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Kinks, solitons, and nonlinear transport in solids

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Exact solutions for solitonlike motion of interacting particles in a periodic potential are found to exhibit curious properties. A kink corresponding to a vacancy or domain wall in this model propagates through the system only if it is subjected to an external force. The force must exceed a minimum value, and the kink which propagates most easily moves with a fairly high velocity (comparable with the speed of sound). Kinks exhibiting this type of behavior will lead to strongly nonlinear transport coefficients. This may relate to the observed nonlinear conductivity in some quasi-one-dimensional metals.

A wide variety of phenomena in solid-state physics has been related to the concept of the soliton. For example, it has been argued that solitonlike motion may be exhibited by dislocation lines in imperfect crystals,[1] domain walls in displacive phase transitions,[2,3] ions in some superionic conductors,[4-6] and charge-density waves in some metals.[7-9] In these physical situations, the word "soliton" must be interpreted loosely. Ideal solitons are undamped particles which survive collisions virtually unchanged. "Kink"[1] may be a more appropriate word to use in describing the solitonlike excitations in many solids.

One must make a "continuum approximation" to justify the soliton picture. This approximation involves replacing a set of particle coordinates u_n by a continuous function $u(x)$ and approximating differences in the particle coordinates by derivatives of the continuous function. It is not easy to investigate models of discrete systems without making the continuum approximation. In order to gain insight into solitonlike motion in discrete systems, a model is presented here for which the steady-state velocity of a kink in an external field can be obtained exactly. When this new model is treated in the continuum approximation, one obtains some standard results: solitonlike kinks are found which propagate with no intrinsic damping. However, when the same model is solved exactly, one finds that the kinks are always damped. They lose their energy through a coupling to phonons so that a "phonon wake" trails behind the kink. Kink damping has been approximately calculated before,[1,10,11] but one advantage of the exact treatment is that the peculiar velocity dependence of the kink damping can be easily seen. Results to be presented here will show that fairly rapidly moving kinks offer the least frictional drag, and a small driving force will not sustain solitonlike motion. These results contradict some phenomenal kink-damping approximations[4,5] and predict a nonlinear transport coefficient.

The discrete model considered here describes particles coupled by nearest-neighbor harmonic forces subject to an additional periodic background potential. The periodic potential $V(u)$ is taken to be an array of parabolas instead of the standard sinusoidal potential:

$$V(u) = \tfrac{1}{2}u^2 \quad \text{for} \quad -\tfrac{1}{2} \leq u \leq \tfrac{1}{2} \tag{1}$$

and $V(u+n) = V(u)$, where u is the particle position and n is any integer. This form for the potential determines length and energy units since the lattice spacing is unity and the potential well depth is $\frac{1}{8}$. The mass of the particles is also taken to be unity.

The equation of motion for the interacting particles is

$$\frac{d^2u_n}{dt^2} = \frac{-dV(u_n)}{du_n} - K(2u_n - u_{n+1} - u_{n-1}) - \frac{\gamma\, du_n}{dt} + F\,. \tag{2}$$

Here u_n is the displacement of the nth particle from the nth-potential-well minimum, K is the spring constant for the nearest-neighbor harmonic interaction, $-\gamma\, du_n/dt$ is a phenomenological frictional force, and F is an applied force. Only the case of N particles in $N+1$ potential minima, periodic boundary conditions, and $N \to \infty$ will be considered here. This case corresponds to a single vacancy (domain wall, etc.).

The equation of motion [Eq. (2)] will be investigated first in the continuum approximation. Then the approximate continuum results will be compared with the exact solution of the discrete problem.

In the continuum approximation,

$$u(t)_n \to u(x,t)\big|_{x=n}\,,$$

$$2u(t)_n - u(t)_{n+1} - u(t)_{n-1} \to -\frac{\partial^2 u(x,t)}{\partial x^2}\bigg|_{x=n}\,,$$

and Eq. (2) becomes

$$\frac{\partial^2 u}{\partial t^2}=\frac{-\delta V}{\delta u}+K\frac{\partial^2 u}{\partial x^2}-\gamma\frac{\partial u}{\partial t}+F\,. \tag{3}$$

The simple form for the periodic potential $V(u)$ makes it easy to find kink solutions of Eq. (3) even when the damping γ is nonzero. A solution corresponding to a kink moving with a constant velocity v is

$$u-\tfrac{1}{2}=\begin{cases}(-\frac{1}{2}+F)(1-e^{a_+(x-vt)}) & \text{for } (x-vt)\geq 0\\ (+\frac{1}{2}+F)(1-e^{a_-(x-vt)}) & \text{for } (x-vt)\leq 0\end{cases} \tag{4}$$

with

$$a_\pm=-\tfrac{1}{2}\{\gamma v\pm[4(K-v^2)+(\gamma v)^2]^{1/2}/(K-v^2)\,.$$

The dependence of the kink velocity on the applied force can be obtained from the condition that $u(x,t)$ have a continuous derivative. The result is

$$v=2\sqrt{K}\,F/\{(\tfrac{1}{2}\gamma)^2[1-(2F)^2]+(2F)^2\}^{1/2}\,. \tag{5}$$

This continuum approximation for $v(F)$ is shown as the dashed curve in Fig. 1 for $K=4$ and $\gamma=0.1$. Of course when $\gamma=0$, no force is necessary for continuum kink motion. An undamped continuum kink has a pseudorelativistic energy

$$E(v)=K/4(K-v^2)^{1/2}\,. \tag{6}$$

Some properties of the original discrete system of Eq. (2) can be obtained without resorting to the continuum approximation. The simplest motion of the particles corresponds to small amplitude vibrations or phonons. The dispersion relation for these phonons for $\gamma=0$ and no vacancy is

$$\Omega(q)=\{1+2K[1-\cos(q)]\}^{1/2}\,, \tag{7}$$

where Ω is the phonon frequency and q is the phonon wave vector.

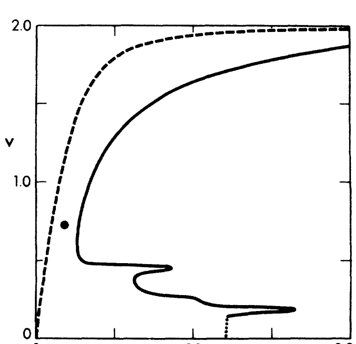

FIG. 1. Force F necessary to move a kink at a velocity v. The dotted line corresponds to the continuum approximation and the full curve is the exact solution. The spring constant K is 4 and the damping γ is 0.1 for both curves. The dot corresponds to the minimum force and optimum velocity of a kink when $\gamma=0$.

A kink in this model can be thought of as the motion of the vacancy through the system. Assume the kink corresponds to a vacancy traveling in the $-x$ direction. If the kink passes the particle with coordinate u_0 at time $t=0$, this particle moves from the potential well centered at $x=0$ to the potential well centered at $x=1$ at $t=0$. This means the force on this particle due to the background potential is

$$\frac{-dV(u_0)}{du_0}=-u_0+\Theta(t)\,, \tag{8}$$

where $\Theta(t)$ is the Heaviside step function. If the kink moves with a velocity v, then after a time $\tau=1/v$, the system will be unchanged except for a translation by one unit in the $-x$ direction. This means

$$u(t+1/v)_n=u(t)_{n+1}\,. \tag{9}$$

Having specified the initial position [Eq. (8)] and velocity [Eq. (9)] of the kink, the equation of motion for u_0 [Eq. (2)] becomes

$$\frac{d^2u(t)_0}{dt^2}=-u(t)_0-K\times[2u(t)_0-u(t+1/v)_0-u(t-1/v)_0]-\frac{\gamma du(t)_0}{dt}+\Theta(t)+F\,. \tag{10}$$

A Fourier transform further simplifies the problem. Let

$$U(t)=u(t)_0-\tfrac{1}{2}-F$$

and

$$\hat{U}(\omega)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}U(t)e^{-i\omega t}\,. \tag{11}$$

Then Eq. (12) becomes

$$\omega^2\hat{U}(\omega)=\{1+2K[1-\cos(\omega/v)]+i\gamma\omega\}\hat{U}(\omega)+\frac{i}{\sqrt{2\pi}\omega}\,. \tag{12}$$

One can see from this equation that $\hat{U}(\omega)$ will be peaked at special frequencies ω_n when γ is small. These frequencies satisfy the relation $\omega_n=\Omega(\omega_n/v)$. By making the change of variable $q=\omega/v$, the condition which determines the special frequencies becomes

$$v=\Omega(q_n)/q_n\,. \tag{13}$$

This describes the matching of the kink velocity v with a phonon "phase velocity" $\Omega(q)/q$. For small v there may be several solutions to Eq. (13), and the q_n may lie outside the first Brillouin zone. The peaks in $\hat{U}(\omega)$ at $\omega=\omega_n$ correspond to oscillations in $U(t)$ for positive time. When viewing the whole string of particles, these oscillations in

$U(t)$ appear as a phonon wake which trails behind the kink. The ω_n do not correspond to the minimum phonon frequency as was suggested in Ref. 10.

The force necessary to drive a kink with velocity v is $-[U(0)+\frac{1}{2}]$ because $U(t)=u(t)_0-\frac{1}{2}-F$ and u_0 was assumed to be $\frac{1}{2}$ at $t=0$ [see Eqs. (8) and (11)]. The inverted Fourier transform of $\hat{U}(\omega)$ gives

$$F=\frac{1}{\pi}\int_0^\infty \frac{\gamma}{[\omega^2-\Omega(\omega/v)^2]^2+(\gamma\omega)^2}d\omega \ . \tag{14}$$

This force-velocity relation is a central result. Typical data obtained from Eq. (14) for the case $K=4$ and $\gamma=0.1$ are shown in Fig. 1 and compared with the continuum approximation results discussed earlier. The complicated structure of this curve in Fig. 1 shows that the physics of kinks in discrete systems is not simple. The figure shows that a minimum force F_m is needed to move the kink at any velocity, and the kink which propagates with the least drag moves with a relatively high velocity v_m. For the case shown here, $v_m \approx 0.3\sqrt{K}$ and $\sqrt{K}$ is associated with a sound velocity in the continuum approximation.

Some simple analytic results can be obtained when the damping is zero [$\gamma \to 0$ in Eq. (2)]. In this case, the force-velocity relation of Eq. (14) becomes

$$F=\sum_n \left(2vq_n^2\left|v-\frac{d\Omega}{dq_n}\right|\right)^{-1}, \tag{15}$$

with the q_n given by Eq. (13). Solving the above equation for the minimum force F_m and the corresponding velocity, v_m of the kink with the least friction yields

$$F_m=\tfrac{1}{2}/(1+6.8154K)\,,$$
$$v_m=(1+2.4344K)^{1/2}/4.4934\,, \tag{16}$$

where 4.4934 is a solution to $x=\tan(x)$, $2.4344=2[1-\cos(x)]$, and $6.8154=2[1-\cos(x)]-x\sin(x)$. The minimum force and optimum velocity for $K=4$ are displayed as the large dot in Fig. 1. The dot does not lie on the solid curve because this point corresponds to the intrinsic minimum resistance for $\gamma=0$ instead of $\gamma=0.1$.

I believe the results obtained here suggest that kinks moving at high velocities ($v>v_m$) are solitonlike. Fast kinks exhibit only a small resistance to an applied force, provided their velocity does not approach the speed of sound ($\sim\sqrt{K}$). They are stable in the sense that they can be driven by an applied force. In the absence of any external force, fast kinks probably slowly decelerate by losing energy to their phonon wake. On the other hand, slow kinks with $v<v_m$ appear to be less solitonlike. Their stability is questionable since $\partial v/\partial F$ may be negative. This means "the harder you push the slower they go." Slow kinks may be able to rapidly decelerate by some pinning mechanism.

The model presented here clearly predicts a nonlinear contribution to transport coefficients since sustained kink motion can only take place for applied forces greater than F_m. Of course, there could still be linear contributions to transport especially at nonzero temperature where some diffusive motion seems likely. Nonlinear transport has been observed in quasi-one-dimensional TTF-TCNQ (tetrathiafulvalenium-tetracyano-p-quinodimethanide),[12] and this behavior has been related to charge-density waves and solitons.[7-9] The model results presented here suggest a somewhat different interpretation of the data. The experimentally observed critical field which produces a large increase in the current in TTF-TCNQ could be associated with the minimum field necessary to sustain kink motion F_m. For large K, F_m can be very small. Static kinks may be present even at low temperatures. If this is the case, the observed activation energy may correspond to the energy necessary to accelerate a kink to the velocity v_m where its behavior is solitonlike. This energy would be much less than the energy necessary to create kink-antikink pairs.

One should keep in mind that the model solved here is classical. It is possible, however, that a classical model can explain electronic conductivity. From one point of view, change-density-wave motion is primarily an ionic phenomenon. If the electron gas is treated in the Born-Oppenheimer approximation, the electrons are merely the source of the periodic potential $V(x)$ which influences the ionic motion. Possible applications of this model to ions in change-density-wave systems is clearly speculative and one should bear in mind that the basic nonspeculative conclusion of this paper is that kinks move best when they move fast.

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