Interaction-induced persistent-current enhancement in frustrated bosonic systems

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We investigate the effect of next-nearest-neighbor hopping on the zero-temperature Drude weight or superfluidity in mesoscopic one-dimensional systems of (a) a single particle with quasidisorder (Aubry-André model) and (b) hard-core bosons with nearest-neighbor interaction. We show that there is an interaction-induced enhancement of the Drude weight when the next-nearest-neighbor hopping is frustrated for the many-body system. The observed nonmonotonic behavior of the Drude weight occurs because the repulsive interactions first suppress the frustration in the system, leading to a rise in the Drude weight, whereas at much larger interaction strengths the charge density wave fluctuations set in the insulator and the Drude weight drops. The present paper reveals a scenario in which a persistent flow enhancement is plausible in the presence of kinetic frustration and repulsive interactions.

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I. INTRODUCTION

An important feature distinguishing quantum-mechanical systems from classical systems is the Aharonov-Bohm effect [1], wherein a charged particle picks up a phase while moving through a field-free region which encloses a finite magnetic flux. Such a flux is proportional to the vector potential along the path of the particle and perturbs the energy levels of the quantum-mechanical system [2]. A notable example of this effect occurs in low-temperature mesoscopic rings in the presence of a static magnetic field where the electronic wave function can retain the Aharonov-Bohm phase acquired throughout the ring and coherently extend over the whole system, thereby generating a persistent current [3,4]. This is true even if the material is not superconducting as had been predicted by theoretical studies and corroborated by experiments on copper [5] and gold [6] rings, although these persistent currents are orders of magnitude smaller than those in superconductors [4]. Remarkably persistent currents can also be generated in systems of neutral particles where an artificial gauge field [7–9] or a rotation of the system causes the particles to acquire an Aharonov-Bohm phase. Indeed, a persistent flow has been achieved in an ultracold setup of Bose-Einstein condensed (BEC) atoms trapped in a toroidal geometry by transferring orbital angular momentum to the atoms of the system [10].

A primary question in past studies, prompted mainly by the disagreement between experimental findings in small metallic rings and single-particle calculations, has been to discern the influence of interactions and disorder on the persistent currents in one-dimensional (1D) and two-dimensional model systems, see, e.g., Refs. [11–15] and references therein. It is generally understood that repulsive interactions can counteract the localizing effects of disorder, thereby increasing the persistent current in the system [11–13]. However, such an interaction-induced enhancement of the current is by no means predicted in all model systems [14], or it is expected only to a weak extent [15,16]. With the observation of a BEC superflow and the ability to artificially gauge model Hamiltonians, ultra-cold-atomic setups seem ideal to investigate the effects of interactions and disorder on the persistent current in various physical models.

In this paper we investigate the zero-temperature Drude weight or conductivity stiffness (which determines the persistent response to an external field and which is precisely defined below) in two prototypical systems that have been realized in cold-atom experiments: the single-particle model with an incommensurate potential (Aubry-André model) [17] and the hard-core boson model [18–20] at and away from half-filling. In particular, we ask what the effect of a longer-range hopping of the particles will be on the properties of each of these models defined on ring geometries. Our motivation for this specific question is twofold: (i) the capability to generate artificial gauge fields [7–9], persistent flows [10], and tunable nearest- and next-nearest-neighbor (NNN) hopping amplitudes [21] in ultracold systems raises the question of how longer-range interactions and hopping processes of the gauged particles will affect the experimentally observable results; (ii) ladder materials, for which our long-range hopping one-dimensional systems are equivalent, realize rich physics through a variety of spin models[22]. Moreover, their bosonic analogs have been studied in the literature, and novel phases, such as a supersolid, have been recently predicted [23,24].

We now briefly summarize previous related work and results. Although the problem of a longer-range hopping has been addressed before for the aforementioned models [23,25–28], these works focused largely on critical gap and localization properties. We will uncover some novel aspects missed in these earlier studies, namely, that the interplay between kinetic frustration and nonlocal repulsive interactions produces a nonmonotonic behavior of the Drude weight as the interaction strength is increased. Our results will bear similarities to earlier reports on frustration-induced metallicity [28,29], undertaken in the context of analyzing the phases of the transition-metal oxide $PrBa_2Cu_4O_8$ and of two-dimensional organic conductors. In these studies: (i) The

Ising gap was seen to vanish for a range of frustrated interaction strengths in a spin system on a ladder geometry [28], and such a behavior was interpreted as the onset of a conducting phase due to frustration. However, no analysis of the conductivity within the metallic phase was attempted; (ii) the Drude weight was seen to be enhanced by frustrated interactions in a quarter-filled two-dimensional electronic system [29]. Our paper extends and complements these studies by considering a kinetically frustrated bosonic system where we find the Drude weight or superfluid density (and hence the persistent flow) to be enhanced by repulsive interactions, even in the thermodynamic limit; that is, *in the presence of frustration interactions can indeed enhance conductivity*. We also explicitly demonstrate how such an effect is absent both for a single-particle one-dimensional system which undergoes a genuine conductor-insulator transition and for the many-body system in the absence of frustration. A recent study [30] of interacting one-dimensional bosons in the continuum with a localized and moving barrier in a ring reached a qualitatively similar conclusion: that there is an optimal on-site interaction for which the persistent flow is maximal.

Drude weight and superfluid density

The persistent flow in a normal metal, superconductor, or superfluid may be induced by threading a flux through a toroidal or ring system. Here we consider a ring of L sites threaded by a flux ϕ. This flux gives rise to a static vector potential along the path of the particles, which modifies the hopping amplitudes by a Peierls phase factor [31] ($t \to te^{\pm\phi/L}$) and perturbs the energy levels of the quantum-mechanical system [2]. This sensitivity of the ground-state energy E to the external flux produces a thermodynamic persistent flow $I \propto -dE/d\phi$ around the ring [4,32].

The response of the ground-state energy to an infinitesimal flux is measured by the Drude weight πD, which quantifies the strength of the zero-frequency peak in the real part of the Kubo conductivity. In one-dimensional systems it is given by [2,33–35]

$$D = \frac{L}{2}\frac{d^2E(\phi)}{d\phi^2}\bigg|_{\phi=\phi_0} \approx \frac{L[E(\phi)-E(\phi_0)]}{(\phi-\phi_0)^2} \equiv \frac{1}{2}\left(\frac{\rho}{m}\right)^*, \quad (1)$$

where ϕ_0 is the flux at which the ground-state energy is minimum and $(\rho/m)^*$ is the effective ratio of the density of mobile carriers to mass. Thus, for an infinitesimal flux, the Drude weight provides a way of quantifying the persistent flow in the ring [11]. Equivalently, the Drude weight can be understood as a measure of the sensitivity of the ground state to a small twist ϕ in the boundary conditions. Consequently, a vanishing (finite) Drude weight signals an insulating (conducting) phase at zero temperature [2]. Finally, we point out that the superfluid density is defined very similarly as the Drude weight in Eq. (1). Specifically, it corresponds to calculating first the ground-state energy in the thermodynamic limit and then its second derivative with respect to the flux [34]. Nonetheless, in (quasi-) one-dimensional systems D and the superfluid density are equal due to the finite number of energy-level crossings in the thermodynamic limit [34,36]. Therefore, our results for the Drude weight may also be interpreted as a measure of the superfluid density in the system.

In what follows we compute, using exact diagonalization, the ground-state energy of the two aforementioned models (both with and without a flux) defined on chains of length L with periodic boundary conditions. The largest matrix we diagonalize has a linear dimension of about 10^7.

II. SINGLE-PARTICLE SYSTEM

In this section we extend the results presented in Ref. [25] as regards the superfluid density or Drude weight of the Aubry-André model [37] to the case with NNN hopping. The model, defined on a ring of L sites, reads

$$H = -t_1\sum_j^L(b_j^\dagger b_{j+1} + \text{H.c.}) - t_2\sum_j^L(b_j^\dagger b_{j+2} + \text{H.c.}) + \sum_j^L \epsilon_j \hat{n}_j, \quad (2)$$

where j runs over the lattice sites, $b\,(b^\dagger)$ is the standard annihilation (creation) operator, and $\hat{n}$ is the corresponding particle number operator. The hopping amplitudes to the nearest- and next-nearest neighbors are set by t_1 and t_2, respectively, and $\epsilon_j = V\cos(2\pi jg)$ with V as the potential strength and $g = (\sqrt{5}+1)/2$ as the golden ratio. We note that the sign of t_1 in Eq. (2) does not have any effect on the physics of the model. On the other hand, a negative value of t_2 does not allow the energy associated with nearest- and next-nearest-neighbor hopping processes to be simultaneously minimized, i.e., it yields kinetic frustration.

For a single particle with no incommensurate potential ($V = 0$), Eq. (1) may be readily evaluated to give $D = (t_1 + 4t_2)/L \equiv t_{\text{eff}}/L = \rho/2m$, where ρ and m are the system's density and the particle's bare mass. In order to facilitate comparison of results between different t_2 values, we define a renormalized Drude weight $\tilde{D} := LD/(t_{\text{eff}})$ which yields $\tilde{D} = 1$ for a single particle in the absence of disorder for any value of t_2.

We consider a chain length of Fibonacci number $L = 610$ in order to impose periodic boundary conditions [25] and compute the Drude weight for the single-particle Aubry-André model with NNN hopping amplitudes $t_2 = 0, \pm 0.2t_1$. Our results are shown in Fig. 1 and bear out the following expectations: (i) There is a genuine conductor-insulator transition as a function of the potential strength V in the ground state as seen by the sharp drop in the Drude weights. Indeed, the transition point $V = 2t_1$ is known exactly for the nearest-neighbor Aubry-André model; (ii) a negative value of the hopping t_2 yields a reduced t_{eff} and works as a localizing mechanism. Consequently, a weaker quasidisorder is sufficient to fully localize the wave function. In contrast, the critical disorder strength increases for a positive t_2. These results are in quantitative agreement with inverse participation ratio (IPR) and Shannon entropy calculations [27]. However, we note that through our Drude weight calculations the conductor-insulator transition in the ground state may be pinpointed more accurately than through IPR calculations. The primary result of this section—that the localizing effect of the incommensurate potential always produces a monotonic decay

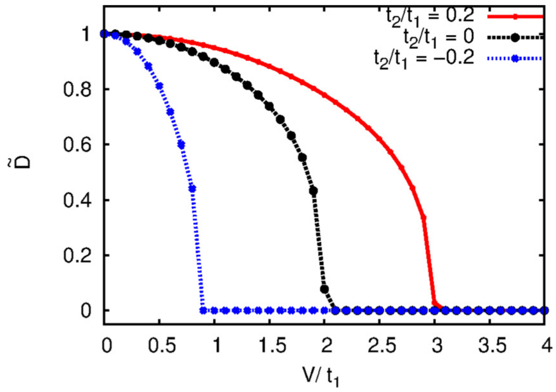

FIG. 1. (Color online) Renormalized Drude weight $\tilde{D}$ (see text) in the extended Aubry-André model as a function of the quasicommensurate potential strength V.

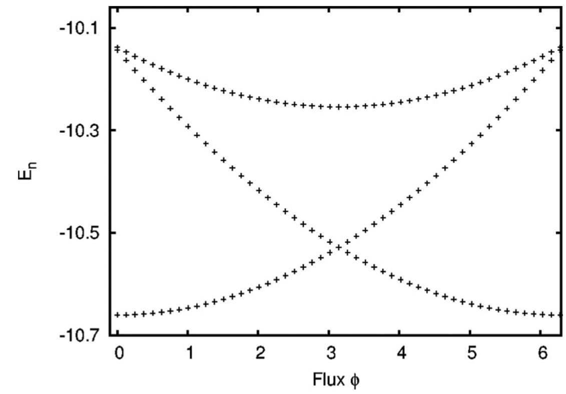

FIG. 2. Energy levels as a function of flux in a 16-site ring with two hard-core bosons and system parameters $t_2/t_1 = 0.2$, $V/t_1 = 1$.

of the Drude weight, although much slower for the unfrustrated system—will be contrasted with the delocalizing effect of the nonlocal repulsive interaction (and its corresponding effect on the persistent flow) while competing with kinetic frustration: In particular, the competition between interaction and frustration will be shown to produce a nonmonotonic decrease in the Drude weight before the conductor-insulator transition sets in.

III. HARD-CORE BOSON SYSTEMS

Next we consider a system of hard-core bosons described by the Hamiltonian,

$$H_{\text{hcb}} = H + V \sum_i \hat{n}_i \hat{n}_{i+1}, \quad (3)$$

where V now sets the strength of nearest-neighbor interaction, $\epsilon_j = 0$, and the particle operators satisfy the usual hard-core boson commutation relations. Such a model has been extensively investigated recently [23,24] in the context of analyzing the competition between quantum fluctuations and kinetic frustration induced by the t_2 hopping term and whether such a scenario can lead to exotic phases. We will work along a contour of the phase diagram presented by Mishra *et al.* (Fig. 2 in Ref. [23]) and uncover some unique properties of the system in the conducting phase.

Given that the second derivative in Eq. (1) is evaluated at the location ϕ_0 where the ground-state energy $E(\phi)$ is minimum, the dependence of the many-body energy levels on the flux deserves some explanation. In the absence of next-nearest-neighbor hopping, the hard-core boson model is exactly solvable, and the Drude weight may be written in closed form [33]. The model may also be Jordan-Wigner transformed to a system of spinless electrons, and most results from the bosonic model transfer to the fermionic one. However, when a flux ϕ threads the ring of electrons the energy is minimum either at $\phi = 0$ or at π, depending on whether the number N of electrons on the ring is odd or even, respectively. This shift in energy is due to the statistical phase that arises when an electron goes around the ring, thereby changing its place with the other $N - 1$ electrons. Such a parity effect does not arise in the corresponding hard-core bosonic system whose many-body wave function is symmetric under particle interchange. Thus, the energy minimum is at $\phi_0 = 0$, and this is the point about which Eq. (1) is evaluated. The location of the energy minimum when NNN hopping is included has also been found to be at $\phi_0 = 0$, provided the system is not in the incommensurately ordered phase obtained in Ref. [24]. In Fig. 2 we show a representative plot of the flux dependence of the first three energy levels for a system of two hard-core bosons over a 16-site ring with $t_2 = 0.2\,t_1$ and $V = t_1$. The energy crossing at $\phi = \pi$ results in a jump discontinuity of the persistent flow, and the energy levels—as well as all physical properties—will clearly be periodic functions of ϕ with period 2π.

Conductor-insulator transition

A transition from a conducting to an insulating (charge density wave) phase is expected as the nearest-neighbor repulsive interaction strength V is increased, and this is true whether t_2 is present or not [23,33]. In the latter case, the Berezinskii-Kosterlitz-Thouless (BKT) transition point is known to be exactly at $V = 2\,t_1$ for a half-filled system. On the other hand, in the presence of NNN hopping, the BKT transition points have been computed numerically by Mishra *et al.* [23] from the behavior of the single-particle excitation gap using the density-matrix renormalization-group technique. Here we focus on the conducting phase of the system at half-filling and consider the representative frustrated value of $t_2 = -0.2\,t_1$ for which the phase transition was predicted [23] to occur at $V_c \approx 1.4t_1$. Our main results are summarized in Fig. 3 for a range of system lengths. As expected from previous works [2,14,38,39], we find the Drude weight to scale polynomially $D(L) = D + a/L + b/L^2$ in the conducting phase and exponentially $D(L) = C\,\exp(-L/\xi)$ in the insulating phase, where ξ is the localization length which diverges at the transition as shown in the bottom panel of Fig. 3.

We point out that we do not, nonetheless, employ the scaling laws to identify the transition point. Instead, we assume the transition takes place at $V_c = 1.4\,t_1$ [23] and perform a polynomial extrapolation to the thermodynamic limit of the computed Drude weights within the conducting phase. Such an extrapolation, shown as the full line in the top panel of Fig. 3, works well both for $t_2 = -0.2t_1$ and for the exactly solvable case of $t_2 = 0$ (the inset of the figure, showing agreement of

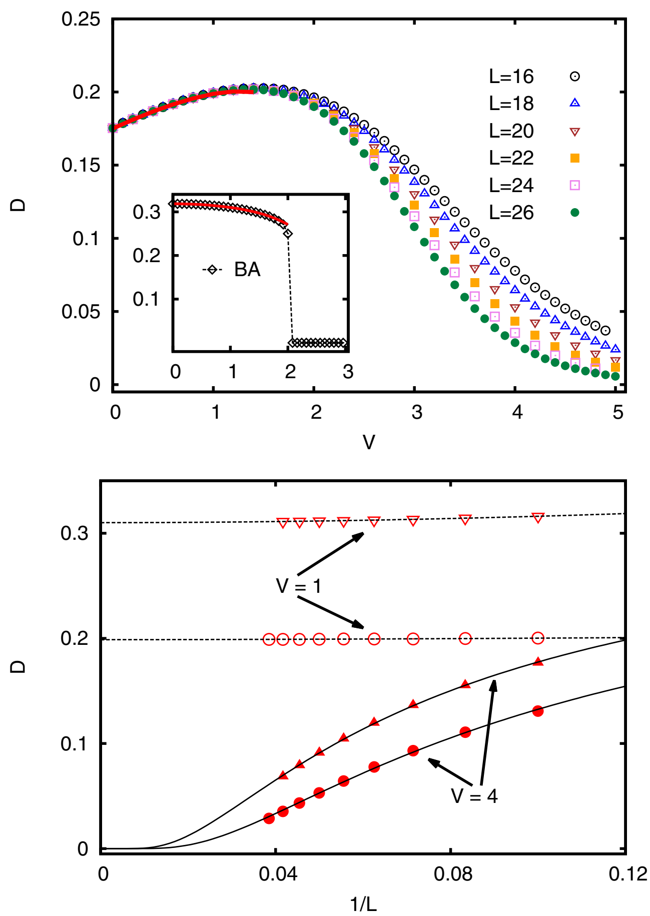

FIG. 3. (Color online) Drude weight of half-filled bosonic rings for various chain lengths L. Top panel: nonmonotonicity of the Drude weight with increasing interaction for frustrated nearest-neighbor hopping $t_2 = -0.2t_1$ and polynomial extrapolation (full lines) from data for $L = 10,12,\ldots,26$ in the conducting phase. The inset shows results from a similar extrapolation for $t_2 = 0$ compared to Bethe ansatz (BA) results. Bottom panel: scaling of the Drude weight for $t_2 = 0$ (triangles) and $t_2 = -0.2t_1$ (circles) as a function of inverse system length for interaction strengths $V = 1$ (open symbols) and $V = 4$ (closed symbols). Full lines are exponential fits $D(L) = C\,\exp(-L/\xi)$, and dashed lines are polynomial fits $D(L) = D + a/L + b/L^2$ to the thermodynamic limit $L \to \infty$. The fits for $V = 4$ give a localization length $\xi \approx 15,11$ for $t_2 = 0, -0.2t_1$, respectively. As V decreases the fits give increasing estimates for the localization lengths ξ.

the extrapolation with Bethe ansatz results [33]). For a finite t_2 a similar sharp jump in the Drude weight should occur as $L \to \infty$, which expectation is borne out from the plots.

We now expatiate on the singular interplay of interactions and frustration and its effect on the Drude weight. The most important feature of the results shown in Fig. 3 is the rise of the Drude weight as the nearest-neighbor interaction is increased, which translates as an enhancement of the persistent flow in the ring. As pointed out in the Introduction, an interaction-induced enhancement of persistent flows and conducting behavior has been reported in earlier theoretical studies of strongly correlated electronic [11–13,29], hard-[28], and soft-core bosonic [30] systems in different [11–13] and similar [28–30] scenarios. Here we uncover a mechanism which produces an enhancement of the Drude weight in ladder geometries as a consequence of the competition between nonlocal repulsive interactions and kinetic frustration within the conducting phase, even after a finite-size scaling to the thermodynamic limit is performed. Indeed, kinetic frustration favors a situation in which the hard-core bosons gain kinetic energy by hopping back and forth between a pair of nearest-neighbor sites and decoupling from the rest of the system [23]. The repulsive nearest-neighbor interaction V, on the other hand, favors a charge density wavelike ordering where the particles tend to avoid sitting next to each other. Thus, initially increasing V causes a spread of the particles and a concomitant increase in charge density wave fluctuations, which in turn reduces the effective frustration, thereby increasing the Drude weight. However, upon a further increase in V the insulating behavior dominates, and the Drude weight drops accordingly. And crucially, as seen in Fig. 3, such a scenario of interaction-induced enhancement of D is valid for finite rings as well as in the thermodynamic limit.

This result is in fact more generic, and we have checked its validity away from half-filling. The main difference in that case being a much more gradual decay of the Drude weight after it reaches its maximum, which is presumably due to the absence of an insulating phase away from half-filling. We have also simulated a system with unfrustrated hopping ($t_2 > 0$) and found a monotonic decay of D with increasing interaction, thereby confirming the crucial role played by the frustration: In the absence of kinetic frustration only one localizing mechanism is present.

IV. CONCLUSIONS

We have studied the interplay of kinetic frustration with quasidisorder and interactions on the Drude weight of single-particle and many-body (quasi-) one-dimensional systems, respectively. For the single-particle Aubry-André model, we found that the Drude weight drops monotonically with an increase in the strength of the incommensurate potential and that, in agreement with earlier work [27], kinetic frustration allows for a quicker onset of the delocalization-localization transition.

For the many-body system of nearest-neighbor hard-core interacting bosons, we found that a frustrating nearest-neighbor hopping causes an interaction-induced enhancement of the Drude weight in the conducting phase. This effect arises because of the degradation of the frustration by the nearest-neighbor interaction, causing an increase in the Drude weight; as the nonlocal repulsive interactions are further increased the insulating behavior sets in, and the Drude weight drops. Our study on kinetically frustrated hard-core bosons is complementary to an earlier study of a 1D spin system [28] where frustrated interactions was seen to destroy the single-particle gap and a later related work [29] which showed the enhancement of the Drude weight by frustrated interactions in quarter-filled two-dimensional electronic systems.

Our paper therefore provides evidence for a unique situation where the conductivity is enhanced in simple kinetically frustrated bosonic systems and opens up the possibility for future cold-atom experiments and theoretical studies wherein the competition between interaction and frustration could produce novel effects in the Drude conductivity and persistent flows, even in the simplest of (quasi-) one-dimensional systems. In fact, studies and experimental realizations of interacting and frustrated systems in low dimensions are many and varied in the present day. Moreover, there still remains much to be gleaned about the additional effect of disorder on the conductivity of these kinetically frustrated systems and on the effects of such a competition in the predicted supersolid phase [23].

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