Devil's staircases and supersolids in a one-dimensional dipolar Bose gas

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We consider a single-component gas of dipolar bosons confined in a one-dimensional optical lattice, where the dipoles are aligned such that the long-ranged dipolar interactions are maximally repulsive. In the limit of zero intersite hopping and sufficiently large on-site interaction, the phase diagram is a complete devil's staircase for filling fractions between 0 and 1, wherein every commensurate state at a rational filling is stable over a finite interval in chemical potential. We perturb away from this limit in two experimentally motivated directions involving the addition of hopping and a reduction in the on-site interaction. The addition of hopping alone yields a phase diagram, which we compute in perturbation theory in the hopping, where the commensurate Mott phases now compete with the superfluid. Further softening of the on-site interaction yields alternative commensurate states with double occupancies which can form a staircase of their own, as well as one-dimensional "supersolids" which simultaneously exhibit discrete broken symmetries and superfluidity.

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I. INTRODUCTION

The unprecedented control over experimental parameters in trapped ultracold atomic gases has substantially widened the range of possible exotic phases of matter that can be explored. Optical lattices can be used to simulate simple lattice models and/or vary the system dimensionality while the interatomic interactions can be varied via a magnetically tunable Feshbach resonance.[1] Thus far, the focus has largely been on *contact* interactions since these generally provide a good description of atom-atom scattering in the low-energy limit. However, with the realization of atomic gases with strong magnetic dipole moments[2] and the prospect of working with molecules that exhibit electric dipole moments,[3,4] there is now substantial interest in examining the physics of long-ranged interactions in these systems.[5]

One important feature of long-ranged interactions is that they can produce exceptionally intricate ground-state structures in the classical, or strong-coupling, limit. A particularly elegant example of this is the case of classical particles in a one-dimensional (1D) lattice interacting via an infinite-ranged convex potential studied by Pokrovsky and Uimin, and Hubbard (PUH).[6–8] Here, it can be shown that the ground-state filling fraction as a function of chemical potential μ is a complete devil's staircase,[9] in which every rational filling fraction between 0 and 1 is stable over a finite interval in μ, and the total measure of all such intervals exhausts the full range of μ.

In this work, we show that the devil's staircase of PUH has dramatic consequences for the physics of quasi-1D atomic gases. Building on the existing understanding of this classical limit, we consider two perturbations of the devil's staircase that arise naturally in the experimental setting of ultracold atomic gases. The first of these is the introduction of a quantum kinetic energy which now renders the problem sensitive to particle statistics—which we take to be bosonic, given that this case can currently be realized with either atoms or molecules. The second perturbation involves tuning the on-site interaction independently of the rest of the interaction. This allows for a controlled departure from convexity, and hence from the PUH states considered previously. The first perturbation has the well-understood effect of initiating a competition between the crystalline, Mott phase that exists at zero hopping and the superfluid (Luttinger liquid in $d=1$) that must exist at all fillings at sufficiently large hopping. By means of strong-coupling perturbation theory similar to that previously studied in the Bose-Hubbard model,[10] and in extended Bose-Hubbard models with nearest-neighbor interactions,[11,12] we derive a phase diagram that exhibits this evolution and which we supplement by standard wisdom from the Luttinger liquid description of the transitions. The second perturbation introduces doubly occupied sites in the classical limit. While describing the resulting phase diagram in complete and rigorous detail is beyond the approaches we take in this paper, we give an account of the "staircase" structure of the initial instability and of regions of the phase diagram where the classical limit states exhibit superlattices of added charge built on underlying PUH states. At least some of these regions exhibit devil's staircases of their own. Finally, upon introducing hopping we are led to an infinite set of "supersolids"—which in this context are phases that are both Luttinger liquids and break discrete translational symmetries.

II. THE MODEL

The Hamiltonian we will study is

$$H = V_0 \sum_{i<j} \frac{1}{r_{ij}^3} n_i n_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i - t \sum_i c_i^\dagger c_{i+1} + \text{H.c.} \quad (1)$$

This model describes bosons in a deep 1D optical lattice with hopping amplitude t, on-site interaction energy U, and an infinite-ranged dipole-dipole interaction V_0/r^3. In cold-atom systems, the hopping potential t is controlled by the depth of

TABLE I. Experimentally attainable values of the hopping t/V_0 as a function of the lattice constant and laser intensity in the approximate range of experimentally realizable values. Here we use parameters relevant to polar molecules–an electric dipole moment of 0.6 D, and the mass of $^{41}K^{87}Rb$. The corresponding values for ^{52}Cr are larger by a factor of ≈300.

a (nm)	300	400	500
	A/E_r		
5	0.184	0.25	0.306
10	0.048	0.065	0.081
15	0.016	0.021	0.026
20	0.006	0.008	0.010

the optical lattice, and hence can be tuned over a wide range of values. In the cases where the bosons are atoms, e.g., ^{52}Cr (Ref. 2), the on-site interaction U may also be easily tuned using Feshbach resonances. We set the dipolar interaction to be maximally repulsive by aligning the dipoles perpendicular to the 1D chain. We also note that though dipolar interactions will couple the different tubes, aligning the dipoles at an angle such that $\cos(\theta)=1/\sqrt{3}$ cancels this interaction in one of the two remaining dimensions. Hence to access the 1D régime, one would ideally work with a single two-dimensional array of optical tubes.

It is instructive to ask what range of parameters can be attained in current experiments. Assuming that the atoms can be cooled such that the temperature is small relative to the other energy scales, the relevant dimensionless ratios are t/V_0 and U/V_0. Current ultracold bosonic molecules have electric dipole moments on the order of $d \approx 1$ D.[13] The dipolar interaction strength at a distance of n lattice spacings is

$$V_{dip} = \frac{1}{n^3}\frac{d^2}{4\pi\epsilon_0 a^3} \approx \frac{1}{n^3 a^3} 1.00141 \times 10^{-22} \text{ Nm}, \quad (2)$$

where a is the optical lattice spacing in nm. The hopping t is given by[14]

$$t = \frac{4E_r}{\sqrt{\pi}}\left(\frac{A}{E_r}\right)^{3/4} e^{-2\sqrt{A/E_r}}, \quad (3)$$

where A is the intensity of the laser beam and E_r is the recoil energy of a single atom, $E_r=h^2/(8ma^2)$. Current experiments can attain lattice spacings of order $a=500$ nm at laser intensities on the order of 10–20 recoils. This gives a range of hopping parameters listed in Table I. Thus with currently realizable optical lattices, fractions $t/V_0 \sim 10^{-2}$ would be within the range of experiments on for cold dipolar molecules. As we shall see in Fig. 2, this suggests that such experiments would find commensurate states at 1/2 and 1/3 filling (as well as integer fillings), stabilized by the dipolar interactions.

Zero-hopping solutions in the convex limit

If U is sufficiently large, the potential is everywhere convex[15] and the $t=0$ (classical) ground states of Eq. (1) are those of a PUH Hamiltonian. For every rational filling fraction $\nu=p/q$, the ground state is periodic with period q (Ref. 6). Each such ground state is unique up to global lattice translations.[16] We denote these states *commensurate ground states* (CGS). A few of these states are shown in Table II. Adding or removing a single particle from a CGS in the infinite volume limit produces a *q -soliton state* (qSS) containing q fractionally charged solitons of charge $1/q$. Each soliton is a distortion of the periodic ground state which alters the distance between one pair of adjacent particles by 1 (see Table II). For every commensurate state, there is a unique distortion of this type which minimizes the potential energy.

TABLE II. Ground states and solitons of the PUH Hamiltonian for a few simple filling fractions. Here q denotes an interparticle separation of q lattice sites, and repetition of a pattern is indicated by an overline. For example, the state $\overline{2}$ has occupancy pattern…101010…, the state $\overline{23}$ has occupancy pattern…1010010100…, and so forth. In the case of the soliton, only the occupancy pattern of the soliton itself is indicated; the rest of the pattern is identical to that of the CGS.

Filling	CGS	Particle soliton	Hole soliton
$1/q$	$\overline{q}$	$q-1$	$q+1$
2/5	$\overline{23}$	22	33
3/7	$\overline{223}$	222	323
5/12	$\overline{23223}$	22322	32323

The range of μ over which each CGS is stable is given by the difference between the energy gaps for adding or removing a single particle. These gaps are simply the energy difference between the particlelike or holelike qSS and the CGS states. For a state of filling fraction p/q at $t=0$, this gives an interval of stability

$$\Delta\mu = \sum_{n=1}^{\infty} \frac{nq}{(nq+1)^3} + \frac{nq}{(nq-1)^3} - \frac{2nq}{(nq)^3}. \quad (4)$$

Though $\Delta\mu$ falls off sharply as a function of q, these intervals cover the entire range of μ pertinent to fillings less than unity. This results in the devil's staircase structure shown in Fig. 1, which describes the filling fraction as a function of chemical potential.

With this brief review of the zero-hopping solutions in the convex limit, we next direct our attention to the $t \neq 0$ phase portrait at large U, where the potential is everywhere convex. The qualitative behavior of our system in this regime is reminiscent of the Bose-Hubbard model, with commensurate Mott lobes ceding to superfluid states as t increases.[17] A state with large q may be treated as a state with smaller q at a nearby filling in which a crystal of dilute solitons has formed. Hopping tends to liquify dilute crystals of solitons: at large separation the intersoliton repulsion is smaller than the kinetic energy gained from delocalization. The delocalized solitons destroy long-ranged spatial order, creating a Luttinger liquid with full translational symmetry. Hence, as t

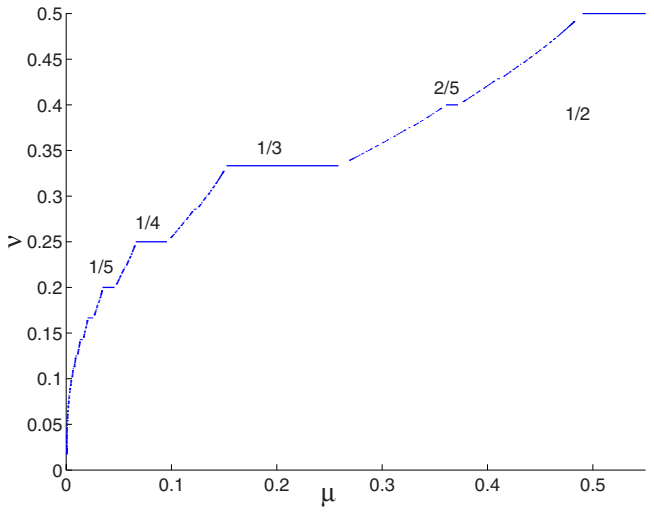

FIG. 1. (Color online) The devil's staircase for $V(r)=1/r^3$, shown for fillings less than 1/2. Each filling fraction is stable over an interval $\Delta\mu$ given in Eq. (4). The resulting function is continuous, has 0 derivative almost everywhere, and possesses a fractal-like structure.

increases, the system undergoes a transition from the Mott insulating CGS to a Luttinger liquid state, with larger q states liquifying at smaller t.

III. STRONG-COUPLING EXPANSION

To find the position of the phase boundary, we generalize the method of Ref. 10 and compare the energies of the CGS and its adjacent qSS to third order in t using standard time-independent perturbation theory. This approach assumes that the phase transition is continuous, so that for a given $t>0$, values of μ for which $E_{\mathrm{qSS}}(\mu)=E_{\mathrm{CGS}}(\mu)$ constitute the phase boundary. This assumption is well founded, since the soliton repulsion ensures that the energy cost of creating multiple solitons is larger than that of a single soliton, thus favoring a second-order transition.

In a finite system one must account for the repulsion between solitons; here we drop these terms and consider the infinite volume limit. In the limit that the solitons are sufficiently well separated that we may neglect their interactions, the qSS is highly degenerate and can be expressed in terms of a band of solitonic momentum eigenstates. Here we consider only the bottom of the band, which lies at zero momentum.

The first- and third-order corrections to the CGS energy are zero. At $\nu=p/q$, the second-order correction in a system of N bosons is given by

$$E^{(2)}=-2\frac{Nt^2}{p}\sum_{i=1}^{p}\frac{1}{\Delta E_i}, \tag{5}$$

where $\Delta E_i=E_i^{(0)}-E_0^{(0)}$ is the difference in potential energies between the ground and the excited state formed by hopping from the ith occupied site in the ground-state configuration. As the ground state is periodic, it suffices to calculate these energies for the p distinct particles in the repeated pattern.

For the qSS at $\nu=p/q$, we consider the infinite volume limit, in which the total-energy correction is simply q times the energy correction for a state with a single soliton. The soliton hops by q sites when a single boson on one of its edges is hopped by one site. The resulting energy corrections are

$$E^{(1)}=-2qt\cos(kqa),$$

$$E^{(2)}=2q\cos(2kqa)\frac{t^2}{\Delta E_{r_1,-1}}-q\sum_{i=1}^{N/q}\sum_{\alpha=\pm1}\frac{t^2}{\Delta E_{r_i,\alpha}},$$

$$E^{(3)}=-2qt^3\cos(kqa)\left[\frac{\cos(2kqa)}{\Delta E_{r_{1,-1}}\Delta E_{r_{1,-1}+q}}-\frac{\cos(2kqa)}{(\Delta E_{r_{1,-1}})^2}\right]$$
$$-2qt^3\cos(kqa)\sum_{i=1}^{N/2}\left[\frac{1}{(\Delta E_{r_i})^2}-\frac{1}{\Delta E_{r_i}\Delta E_{r_{i+1}}}\right]. \tag{6}$$

Here k is the soliton momentum, a is the lattice constant, and q is the denominator of the commensurate filling fraction, which appears here because one hopping displaces the soliton by q lattice spacings. The subscripts on $E_{r_i,\pm1}$ indicate the distance between particle i and the soliton, and the direction of the hopping relative to the soliton. The special distance r_1 describes an excited state in which an antisoliton is sandwiched between two solitons or vice versa. These states contribute extra terms to the energy corrections of the qSS because of the ambiguity as to which soliton is associated with the ground-state qSS.

Figure 2 shows the results of the perturbative calculation for selected filling fractions. The $t=0$ axis corresponds to the classical limit in which the CGS states comprise a complete devil's staircase: every value of μ corresponds to a rationally filled ground state, except for a set of measure 0. The figure shows the resulting Mott lobes: inside each lobe the CGS is stable and the system is in a Mott insulating state. The Mott gap vanishes on the boundary of the lobe; outside of this region solitons proliferate and the system is in a Luttinger liquid phase. We find that the dominant contribution to the lobes is the linear-order correction, and hence expect that our third-order calculation of the phase boundary gives a good description of the phase boundary away from the tip of the lobe where perturbation theory breaks down as t is of the same order as the soliton gap. The estimates in Table I indicate that the 1/2- and 1/3-filled states should be accessible to experiments with dipolar molecules using current optical lattice technology.

For any $t>0$, only a finite number of insulating states exist; the rest are liquid states with a superfluid of condensed solitons. The function $\nu(\mu)$ is no longer a devil's staircase, but rather a piecewise smooth function, with plateaux of constant density separated by liquid phases whose density varies continuously with μ. The size of the commensurate region decreases sharply with q: states of higher q have both smaller ranges of stability in the classical limit and larger energy corrections relative to the CGS. The total volume occupied by liquid states can be estimated from the first-order approximation to the Mott lobe boundaries; we find that for small

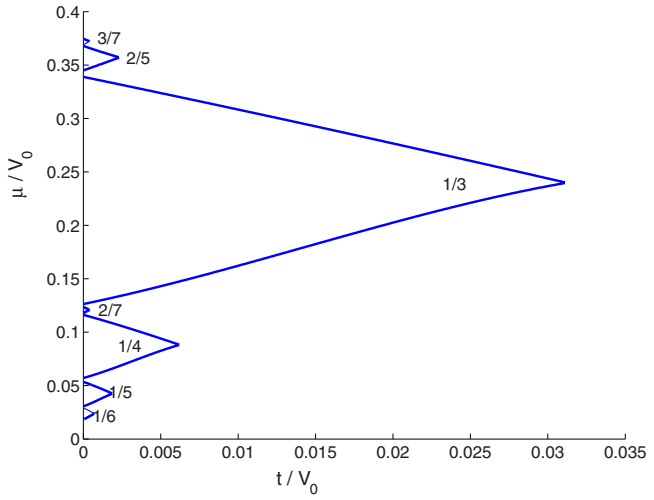

FIG. 2. (Color online) Perturbative calculation of the Mott to SF phase boundary in the (t,μ) plane, shown here for $U=20$. Here the strength of all couplings is measured relative to that of the dipolar interaction strength V_0. Each lobe encloses a Mott insulating region in which the filling is fixed; the region outside the lobes is a superfluid of solitons. The 1/3-, 1/5-, 1/6-, 2/7-, 2/7-, and 3/7-filled lobes are shown here. Every commensurate state of the complete devil's staircase has a Mott lobe, but the range of hoppings over which a state exists falls off sharply with its denominator. Using the values of t/V_0 from Table I, this indicates that commensurate plateaux at 1/2 and 1/3 filling should be experimentally accessible to dipolar molecules.

but fixed t the volume of the liquid region scales as approximately $t^{2/5}$. At sufficiently large t we expect all insulating states to be unstable and the particle density to vary smoothly with μ.

To estimate the fraction of the Mott states lost at hopping t, we estimate the range in μ initially covered by lobes which have disappeared entirely, as well as the fraction of the Mott lobes that remain which has been converted to superfluid states. Using a first order in t approximation to the boundaries of the Mott lobe gives a lobe length of order $1/q^5$ along the t axis. Hence the threshold value of q above which all commensurate states of denominator greater than q have disappeared at hopping t scales as $q_0 \sim t^{-1/5}$. The range of μ covered by a Mott lobe at $t=0$ scales approximately as $1/q^4$ for large q. Summing over $q>q_0$, approximating the multiplicity of states with denominator q by q, gives a net interval of length $1/q_0^2$ in μ. The range in μ covered at $t=0$ by lobes which have disappeared entirely at hopping t therefore scales approximately as $t^{2/5}$. To this, we must add the fraction of each remaining Mott lobe which has been converted to superfluid. Using a linear approximation for the boundaries, we find that a swath of length $2qt$ in μ has been lost from each lobe. Summing over all lobes with $q \leq q_0$ again gives an interval which again scales as $t^{2/5}$ for small t. Thus both contributions contribute a superfluid region in μ which scales as $t^{2/5}$ for small t.

Thus far, our results only apply to a homogeneous system, but we can estimate the effects of a harmonic trapping potential (present in current cold-atom experiments) using the local-density approximation—this assumes that the trapping potential is slowly varying enough that it can be simply incorporated into the chemical potential, resulting in a spatially dependent μ. Trajectories along the 1D chain then correspond to cuts in Fig. 2 at fixed t/V_0. Thus, at $t=0$ we expect different commensurate fillings at different points along the trapped chain with the most stable states (fillings 1/2 and 1/3) occupying the largest regions within the trap. Note, however, that commensurate states with a period q greater than the length scale over which the trapping potential varies do not exist in the trapped system since they violate the local-density approximation. Moreover, in any physically realistic scenario t is nonzero, and we expect islands of Mott states at various fillings p/q (1/2 and 1/3 being most visible), separated by regions of superfluid which interpolate continuously between the two commensurate densities.

Connection to commensurate-incommensurate phase transitions

The qualitative nature of the Mott transition can be deduced from existing knowledge of 1D commensurate-incommensurate phase transitions, which we summarize here. Bosonization can be used to treat the kinetic term and dipolar interactions exactly; the lattice potential must be treated perturbatively. In bosonized form, our system is described by a Hamiltonian that is a sum of a Luttinger piece, accounting for the kinetic term and dipolar interactions,[18] and a sine-Gordon term which emulates the lattice in the continuum limit.

The resulting Hamiltonian is well studied in both the context of the Mott transition[19] and the Frenkel-Kontorowa model of surface interfaces.[20] The upper and lower Mott lobes join in a cusp which is not accurately described by the perturbation theory–since "small" hopping implies that the ratio $t/\delta E_i$ of the hopping relative to the energy gap to the solitonic states must be small, the range of t over which the perturbative treatment is valid decreases with q and never encompasses this point. The bosonized treatment reveals that crossing the edge of the Mott-Hubbard lobe induces one of two different types of phase transitions. At the cusp joining the upper and lower Mott lobes, a constant-density phase transition of the Kosterlitz-Thouless type occurs. Everywhere else the transition is well described by a simple two-band model with quasiparticles that are gapped in the commensurate phase, and with a density increasing as $\sqrt{\mu-\mu_c}$ near the transition on the liquid side.

IV. AWAY FROM THE CONVEX LIMIT

The PUH CGS are the classical ground states so long as the potential is everywhere convex. Since the on-site potential U is tunable experimentally, it is interesting to ask what happens to these states as U is lowered away from convexity and double occupancies begin to form. Of course, as U is lowered still further, triple and higher occupancies will also form but we will not push our analysis that far—the doubly occupied regime has enough challenges of its own. Our results on this are summarized in Fig. 3 and we now describe the analysis behind these.

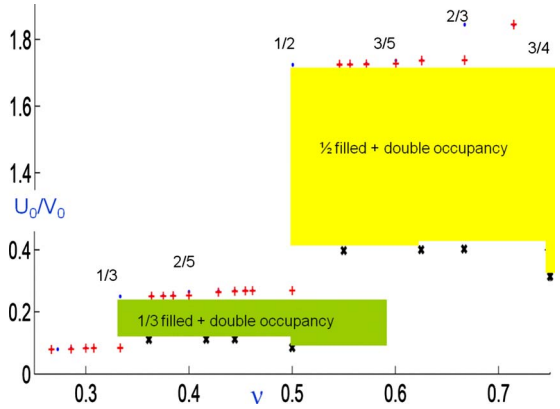

FIG. 3. (Color online) Numerically calculated values of $U_c^{(\mathrm{CGS})}$ (red) and $U_c^{(\mathrm{qSS})}$ (blue), for a selection of filling fractions ν. Quoted values of U are measured relative to V_0. A segment of the y axis between $U_c^{(\mathrm{CGS})}(1/2)$ and $U_c^{(\mathrm{qSS})}(1/2)$ has been removed for better resolution of the rest of the phase diagram. The green and yellow boxes, bordered by black dots, indicate the approximate regions where the ground states consist of double occupancies in the 1/3- and 1/2-filled states, respectively. Between the shaded regions the ground states consist of double occupancies on other, higher-denominator states.

Let $U_c^{(\mathrm{CGS})}(\nu)$ be the thresholds at which the PUH ground states give way to ones with at least one double occupancy—these are marked as the red crosses in Fig. 3. Observe that these thresholds increase monotonically with ν, $U_c^{(\mathrm{CGS})}(\nu') > U_c^{(\mathrm{CGS})}(\nu)$ for $\nu' > \nu$. This behavior can be qualitatively understood by considering the implications of convexity at a given filling. Sufficient conditions for convexity[6] are that, for all x,

$$\frac{1}{2}[V(0)+V(2x)] \geq V(x) \quad \text{and} \quad U \geq \frac{15}{8}V_0\left(\frac{1}{x^3}\right). \tag{7}$$

For convexity to hold everywhere, Eq. (7) must hold for $x=1$; below this threshold double occupancies may occur. However, when perturbing about a given convex solution at fixed μ, solutions will be stable approximately until U violates Eq. (7) *for* $x=r_m$, the minimal interparticle distance. This implies that states with lower filling fractions are more stable against double occupancies, as the potential gain in lattice energy from doubly occupying a site is smaller. This is in contrast to the stability of the commensurate states as t increases, where the denominator of the filling fraction determines stability.

While our primary interest is in ground-state transitions, much insight is gained by also computing a second threshold at a given filling. Past this threshold, $U=U_c^{(\mathrm{qSS})}$ (shown in blue dots in the figure), a particle added to the state goes in as a double occupancy instead of fractionalizing into q solitons. From our above considerations, at fixed filling, the CGS is always more stable against forming double occupancies than the qSS; a simple estimate suggests that the gap separating these instabilities is approximately the difference in energies for adding and removing a particle to the state, which is equal to the interval in μ over which the state is stable at infinite U.

Now consider a filling $\nu' > \nu$. As ν' can be constructed by adding charge to ν, we conclude that $U_c^{(\mathrm{CGS})}(\nu') > U_c^{(\mathrm{qSS})}(\nu)$; the latter corresponds to the threshold at which adding an extra filling $\nu'-\nu$ in the form of the solitons of ν loses out to adding it in the form of double occupancies on top of the PUH state at ν. As filling factors only slightly greater than ν involve a dilute addition of charges, we further conclude that $\lim_{\nu'\to\nu^+} U_c^{(\mathrm{CGS})}(\nu') = U_c^{(\mathrm{qSS})}(\nu)$. A somewhat more involved argument shows that $\lim_{\nu'\to\nu^-} U_c^{(\mathrm{CGS})}(\nu') = U_c^{(\mathrm{CGS})}(\nu)$.[21]

Our considerations so far imply intricate behavior for the location of the initial ground-state instability, namely, that $U_c^{(\mathrm{CGS})}(\nu)$ is a monotone increasing function of ν on the set of rationals with a discontinuity at each rational value of $0 \leq \lambda \leq 1$,

$$\lim_{\nu'\to\nu^+} U_c^{(\mathrm{CGS})}(\nu') > U_c^{(\mathrm{CGS})}(\nu) = \lim_{\nu'\to\nu^-} U_c^{(\mathrm{CGS})}(\nu').$$

We can understand the coarse features of this instability by considering first the most stable states (of denominator $q \leq q_0$, for some q_0 small enough to allow the exact thresholds to be computed) and deducing the expected behavior at fillings close to these. Figure 3 plots $U_c^{(\mathrm{qSS})}$ (blue dots) and $U_c^{(\mathrm{CGS})}$ (red crosses) for states with $q \leq 15$ in the vicinity of half filling. The values of $U_c^{(\mathrm{qSS})}$ shown there are obtained by numerical minimization in the sector with one added charge at the specified filling. The values of $U_c^{(\mathrm{CGS})}$ are obtained by numerical minimization over configurations *at* the specified filling that contain exactly one double occupancy. This is the correct answer for all $\nu=p/q$ for which p and q are not both odd. In such cases the double occupancy and its surrounding charge rearrangements give rise to even moments starting with a quadrupole. Consequently, double occupancies repel at all distances and enter via a continuous transition at the computed threshold. However, when p and q *are* both odd, the double occupancy has a dipole moment and the transition goes first order which causes the true $U_c^{(\mathrm{CGS})}$ to lie above our numerically determined value. This gap is not very large though, and vanishes at large q at least as $1/q^3$ and we ignore it here.

At any given filling, tracking the evolution of the ground state with decreasing U after double occupancies have been introduced is a problem of considerable complexity. Here we use the ideas developed thus far to identify a family of regions in the (ν, U) plane where simpler descriptions emerge—these are indicated, in two simple cases, by the shaded regions on the figure. The basic idea is that once the $\nu=p/q$ qSS becomes unstable to double occupancy, any particles added to the $\nu=p/q$ state will be added as double occupancies, since these repel less strongly than solitons. Hence at first sight we expect, in the region $U_c^{(\mathrm{qSS})}(p/q) > U > U_c^{(\mathrm{CGS})}(p/q)$, states of filling $\nu > p/q$ to consist of double occupancies in the $\nu=p/q$ state. At rational fillings the double occupancies will arrange themselves in a crystal thus generating a commensuration distinct from that of the underlying p/q state—we will refer to these as doubly commensurate states. However, for any given ν this argument becomes less reliable as the density of added charge increases since the background parent state itself becomes less stable to forming extra double occupancies. This can lead to

transitions in which the structure of the CGS collapses to a crystal of double occupancies over a background of significantly smaller filling. We have carried out a simple analysis of the location of this instability for the 1/2 and 1/3 plus double occupancy regions in Fig. 3 at selected fillings and these are marked by the black x's in the figure.[22] While this indicates that there are sizeable regions which can be described as simple descendants of the 1/2 and 1/3 states, we are not at present able to estimate the sizes of analogous regions for higher denominator fractions. Of course, to have a full solution of this would be equivalent to tracking the evolution of each ν as U is decreased from $U_c^{(\mathrm{CGS})}$.

As the barrier to triple occupancies is $3U$, instabilities toward triple occupancy at a given filling will set in at approximately one third the value of U for instabilities to double occupancy. For U close to $U_c^{\mathrm{qSS}}(1/2)$, triple occupancies will not be favored at any filling fraction.

New staircase

The above discussion has led us to the doubly commensurate states in the (ν, U) phase diagram: we remind the reader that such states are constructed by periodically doubly occupying some fraction of the sites in a CGS. We now observe that in at least some cases these doubly commensurate states can form a devil's staircase of their own.

First consider states constructed from double occupancies in the 1/2-filled state, which exist in the region shaded in yellow in Fig. 3. The energetics of such states can be divided into (a) the constant interaction of the parent 1/2-filled PUH configuration with itself, (b) the constant interaction of the added charges, irrespective of their location, with the parent 1/2-filled configuration, and (c) the interaction of the added charges with themselves. This last part involves an interaction between the added charges which is convex again and thus leads to PUH configurations sitting on a lattice with a doubled lattice constant. The energy cost of adding a single double occupancy is $U+V_d$, Hence the doubly occupied sites comprise a devil's staircase with $\mu \to \mu + U + V_d$, and the widths of all intervals decreased by a factor of 8. Here $V_d = \frac{1}{8}\Sigma_{n=1}^{\infty}\frac{1}{n^3}$ is the interaction energy of each double occupancy with the underlying 1/2-filled state. At fixed U, this staircase is complete over the range of fillings for which increasing the particle density infinitesimally does not induce "excess" double occupancies to form in the half-filled background lattice. In the case of the 1/2-filled state, for U sufficiently close to the upper cutoff this gives a complete staircase on $1/2 \leq \nu \leq 1$. Similar structures exist for all $1/q$-filled states in the appropriate range of U. As mentioned before, we do not, at present, understand the situation for doubly commensurate descendants of general rational fillings.

V. "SUPERSOLIDS"

Thus far our considerations away from the convex limit have been purely classical. But we can equally consider states obtained from these modified classical states upon the introduction of hopping. Specifically, let us consider the fate of the doubly commensurate descendants of the PUH $1/q$ states considered above.

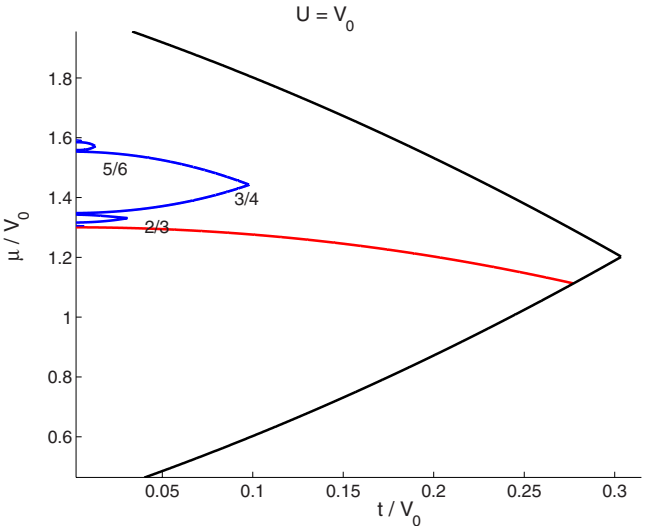

FIG. 4. (Color online) Phase portrait in the vicinity of doubly commensurate states about 1/2 filling at $U=V_0$. Again, μ, t, and U in the figure are measured relative to V_0. The black lines indicate the boundaries of the Mott lobe at $U=20$. The red curve shows the chemical potential at which it becomes energetically favorable to add particles to the half-filled state as double occupancies for $U=V_0$. The blue curves show some Mott lobes of the doubly occupied staircase region; the region between these and the black lines (which delineate the region of stability of the 1/2-filled state at infinite U) is a supersolid state.

In a manner entirely analogous to the problem with which we began this paper, the superlattice of added charges can melt via the motion of *its* solitons as t is increased resulting in a phase transition between the doubly commensurate state and a "supersolid" like phase in which the background $1/q$-filled CGS coexists with a Luttinger liquid. This is, in a sense the $d=1$ version of the supersolid in higher dimensions but it is worth noting that the $d=1$ version in our problem exhibits a more divergent CDW susceptibility than superfluid susceptibility as $T \to 0$.

To get a more quantitative account of these new phases, we may repeat the strong-coupling treatment above. Figure 4 shows the phase portrait at intermediate values of U near $\nu = 1/2$. The black line traces the infinite-U Mott lobe, over which the background 1/2-filled state is stable against forming solitons. The red line shows the threshold at which it is energetically favorable to add a single double occupancy to the 1/2-filled state. The blue curves show the positions of the Mott lobes for the doubly commensurate states. The presence of double occupancies stabilizes the 1/2-filled state against proliferation of solitons, so that the background remains commensurate at least within the infinite-U 1/2-filled Mott lobe, shown in black. This 1/2-filled supersolid phase has also been shown to exist in an extended Bose-Hubbard model with second-neighbor repulsion;[23] these numerical results are consistent with the phase portrait shown here for small t/V.

VI. CONCLUDING REMARKS

The long range of the dipolar interaction does produce, as promised, intricate phase diagrams for the one-dimensional dipolar bosonic gas. Particularly striking are the singular staircase functions that showed up in our analysis in three different settings: in the $\nu(\mu)$ curve for the exactly dipolar classical problem, in the function $U_c^{(\mathrm{CGS})}$ which marks the instability of the PUH states when the on-site U is tuned down and in the $\nu(\mu)$ curves in selected regions of the (ν, U) plane. The other main set of results pertain to the presence of a large, indeed, infinite number of transitions between Mott crystals and Luttinger liquids or supersolids. The challenge of observing some of this physics in cold atomic gases is not trivial—the major obstacles are getting a reasonable simulacrum of a one-dimensional gas of infinite extent, as well as cooling and trapping polar molecules with sufficiently large electric dipole moments. On the positive side, the control parameters we study here are eminently tunable and some of the physics described above should be within the reach of experiments. We hope that the intricate effects described above will motivate our experimental colleagues to invest in exploring the behavior in these and other, potentially richer, regions of parameter space.

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[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[2] T. Lahaye, T. Koch, B. Fröhlich, M. Fattori, J. Metz, A. Griesmaier, S. Giovanazzi, and T. Pfau, Nature (London) **448**, 672 (2007).
[3] J. M. Sage, S. Sainis, T. Bergeman, and D. DeMille, Phys. Rev. Lett. **94**, 203001 (2005).
[4] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Pe'er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science **322**, 231 (2008).
[5] For a review of the current understanding of dipolar interactions, and the parameter regime currently accessible to experiments, see Refs. 13 and 24.
[6] J. Hubbard, Phys. Rev. B **17**, 494 (1978).
[7] V. L. Pokrovsky and G. V. Uimin, J. Phys. C **11**, 3535 (1978).
[8] V. L. Pokrovsky, Solid State Commun. **26**, 77 (1978).
[9] P. Bak and R. Bruinsma, Phys. Rev. Lett. **49**, 249 (1982).
[10] J. K. Freericks and H. Monien, Phys. Rev. B **53**, 2691 (1996).
[11] T. D. Kühner, S. R. White, and H. Monien, Phys. Rev. B **61**, 12474 (2000).
[12] P. Niyaz, R. T. Scalettar, C. Y. Fong, and G. G. Batrouni, Phys. Rev. B **44**, 7143 (1991).
[13] C. Menotti, M. Lewenstein, T. Lahaye, and T. Pfau, *Dynamics and Thermodynamics of Systems with Long Range Interactions: Theory and Experiments*, AIP Conf. Proc. No. 970, edited by A. Campa, A. Giansanti, G. Morigi, and F. Sylos Labini (AIP, New York, 2008).
[14] N. Dupuis and K. Sengupta, Physica B (Amsterdam) **404**, 517 (2009).
[15] A potential is convex if it obeys $V(x) \leq \lambda V(x-1+\lambda)+(1-\lambda)V(x+\lambda)$ for $0 \leq \lambda \leq 1$.
[16] S. Burkov and Y. Sinai, Russ. Math. Surveys **38**, 235 (1983).
[17] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[18] Though the potential is infinite ranged, it falls off quickly enough that the qualitative description is identical to that for short-ranged interactions (Ref. 19).
[19] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford University Press, New York, 2004).
[20] H. J. Schulz, Phys. Rev. B **22**, 5274 (1980).
[21] The argument is as follows: we have $\lim_{\nu' \to \nu^-} U_c^{(\mathrm{qSS})}(\nu') = U_c^{(\mathrm{CGS})}(\nu)$, as the state at filling $\nu - \delta$ is the state at filling ν with a density δ of holelike solitons; as this density decreases a single particle added as a double occupancy will induce a charge configuration increasingly similar to that of forming a double occupancy in the half-filled state (which can be thought of as forming q holelike solitons by removing a single particle, then reinserting this particle as a double occupancy and letting the charge settle into its optimal distribution.) Further, the gap between $U_c^{(\mathrm{qSS})}(\nu')$ and $U_C^{(\mathrm{CGS})}(\nu')$ vanishes as the denominator of the state ν' goes to infinity, implying continuity of $U_C^{(\mathrm{CGS})}$ from the left.
[22] The result is not monotonic in filling, as once at least half the sites are doubly occupied, the dipolar interaction of an extra double occupancy with the existing double occupancies becomes comparable to the energetic gain of creating holelike solitons in the CGS.
[23] G. G. Batrouni, F. Hébert, and R. T. Scalettar, Phys. Rev. Lett. **97**, 087209 (2006).
[24] C. Menotti and M. Lewenstein, *Recent Progress in Many-Body Theories*, Series on Advances in Quantum Many-Body Theory Vol. 11, edited by J. Boronat, G. Astrakharchik, and F. Mazzanti (World Scientific, Singapore, 2008).