt{2} + i(\hat{p}_k - l_z)/\sqrt{2}\xi$, and $\xi^2 = t/(\pi\lambda|\epsilon|)$. Since a_k satisfies $[a_k, a_k^\dagger] = 1$, it is a ladder operator. Remarkably, this momentum-space Hamiltonian is similar to that of the two-dimensional (2D) massless Dirac equation in the presence of a perpendicular magnetic field in the Landau gauge. Using the ladder operators, we find that the energy spectrum of H^{valley} is $\pm\sqrt{8nt}/\xi$, where $n = 0, 1, \dots$ [36]. In particular, there is a zero-energy solution with an eigenstate

$$|l_z\rangle \approx (\pi\xi^2)^{-1/4} \sum_{j=1}^L (s_z)^j S_j e^{-(j-l_z)^2/2\xi^2} |j\rangle, \quad (5)$$

where $|j\rangle = c_j^\dagger |\text{vacuum}\rangle$, $S_j = \sqrt{2} \cos(j\pi/2 - \pi/4) = \dots, 1, 1, -1, -1, 1, 1, \dots$, and we used the fact that $\xi \gg 1$. This wave function is confined to a Gaussian of width ξ around l_z . Notably, the wave functions of the excited states are also confined with the same Gaussian, similar to the eigenstates of the harmonic oscillator [36].

Turning back to the original noninteracting Hamiltonian, there is a superlattice of valleys, each with its corresponding zero-energy state. We expect these states to hybridize and form the central band. The $|l_z\rangle$ states form a basis for this subspace, since $\langle l_z | l_{z\pm 1} \rangle = 0$ and $|\langle l_z | l_{z'} \rangle| \leq e^{-(l_z - l_{z'})^2/2\xi^2} \ll 1$. We can therefore project the Hamiltonian to this subspace. The projected Hamiltonian is given by the matrix elements $\langle l_z | H(U=0) | l_{z'} \rangle$. The diagonal elements $z' = z$ vanish, since $|l_z\rangle$ is of zero energy. The Gaussian decay implies that for $|z' - z| \geq 2$, the matrix elements are negligible. We are therefore left only with $\langle l_z | H(U=0) | l_{z\pm 1} \rangle$, namely, hopping between neighboring valleys. The resulting effective Hamiltonian for the central band is [36]

$$H^{\text{central}} = -\bar{t} \sum_{z=1}^{L_z} c_{l_z}^\dagger c_{l_{z+1}} + \text{H.c.}, \quad (6)$$

where $L_z = [2|\epsilon|L]$ is the number of valleys, and $\bar{t} \approx e^{-\xi^2/(4\xi^2\epsilon^2)} \{2te^{-1/4\xi^2} \sinh[(4\xi^2|\epsilon|)^{-1}] - \lambda e^{-\pi^2\epsilon^2\xi^2}\}$.

Notably, we obtain $\bar{t} \approx 0.0012$, which is slightly smaller than the numerically observed $\bar{t} \approx 0.0019$ [cf. the inset of Fig. 1(a)]. The small discrepancy arises from using the linear approximation of the potential also between the valleys, leading to a too fast decay of the wave function. Substituting $1.16\xi^2$ for ξ^2 in the expression of $\bar{t}$ corrects the bandwidth.

For a periodic boundary condition, the eigenstates of H^{central} are plane waves $|k\rangle = L_z^{-1/2} \sum_{z=1}^{L_z} e^{ikz} |l_z\rangle$ with spectrum $E^{\text{central}}(k) = -2\bar{t} \cos k$, where $k = 2\pi n/L_z$ with $n = 1, \dots, L_z$. Note that these are plane waves of valley Gaussians, as can be seen from Fig. 2(b), which depicts the total density of the central band. Notably, the bandwidth of the central band $4\bar{t}$ is much smaller than the gap to the bands of the first excited states $\sqrt{8t}/\xi$, as seen in Fig. 1(a). Therefore weak interactions and low temperatures will not mix it with the other bands.

At the presence of the repulsive interaction U , the effective model of the central band enables us to describe the increase in compressibility using mean-field theory. Here, $\sum_j n_{j+1} n_j$ is approximated by $\sum_j j[(\langle n_{j+1} \rangle + \langle n_{j-1} \rangle) n_j - \langle n_j \rangle \langle n_{j+1} \rangle - \langle p_j \rangle c_{j+1}^\dagger c_j - \langle p_j \rangle^* c_j^\dagger c_{j+1} + |\langle p_j \rangle|^2]$, with $\langle n_j \rangle$ as the background density, and $\langle p_j \rangle = \langle c_j^\dagger c_{j+1} \rangle$ as the background exchange energy, both created by the occupied satellite bands below the central band. The constant terms do not contribute to $\Delta_2(N)$, and will therefore be ignored. The mean-field approximation adds effective single-particle terms, both on-site potential and hopping, which are modified according to the background density and exchange energy.

We therefore turn to estimate $\langle n_j \rangle$ and $\langle p_j \rangle$, and begin by solving the simplest Hamiltonian of Eq. (1) with $U = \epsilon = 0$. This Hamiltonian describes a uniform staggered potential $(-1)^j \lambda \cos \phi$. Its spectrum is gapped, unless the staggered potential is turned off at $\phi = \pi/2$. If the lower band is fully occupied, then the many-body density is also staggered, $\langle n_j \rangle|_{\epsilon=0} = 1/2 - (-1)^j \bar{n}(\lambda \cos \phi/2t)$, whereas the many-body exchange energy is constant in space $\langle p_j \rangle|_{\epsilon=0} = \bar{p}(\lambda \cos \phi/2t)$, where

$$\bar{n}(x) = \pi^{-1} \text{sgn}(x) K(-x^{-2}), \quad (7)$$

$$\bar{p}(x) = -\pi^{-1} |x| [E(-x^{-2}) - K(-x^{-2})], \quad (8)$$

and $K(x)$ and $E(x)$ are the complete elliptical integrals of the first and second kind, respectively [36].

For $\epsilon \neq 0$, the on-site potential corresponds locally to $(-1)^j$, while $\lambda \cos \phi$ varies slowly in space. Therefore, we expect that the above expressions to remain valid locally and vary slowly in space,

$$\langle n_j \rangle \approx 1/2 - (-1)^j \bar{n}[\lambda \cos(2\pi\epsilon j + \phi)/2t], \quad (9)$$

$$\langle p_j \rangle \approx \bar{p}[\lambda \cos(2\pi\epsilon j + \phi)/2t]. \quad (10)$$

Figure 2(b) depicts the background density $\langle n_j \rangle$ obtained both numerically and analytically, according to Eq. (9), and they fit very well. It can be seen that $\langle n_j \rangle$ follows the cosine modulation. Therefore, between the valleys, $\langle n_j \rangle \approx 1/2 - (-1)^j \bar{n}(\lambda/2t) \cos(2\pi\epsilon j + \phi)$, to first approximation. The background exchange energy $\langle p_j \rangle$ is approximately uniform in space, and thus $\langle p_j \rangle \approx \bar{p}(\lambda/2t)$.

Substituting these simplifications in the mean-field approximation of H , we find that the background density increases the

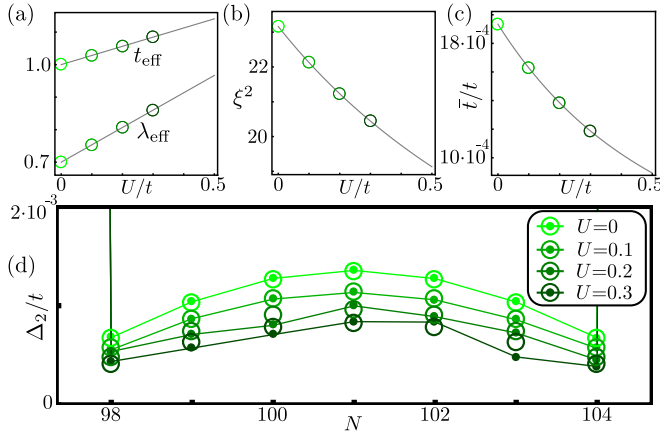


FIG. 3. (Color online) Mean-field theory: (a)–(c) The effect of interaction between the central band and the background density, parametrized by the strength U , on (a) the effective on-site and hopping amplitudes λ_{eff} and t_{eff} for bare $t = 1$ and $\lambda = 0.7$ [cf. Eq. (11)], (b) the width of the single-valley Gaussian ξ^2 [cf. Eq. (5)], and (c) the resulting hopping amplitude $\bar{t}$ of the central band's effective model [cf. Eq. (6)]. (d) The inverse compressibility of the central band obtained by the effective model of the central band (open circles) compared to that obtained by DMRG (solid lines and dots; cf. Fig. 1). An increasing interaction corresponds to darker (green) shades.

modulated on-site potential, and the exchange energy enhances the hopping,

$$H^{\text{MF}} = \sum_{j=1}^L [t_{\text{eff}} c_j^\dagger c_{j+1} + \text{H.c.}] + \lambda_{\text{eff}} \cos(2\pi b j + \phi) n_j + U n_j, \quad (11)$$

where $\lambda_{\text{eff}} = \lambda + 2U\bar{n}(\lambda/2t)$ and $t_{\text{eff}} = t + U\bar{p}(\lambda/2t)$. Similar to $H(U = 0)$, H^{MF} has a central band of superlattice states. Nevertheless, the width of the valley states ξ and their hopping amplitude $\bar{t}$ are here determined by λ_{eff} and t_{eff} , rather than by λ and t . Although both λ_{eff} and t_{eff} increase with U , λ_{eff} grows faster. Therefore, $\xi = \xi(t_{\text{eff}}/\lambda_{\text{eff}})$ decreases as a function of U , making the Gaussians squeezed. Consequently, $\bar{t}$ also reduces,

and the central band becomes narrower [see Figs. 3(a)–3(c)]. Intuitively, it is caused by the fact that the background density follows the on-site potential, whereas the states of the central bands are localized in its valleys. Therefore, the repulsion from the background density squeezes the Gaussians and reduces their overlap.

In order to recover the enhanced compressibility in the interacting case, one can diagonalize the effective noninteracting model of the central band H^{central} [cf. Eq. (6)] with $\bar{t}(t_{\text{eff}}, \lambda_{\text{eff}})$, and extract Δ_2 . Figure 3(d) depicts $\Delta_2(N, U)$ that is obtained following this procedure. Clearly, it fits nicely to the one observed by DMRG. We note that the low-energy excitations of the satellite bands are also composed of valley states, and therefore they also have decreasing compressibility, as implied by Fig. 1(b). However, since the gap that separates them from the background states is much smaller, they will mix for a much weaker interaction and lower temperatures.

To summarize, we study an unusual increase of compressibility due to a repulsive interaction, which does not fit the standard paradigm on the influence of an e - e interaction on a metallic state in 1D. In turn, we expect an interesting flow to localization by interactions. Our analysis is readily extended to any potential that has fast oscillations times a slowly modulated envelope, be it ordered or random. Such potentials will exhibit localized states within the potential valleys—states that would get squeezed by the interaction with the background. As such, this may be an appropriate model for describing granular disordered metals, and an inhomogeneous background potential of quantum dots. For the latter, it captures the essential ingredients for the solution of that long-standing puzzle: The experiments show increasing compressibility with repulsive interactions, and evidence that consecutive electrons that enter the system at a very close chemical potential reside in different regions of the sample [15,16]. Last, it would be interesting to study the effects of an interaction on similar 2D models [37].

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