Statics and dynamics of a one-dimensional quantum many-body system

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The macroscopic zero-temperature behavior of weakly incommensurate systems in one dimension is described in terms of solitons. The soliton density n obeys equations displaying several types of singular interfacelike solutions: (i) equilibrium or moving boundary between the $n=0$ and finite n regions, and (ii) stationary or moving annihilation front separating solitons from antisolitons.

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I. SOLITON DESCRIPTION OF WEAKLY INCOMMENSURATE SYSTEMS IN ONE DIMENSION

Low-dimensional materials provide a testing ground for the theories of strongly correlated systems.[1] Recently there have been several attempts to manufacture truly one-dimensional systems with periodically modulated parameters. Kouwenhoven *et al.*[2] built a one-dimensional wire of spinless electrons with a 200 nm periodic potential. Upon varying the electron density with a gate voltage they observed suppression of conductance at some rational fillings. Recently Tarucha[3] has succeeded in introducing a shorter period potential.

A different path was undertaken by van Oudenaarden and co-workers[4] who modeled a one-dimensional quantum liquid placed in a periodic potential by a very long and narrow array of small Josephson junctions placed in a magnetic field. The field determines the density of Josephson vortices in the array; these behave like quantum particles. A suppression of the array resistance (implying immobilization of the vortices) at some rational fillings was observed, and interpreted in terms of a Mott transition.

Another relevant experimental system would be a weakly-doped nanotube at low temperature. Bundles of carbon nanotubes themselves can play a role of hosts[5] in which adsorbed helium atoms form strictly one-dimensional systems placed in an external potential that can be tuned over a range of amplitudes and periods. In the bundles helium atoms can be bound in the interstitial channels or within the tubes themselves.[6] Recent work[7] has demonstrated that the competition between the helium-helium interaction and the corrugation in the external periodic potential can induce a commensurate-incommensurate transition in the system.

In each of these examples, the fundamental model is a one-dimensional quantum liquid—spinless fermions, or bosons with a short-ranged repulsive interaction—at zero temperature, placed in an external periodic potential.[8,9] We exclude from consideration the case of long-ranged interactions. For the electronic systems that we consider, this implies that the Coulomb interaction is screened. The possible phases are classified as follows.[8]

(1) When the interactions between particles are not strongly repulsive, quantum fluctuations will render the periodic potential irrelevant, and the system will always be a conductor.

(2) Strongly repulsive particles will become immobilized even by a weak commensurate potential, and the resulting state has long-ranged order, so that we may idealize this structure as being a crystal of particles in registry with the periodic potential. This state is called a Mott insulator.[10]

(3) When the number of particles per period of the potential is not rational, there can be no commensuration and the system is again a conductor. The macroscopic behavior of such *weakly incommensurate* systems is the subject of this paper, focusing on what happens near commensuration, where the Mott mechanism can play an important role.

In general the Mott state is degenerate: when the number of particles per potential well is $\nu=p/q$ (where p and q are co-prime) there are q different registries of the crystal relative to the potential. An important configuration is the soliton, which is the lowest-energy way of joining two domains of different registry. Although there are $q-1$ such combinations, we will assume that energetic considerations select a preferred sequence of neighboring domains, so that the possibilities reduce to "soliton" and "antisoliton." Then for ν close to p/q the structure may be regarded as a low-density gas of solitons, with density $n=(\nu-p/q)/a$, where a is the periodicity length of the potential. This is a weakly interacting system, even though the original particles are dense and their interactions are not small.

The application of these concepts to the Josephson network is as follows: the "Mott insulator" is a configuration in which the vortices form a regular array, commensurate with the plaquettes of the junction network. With a slightly different density of vortices, there would be regions having this structure but with different registry; the domain walls between these "crystals" are the solitons. Motion of a soliton occurs by motion of a vortex as it crosses a domain wall, leaving one crystallite to join another, and would give rise to dissipation.

We note that in the path-integral representation the gas of quantum solitons is equivalent to a gas of classical lines in two dimensions, and thus describes the behavior of magnetic flux lines in a large area Josephson junction (i.e., a thin normal interface between two superconductors), or steps on the surface of a crystal.

Moving a soliton through the system shifts the Mott crystal by one potential well, and thus at $\nu=p/q$ moving q solitons shifts p particles past a given point, returning the crystal to its original registry: a soliton is a fractional particle.[11]

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II. STATICS

Solitons repel each other with a short-ranged force; in one dimension this can be approximated[12] by treating the solitons as a gas of noninteracting free fermions,[13] with the chemical potential

$$\mu = \epsilon + \pi^2 \hbar^2 n^2 / 2m, \tag{1}$$

where ϵ is the energy cost to introduce a soliton, n is the density of solitons, and m is the soliton mass. The last term is a quantum effect coming from the overlap of soliton wave functions, and is more important than the classical effect coming from the overlap of soliton strain fields when the intersoliton distance n^{-1} exceeds the soliton width ξ.

In equilibrium the chemical potential must be constant along the system, i.e. $\epsilon + \pi^2\hbar^2 n^2/2m = \text{const}$. Depending on the magnitude of the constant this equation can have a solution with n real (the uniform soliton conductor), or may have no real solution at all. The latter means there are no solitons in the system (Mott state, $n=0$) and the condition of equilibrium is irrelevant as there is nothing to equilibrate. The Mott crystal plays a role of a vacuum of solitons/antisolitons.

When the system is placed in an external field that provides a potential energy $U(x)$ for the solitons, the condition of equilibrium becomes[14]

$$\mu + U(x) = \epsilon + \pi^2\hbar^2 n^2/2m + U(x) = \text{const}. \tag{2}$$

In contrast to the translationally-invariant case $U=\text{const}$, this equation allows solutions in which a region occupied by solitons can coexist with the soliton-free vacuum.

For example, let us look at a system of finite length $0 \leqslant x \leqslant L$ placed in a field that exerts a constant force F on each soliton, so that $U(x) = -Fx$. In the context of the periodically moduated Josephson junction the solitons (of the pinned lattice of Josephson vortices) will carry a fractional "charge" (that is, a fractional magnetic flux); then a transport current flowing perpendicular to the line of the contact and the direction of external magnetic field would give rise to such a force. We will also assume the vortices are prevented from leaving the system. Then Eq. (2) has a solution of the form $n^2 = (2mF/\pi^2\hbar^2)(x - x_s)$. For $F>0$ there is a soliton vacuum for $x < x_s$, and the solitons will occupy the $x \geqslant x_s$ half-space with a sharp boundary between the two regimes located at $x = x_s$. However, solitons and antisolitons are oppositely charged, so that the same constant force will push antisolitons in opposite directions, and there can be a second region for $x < x_a$ where there is a finite density of antisolitons. We will associate $n>0$ with a density of solitons (an excess of the original particles) and $n<0$ with antisolitons (a particle deficit). Then the equilibrium distribution is

$$n(x) = \begin{cases} \sqrt{2mF(x-x_s)/\pi^2\hbar^2}, & x > x_s \\ -\sqrt{2mF(x_a - x)/\pi^2\hbar^2}, & x < x_a. \end{cases} \tag{3}$$

The values of x_s and x_a are constrained by the condition of conservation of particles, which is also a constraint on the integral of $n(x)$.

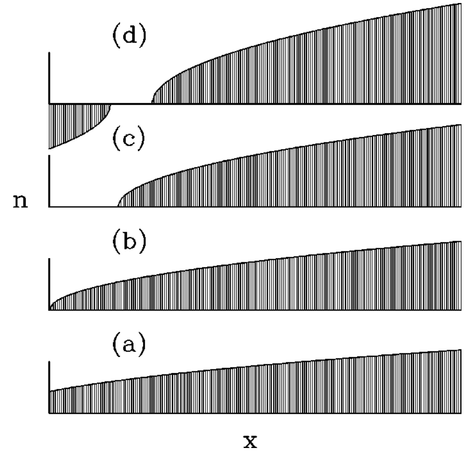

FIG. 1. Soliton distribution in a soliton conductor for various applied fields. (a) For small fields, the soliton distribution is nonuniform but everywhere nonzero. (b) There is a critical value of the field, where the soliton density is zero at one end of the system; (c) For larger fields, there is a region where $n(x)=0$. (d) For even larger fields, soliton-antisoliton pairs nucleate.

(i) Assume that for $F=0$ the ground state is the Mott crystal with no solitons present. A nonzero field F will promote the creation of soliton-antisoliton pairs. The change of the system energy upon creation of a soliton-antisoliton pair is given by $\epsilon(y) = 2\epsilon - Fy$ where the first term is the energy cost to create two solitons of opposite kind separated by a distance $y \gg \xi$ while the second term is the energy gain in external field. The pairs for which $\epsilon(y) \leqslant 0$, i.e., those separated by a distance bigger than $2\epsilon/F$ will be present in equilibrium. As a result the external field F polarizes the Mott insulator by creating and spatially separating solitons and antisolitons. If the field F pushes solitons to the right and antisolitons to the left, the density distribution $n(x)$ is odd in x about $x=0$, and we have $n=0$ for $0<x<\epsilon/F$ and $n = (2mF/\pi^2\hbar^2)^{1/2}(x-\epsilon/F)^{1/2}$ for $x \geqslant \epsilon/F$: a strip of Mott phase of width $2\epsilon/F$ separates solitons from antisolitons. This conclusion is only true for a sufficiently large system whose size L exceeds the size of the Mott strip $2\epsilon/F$; otherwise pair creation is not profitable and the vacuum is the lowest-energy state. As the field increases, the Mott strip shrinks, and our description fails at very large fields of order ϵ/ξ when the size of soliton-free region becomes comparable with the soliton width ξ.

(ii) Assume that for $F=0$ the ground state is a soliton conductor. A sufficiently small nonzero field F pushing solitons to the right will turn the uniform soliton distribution into $n = (2mF/\pi^2\hbar^2)^{1/2}(x-x_s)^{1/2}$ illustrated in Fig. 1(a) (for this case x_s is outside of the physical region). As the field increases, at some F there will be a marginal configuration ($x_s=0$) [shown in Fig. 1(b)] where the soliton density vanishes at the left end of the system. At larger fields ($x_s>0$) a soliton-free Mott strip forms at the left end of the system [Fig. 1(c)]. Upon further increase of the field when solitons get pushed sufficiently far away from the left, there will be another marginal configuration for which the size of the Mott strip is exactly $2\epsilon/F$. At largest fields, antisolitons nucleate at the left end of the system ($x_a>0$), the number of solitons at the right increase by the same amount, and the size of the Mott strip stays equal to $2\epsilon/F$ thereafter [Fig. 1(d)].

The equilibrium configurations of solitons in an external field are related to the equilibrium crystal shapes of three-dimensional crystals, since the latter system can be viewed as equilibrium of atomic steps.[15]

III. DYNAMICS

We now turn to a discussion of nonequilibrium effects, and hereafter we assume that there are no external fields present. The force exerted on a given soliton by its neighbors is $-\partial\mu/\partial x$, which will cause it to drift with the velocity $u=-\gamma\partial\mu/\partial x$, where γ is phenomenological friction constant. The resulting current of solitons is

$$j=nu=-\gamma n\partial\mu/\partial x=-\Gamma\partial\mu/\partial x=-bn^2\partial n/\partial x, \quad (4)$$

where $\Gamma=\gamma n$ is the system mobility, $b=\gamma\pi^2\hbar^2/m$ is a dynamical parameter, and we used Eq. (1) to compute $\partial\mu/\partial x$. The mobility Γ is linear in the soliton density n, which implies that the conductivity of the system vanishes linearly in deviation from commensuration as the Mott insulator phase is approached from the conductor side. This transport theory explains the linear drops in resistance seen by van Oudenaarden and co-workers[4] in the vicinity of the Mott phases, and parallels the flux line mechanism of resistivity of a type-II superconductor in the vortex state,[16] and the growth regime of vicinal crystal surfaces via the motion of steps.[15]

Conservation of soliton number within a region implies a continuity equation, which provides an equation of motion for $n(x,t)$:

$$\partial n/\partial t=-\partial j/\partial x=b\frac{\partial}{\partial x}\left(n^2\frac{\partial n}{\partial x}\right). \quad (5)$$

When the function $n(x,t)$ changes sign (both solitons and antisolitons present) the relaxation within the two regions continues to be described by Eq. (5); however, the behavior at the interface $n=0$ where the solitons and antisolitons annihilate requires further discussion.

When a soliton-antisoliton pair annihilates, an energy 2ϵ is released [first term of Eq. (1)]. Viewed classically, the force that corresponds to this potential energy has only the range of order ξ, since solitons do not communicate beyond this scale. From our macroscopic viewpoint this would imply no interaction between solitons of opposite kind at all, and the dynamics of annihilation would be determined by the rate at which they get pushed together by the excess of particles elsewhere. This overlooks a quantum effect: there always is a finite annihilation probability of a pair whose size is bigger than ξ. This possibility of future annihilations gives an effective longer-range attraction between solitons of opposite type. However, the dominant effect associated with the region where solitons and antisolitons annihilate is that the mobility vanishes [Eq. (4)], so that attractive forces between solitons and antisolitons have no important macroscopic effect on dynamics, and (5) is still valid.

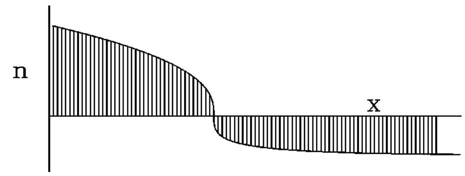

FIG. 2. Annihilation front. Solitons are invading from the left, annihilating a stationary distribution of antisolitons to the right.

Equation (5) resembles the diffusion equation, but the "diffusion constant" $D=bn^2$ is density dependent. This equation has previously appeared in the theories of shock waves, filtration,[17] and dynamics of crystal surfaces.[18]

The most remarkable property of Eq. (5) is that it allows self-similar moving solutions with a sharp front where the soliton density vanishes. Indeed, assume there is such a boundary, moving at constant speed v. The soliton density can be sought in the form $n(x-x_f)$, where $x_f=vt$ is the time-dependent position of the front [defined by $n(x_f)=0$]. It is then an implication of Eq. (5) that the current density has the form $j=j_f+vn$, where j_f is the current density at the front position $x=x_f$. Equation (5) can be integrated to give

$$vn^2/2-j_f n+(j_f^2/v)\ln|(vn+j_f)/j_f|=v^2(x_f-x)/b. \quad (6)$$

The shape of the density profile near the front edge depends on whether j_f is zero or finite.

(i) The case $j_f=0$ has been considered previously.[17] Taking in Eq. (6) the limit $j_f=0$ we find $n^2=(2v/b)(x_f-x)$, which implies that the solitons are present only in the region of space satisfying $v(x_f-x)\geqslant 0$; behind the front, the soliton density is given by[17]

$$n=\pm\sqrt{\frac{2v(x_f-x)}{b}}. \quad (7)$$

The region $v(x_f-x)<0$ is soliton-free.

This type of front describes a cloud of solitons/antisolitons invading a Mott phase, for example when vortices are first injected into a narrow Josephson junction array, or when the array is in any way disturbed away from commensuration. As in the equilibrium case (3), the front has a square-root singularity (7). The steepness of the moving front is determined by the velocity v of the front. The current is given by $j=nv$, and vanishes at the front. In the narrow Josephson array this would be directly measurable as a voltage difference across the narrow dimension of the array. Note that to maintain constant velocity of the moving front, the rate of injection at a fixed boundary will have to vary proportional to $\sqrt{t}$.

(ii) If $n(x_f)=0$ is an annihilation front then solitons and antisolitons get pushed by their neighbors towards $x=x_f$, and the current density j_f will stay finite there. As far as we can tell, this type of shock has not been studied previously. This type of front describes solitons invading an antisoliton conductor (or the other way around); in the Josephson network context, this describes what happens when the vortex density is changed from slightly below commensuration to slightly above (or the other way around). Its form is shown in Fig. 2, for the case $v>0$ so that the front is moving to the right.

Far to the left of the front position, $x \ll x_f$, the front profile is approximately given by Eq. (7). Far to the right, $x \gg x_f$, the density tends to a constant value $n_\infty = -j_f/v$, and then the solution (6) can be approximated by $n = n_\infty\{1 - \exp[(v/bn_\infty^2)(x_f - x)]\}$. This is exactly the density profile one would get ahead of a constant-velocity front using the linearized version of Eq. (5) with the diffusion constant $D = bn_\infty^2$; the size of the perturbed region ahead of the front is given by the diffusion length $D/v = bn_\infty^2/v$.

The soliton density near the front can be found by solving Eq. (6) to lowest-nonvanishing order in $|vn/j_f| \ll 1$,

$$n = [3j_f(x_f - x)/b]^{1/3}\{1 + (v/4j_f)[3j_f(x_f - x)/b]^{1/3}\}. \tag{8}$$

A peculiar feature of Eq. (8) is that the magnitude of the force acting on a soliton $\partial\mu/\partial x \propto n\partial n/\partial x \propto (x_f - x)^{-1/3} \propto n^{-1}$ diverges at the annihilation edge. This divergence offsets the vanishing of the system mobility and thus overcomes a dynamical bottleneck. The cubic-root singularity in n is thus a necessary consequence of having finite-current density at the annihilation edge.

Equation (8) describes both moving and stationary annihilation fronts. In fact, for $v=0$, Eq. (8) provides an exact *steady-state* solution to Eq. (5). In this case the parameter j_f is a fixed current flowing through the system that is the same everywhere. Although these solutions have assumed that the front moves at a constant speed, they characterize the form of the front for more general cases. The essential point is that in the comoving frame the singular derivatives in Eq. (6) can be made to cancel by giving the density the forms (7) and (8), leaving perhaps only a time-dependent amplitude. Below we consider a few more practically relevant examples for which the front velocities are not necessarily constants.

(i) Imagine a Mott insulator for which extra particles have been added to a region of the system. This can be described as a segment of nonzero soliton density embedded between two half-infinite commensurate domains. The number of particles added determines the total number of solitons N, which is conserved: $\int_{-\infty}^{\infty} n(x,t)dx = N$. The parameters b, N and the variables x and t can be combined to form one dimensionless combination bN^2t/x^4. This implies that the size of the region containing the excess particles is of order $x_f \cong b^{1/4}N^{1/2}t^{1/4}$, and that the average soliton density in the region decays as $N/x_f \cong N^{1/2}b^{-1/4}t^{-1/4}$. Another representation of the results is that the boundary of N solitons localized in a region of size x_f will move as a shock front with velocity $v \cong bN^2/x_f$. Arbitary initial particle distributions will relax asymptotically to a common form[17]

$$n(x,t) = \left(\frac{N^2}{\pi^2 bt}\right)^{1/4}\sqrt{1 - \pi x^2/4N\sqrt{bt}}, \tag{9}$$

which has the characteristic square-root singularity (7) at its edges.

(ii) Consider the case that the average density of particles is appropriate for commensuration but the initial distribution is inhomogeneous. For example, we could have a Mott insulator everywhere except in a small region, where there is an excess of particles on one side, and a deficit on the other. In the soliton description, the two regions will contain solitons of different types—solitons and antisolitons— which can be described by a single function $n(x)$. Here are two examples in which soliton-antisoliton annihilation plays a role.

Consider a periodic distribution of solitons of both signs such that the total soliton ''charge'' is zero. The spatial periodicity of the distribution will be preserved by time evolution; this implies that the asymptotic solution to Eq. (5) should be sought in the form[18] $n = t^{-\alpha}f(x)$. It is readily seen that the equation of motion (5) determines the exponent to be $\alpha = 1/2$. The density decays because solitons succeed in getting through the zero-mobility region, by having a singularity in the applied force: the function $f(x)$ has $\Delta x^{1/3}$ singularities at every point where it changes sign[18] in agreement with the general argument leading to Eq. (8).

A related example is a soliton distribution such that $n(-x) = -n(x)$. This symmetry will be preserved by the time evolution. Due to annihilation events at $x=0$, the total number of solitons of either type is not conserved; however, the dipole moment $P = \int_{-\infty}^{\infty} xn(x,t)dx$ is conserved[17] by the equation of motion (5). The parameters b, P and the variables x and t can be combined to form one dimensionless combination bP^2t/x^6, which implies that asymptotically the disturbance expands according to $x_f \cong b^{1/6}P^{1/3}t^{1/6}$, and the total number of solitons of given kind decreases with time as $P/x_f \cong b^{-1/6}P^{2/3}t^{-1/6}$. The expansion rate is smaller than in previous case of the spread of a region of excess solitons because of annihilation of soliton-antisoliton pairs at $x=0$; the envelope decays more slowly than in the periodic case because the solitons are not confined. The analytic solution for this case is[17]

$$n(x,t) = \frac{AP}{x_f^2}\left(\frac{x}{x_f}\right)^{1/3}\left[1 - \left(\frac{x}{x_f}\right)^{4/3}\right]^{1/2}, \tag{10}$$

where $A = 2.08657\ldots$ is a constant and $x_f = (4A^2P^2bt)^{1/6}$ is the limit of the distribution. At the extremal edges, there is again the $\sqrt{\Delta x}$ singularity, (7), but near the origin $n(x) \propto x^{1/3}$ [see Eq. (8)], as is required to have a net current of solitons through the mobility bottleneck.

(iii) Let us start from commensurate phase $(n=0)$, and try to change the average particle density by connecting the $x=0$ end of semi-infinite system to a macroscopic reservoir of particles with their chemical potential selected so that extra particles will be prompted to enter the system (or the particles of the system will be prompted to enter the reservoir). If the new equilibrium particle density is not very different from the old one, then the transient process can be described as a solution to Eq. (5) satisfying $n(x>0,0)=0$, and $n(0,t)=n_0$, where n_0 is a soliton (antisoliton) density fixed at the boundary. The parameters n_0, b, and the variables x and t can be combined to form the one dimensionless combination bn_0t/x^2. This implies that asymptotically the new equilibrium $n=n_0$ is reached through a multisoliton wave traveling across the system; in the vicinity of the front the profile is given by Eq. (7), and the front position evolves with time as $x_f \cong n_0(bt)^{1/2}$. The corresponding self-similar solution to Eq. (5) will have to have the form $n(x,t) = n_0 f(x/x_f)$ and the function $f(y)$ obeying $f(0)=1, f(y \geqslant 1) = 0$, can be found[17] by numerical integration of an ordinary-differential equation for $f(y)$.

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