

independence of the energy ratio (Fig. 3) on surface temperature is also in contradiction with the AA model (the model predicts a decrease of the energy ratio with increasing temperature). On the other hand, the model proposed by Goodman<sup>7</sup> is in qualitative agreement with most experimental data reported here: The dotted line in Fig. 2(a) predicted by Goodman's model for  $T_n = 1916$  K and  $T_t = 1143$  K reflects correctly the experimental trend. The constancy of the energy ratio is, within the limits of the error, not in contradiction with this theory. The only discrepancy appears when looking at the speed ratio values: Goodman's model predicts in all cases  $S = 1$  which is in contradiction with all our data for small  $\theta$  in Figs. 1(b), 2(b), and 3(b).

The fact that the results for  $H_2$ , HD, and  $D_2$  are practically identical is probably valid not only in the particular case of this experiment. It seems that the detailed features of the desorption process (energy distribution, angular dependences, etc.) are due neither to excitations of rotational or vibrational states nor to other molecular mass-dependent phenomena but to the chemisorption mechanism itself. This general observation and the peculiarities of the data presented here might be useful for the construction of more realistic models for the associative desorption process. Further experiments with monocrystalline surfaces and variable sulfur coverage are in progress.

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## Solitons in a Coupled Linear Chain System\*

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The existence of solitons in two or more dimensions is discussed. Solitary-wave solutions are found for a system of discrete chains with a derivative of a periodic coupling between the chains. Relevance of the model to phase solitons in the Peierls condensate and in spin systems is discussed.

Recent studies have indicated the possible importance of solitons and solitary waves<sup>1</sup> in the dynamics of structural phase transitions<sup>2-4</sup> and in the low-temperature conductivity of one-dimensional conductors.<sup>5,6</sup> However, applicability of these ideas to real systems is limited because static soliton solutions were found only in strictly one-dimensional systems. Moreover, for higher dimensional continuous media with an elastic coupling  $(\nabla\phi)^2$  it is known that there are no static, finite-energy solitons.<sup>7,8</sup> In

this Letter, we present two model Lagrangians in two (or more) dimensions which can have soliton solutions and solve them explicitly for a particular potential.

As a first step we consider a system which is continuous in one spatial direction ( $x$ ) and discrete in any other—namely a set of chains. Thus the solutions may be discrete in all space directions except the  $x$  direction. If  $n$  is the chain index, then the field has the form  $\varphi_n(x, t)$ . On each chain we assume a potential<sup>9,10</sup>  $V(\varphi) = V(-\varphi)$  with two or more ground states (say at  $\varphi = \pm 1$ ) so that  $V(\pm 1) = 0 = V'(\pm 1)$  and  $V''(\pm 1) = \omega_0^2 > 0$ . The potential is such that in the absence of interchain coupling it leads to static soliton solutions  $\varphi_s(x)$

$$-c_0^2 \varphi_s''(x) + V'(\varphi_s) = 0, \quad \lim_{x \rightarrow \pm\infty} \varphi_s(x) = \text{sgn} x. \quad (1)$$

For the coupled-chain system we look for solutions which have solitons on some of the chains; more strictly, some of the chains have boundary values which differ at  $x \rightarrow \infty$  and  $x \rightarrow -\infty$ .

A crucial step now is the choice of the interchain coupling. The elastic coupling  $(\varphi_n - \varphi_{n+1})^2$  leads to infinite energies as the size of the system increases, if the fields on adjacent chains differ by a constant finite amount at the boundaries. Thus we choose the following Lagrangian:

$$L = \sum_n \int dx \left\{ \frac{1}{2} [\dot{\varphi}_n(x, t)]^2 - \frac{1}{2} c_0^2 [\varphi_n'(x, t)]^2 - V[\varphi_n(x, t)] - \lambda \varphi_n'(x, t) \varphi_{n+1}'(x, t) \right\}. \quad (2)$$

One can think of  $\varphi_n'(x, t)$  as a charge (as for “ $\varphi$  particles”<sup>6</sup> or for electric dipoles) and the derivative coupling in (2) as the interaction between these charges. By completing the squares of terms quadratic in spatial derivatives we note that the system is stable only for

$$|\lambda| < \frac{1}{2} c_0^2. \quad (3)$$

The equations of motion are

$$\ddot{\varphi}_n(x, t) - c_0^2 \varphi_n''(x, t) + V'[\varphi_n(x, t)] - \lambda [\varphi_{n+1}''(x, t) + \varphi_{n-1}''(x, t)] = 0. \quad (4)$$

Two observations can be made here. First, since we look for solutions of finite energy, we must have  $\lim[\varphi_n(x \rightarrow \pm\infty, t)] = \pm 1$  for all  $n$ . Thus,  $\dot{\varphi}_n(\pm\infty, t) = 0$  for any finite  $t$ , yielding a topological conservation law<sup>8</sup> for each chain separately. Hence a soliton cannot jump from one chain to another, and there is no annihilation. Thus the distinction between a soliton and a solitary wave<sup>1</sup> is not important here, as long as we consider one or no solitons on each chain. Second, the coupling term in Eq. (2), which was chosen on physical grounds, breaks the Lorentz invariance of the uncoupled system. However time-dependent solutions can still be generated from the static solutions  $\varphi_n^s[x; \lambda]$  using  $\lambda$  as a variable. Moving solutions for (4) are  $\varphi_n[(x - vt)/\gamma; \lambda/\gamma^2]$ , where  $\gamma^2 = 1 - v^2/c_0^2$ . Because of the stability condition (3),  $v$  is bounded by  $v^2 < c_0^2 - 2|\lambda|$ .

We wish to find static, localized, and stable solutions  $\varphi_n^s[x; \lambda]$  of (4). Stability means that perturbations  $g_n(x) e^{i\omega t}$  around the solution have frequencies  $\omega^2 \geq 0$ . The linearized equation for  $g_n(x)$  is

$$-c_0^2 g_n''(x) + V''(\varphi_n^s[x; \lambda]) g_n(x) - \lambda [g_{n+1}''(x) + g_{n-1}''(x)] = \omega^2 g_n(x). \quad (5)$$

Equation (4) is easily solved for an infinite array of solitons, and the stable configuration is

$$\varphi_n^s(x) = (-\text{sgn} \lambda)^n \varphi_s[x/(1 - 2|\lambda|/c_0^2)^{1/2}]. \quad (6)$$

The relative signs ensure that neighboring solitons attract each other. The lowest-frequency band of (5) starts at  $\omega^2 = 0$  and corresponds to transverse vibrations of the wall of solitons.

We consider now the important question of a single soliton. For a general  $V(\varphi)$ , only a perturbation approach is feasible. This is discussed below. However, for the particular choice<sup>11</sup>

$$V(\varphi) = \frac{1}{2} \omega_0^2 (|\varphi| - 1)^2, \quad (7)$$

the problem is exactly solvable. Equation (4) takes the form

$$-c_0^2 \varphi_n''(x) + \omega_0^2 \varphi_n(x) - \lambda [\varphi_{n+1}''(x) + \varphi_{n-1}''(x)] = \omega_0^2 \text{sgn} \varphi_n(x). \quad (8)$$

The eigenfunctions of the left-hand side are  $\exp(ikx + iqn)$  with frequencies

$$\omega_{k,q}^2 = \omega_0^2 + (c_0^2 + 2\lambda \cos q) k^2. \quad (9)$$

We try a solution which satisfies

$$\text{sgn}\varphi_n(x) = \begin{cases} \text{sgn}x, & n=0, \\ \eta_n, & n \neq 0, \end{cases} \quad (10)$$

where  $\eta_n$  can be chosen arbitrarily as  $\pm 1$ . Using the Green's function of the left-hand side of (8), we find

$$\varphi_n(x) = \begin{cases} [1 - I_0(x)] \text{sgn}x, & n=0, \\ \eta_n - I_n(x) \text{sgn}x, & n \neq 0, \end{cases} \quad (11)$$

$$I_n(x) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \cos qn \exp \left[ \frac{-\omega_0|x|}{(c_0^2 + 2\lambda \cos q)^{1/2}} \right].$$

Equation (11) represents a static solution with one soliton. The solution is analytic in  $\lambda$  (if  $2|\lambda| < c_0^2$ ), so that a perturbation expansion is valid. The energy of this soliton is given by

$$E = \omega_0 \int_{-\pi}^{\pi} \frac{dq}{2\pi} (c_0^2 + 2\lambda \cos q)^{1/2}. \quad (12)$$

Note that  $E = E(|\lambda|)$  is a decreasing function of  $|\lambda|$  and  $2\sqrt{2}/\pi \leq E/\omega_0 c_0 \leq 1$ . For the stability analysis in Eq. (5) we use the same Green's function method as for Eq. (8). We obtain a single bound state [ $g_0(0) \neq 0$ ] with  $\omega^2 = 0$  and the continuum  $\omega^2 = \omega_{k,q}^2$  for  $g_n(x) = \text{sink}x \exp(iqn)$ . This spectrum covers exactly the same values as the one-dimensional ( $\lambda = 0$ ) solution.

We emphasize that non-negative values of all eigenvalues  $\omega^2$  ensure the stability of the assumed solitary structure.

We have also considered the case of solitons on two distinct chains, say, on  $n=0$  and  $n=N$ . Stability analysis of this solution yields the usual  $\omega^2 = 0$  translational mode and an additional bound state with  $\omega_b^2$ . If the condition

$$\text{sgn}\varphi_N(x) = (-\text{sgn}x)^N \text{sgn}\varphi_0(x) \quad (13)$$

is satisfied, the interaction between the two solitons is attractive and  $\omega_b^2 > 0$ , corresponding to a vibrational mode of the bound pair of solitons. If, however, the two solitons repel,  $\omega_b^2 < 0$ , corresponding to breaking of the pair.

For a general  $V(\varphi)$ , a single-soliton solution for Eq. (4) cannot be obtained analytically. However, we expect some general properties of the exact solution presented above to remain valid. Namely, we expect a single chain soliton solution to exist and be analytic near  $\lambda = 0$ . Thus a perturbative approach (in  $\lambda$ ) seems appropriate. Using Eq. (1) we look for a solution

$$\varphi_n^s(x) = \begin{cases} \varphi_s(x) + f_0(x), & n=0 \\ \eta_n + f_n(x), & n \neq 0 \end{cases} \quad (14)$$

with  $f_n(x \rightarrow \pm\infty) = 0$ . To first order in  $\lambda$ , only the  $n = \pm 1$  chains are affected, and

$$f_{\pm 1}(x) = \frac{\lambda}{2c_0^2} \int_0^{\infty} \exp(-\omega_0 x'/c_0) [\varphi_s'(x'+x) - \varphi_x'(x'-x)] dx'. \quad (15)$$

For  $x \ll \omega_0/c_0$  we obtain  $f_1(x) \simeq -\varphi_s(x)/c_0^2$ ,  $f_0(x) \simeq \lambda^2 x \varphi_s'(x)/c_0^4$ , and  $\varphi_0^s(x) \simeq \varphi_s[x/(1 - \lambda^2/c_0^4)]$ . As in the solution (6), the coupling  $\lambda$  tends to form thinner solitons. The leading correction on the  $n$ th chain ( $n \neq 0$ ) is of order  $\lambda^{|n|}$ ; hence the solution decays exponentially as it moves away from the  $n=0$  chain.

Consider now the stability of (14). The translation mode  $g_n(x) = \varphi_n^s(x)$  is an eigenfunction of (5) with  $\omega^2 = 0$ . [This is shown by differentiating Eq. (4).] Since the potential  $V''(\varphi_n^s[x; \lambda])$  is localized, there are extended wave solutions with  $\omega^2 = \omega_{k,q}^2$ . We now compare this spectrum to the spectrum of (5) with  $\lambda = 0$ . On the  $n \neq 0$  chains we have only the continuum with  $\omega^2 = \omega_0^2 + c_0^2 k^2$ , while the  $n=0$  chain has also a bound state with  $\omega^2 = 0$  and possibly other discrete levels<sup>9,10</sup> with  $0 < \omega^2 < \omega_0^2$ . It is important to note that there is a single eigenfunction with  $\omega^2 = 0$ . This eigenfunction is the translation mode and, as  $|\lambda|$  increases, its frequency stays at  $\omega^2 = 0$ . Also the continuum edge remains at  $\omega_0^2$ . Analyticity in  $\lambda$  implies that for sufficiently small  $\lambda$  there is no level crossing so that  $\omega^2 \geq 0$  and the solution (14) is stable.

As a physical system which can be described by (2) we consider the phases of charge-density waves (CDW) in a Peierls condensate.<sup>6</sup> On each chain a phase soliton creates an excess of charge  $\sim \varphi_n'(x)$ . The Coulomb interaction of this charge with the CDW itself can be neglected if the soliton is much wider than the CDW periodicity. Assuming nearest-neighbor interactions only and neglecting current-current interactions ( $\sim \dot{\varphi}_n \dot{\varphi}_{n+1}$ ), we obtain the nearest-chain local interaction of Eq. (2).

In Ref. 6,  $V(\varphi)$  was assumed to be a commensurability potential. By now we recognize the limitations of this viewpoint and, as we show now, solitons appear also in the incommensurate case because of an interchain coupling in the condensed CDW phase. This coupling must be periodic in the phase differences between chains and should lead to a unique ground state, say  $\varphi_n - \varphi_{n+1} = \pi$ . Let us choose

$$V(\varphi) = \frac{1}{2}\omega_0^2(\varphi - \pi)^2, \quad 0 < \varphi < 2\pi, \quad V(\varphi + 2\pi n) = V(\varphi), \quad n \text{ integer}, \quad (16)$$

and use  $V(\varphi_n - \varphi_{n+1})$  instead of  $V(\varphi_n)$  in (2). We expect this coupling to lead to an effective periodic potential on each chain so that solitons are possible. The main difference is that now the linearized equation of motion has the spectrum

$$\tilde{\omega}_{k,q}^2 = (c_0^2 + 2\lambda \cos q)k^2 + 4\omega_0^2 \sin^2 q/2, \quad (17)$$

which starts at zero. The interchain coupling has no pinning effect and the system still has a Goldstone mode with  $\omega = 0$ .

Using the same methods as for Eq. (8), we obtain an exact single-soliton solution

$$\varphi_n(x) = (-)^n \pi/2 + \pi(\operatorname{sgn} x - 1)\delta_{n,0} - \tilde{I}_n(x) \operatorname{sgn} x, \quad \tilde{I}_n(x) = \int_0^\pi dq \cos qn \exp \left[ \frac{-2\omega_0 \sin q/2}{(c_0^2 + 2\lambda \cos q)^{1/2}} |x| \right]. \quad (18)$$

Stability analysis yields a continuous spectrum  $\omega^2 = \omega_{k,q}^2$  and a bound state with  $\omega^2 = 0$  (the translation mode).

We have also studied a second type of a Lagrangian which can have soliton solutions

$$L = \sum_n \int dx \left\{ \frac{1}{2} [\dot{\varphi}_n(x, t)]^2 - \frac{1}{2} c_0^2 [\varphi_n'(x, t)]^2 - V(\varphi_n - \varphi_{n+1}) \right\}, \quad (19)$$

where  $V(\varphi_n - \varphi_{n+1})$  is periodic. For  $V(\varphi)$  given by (16), obviously (18) with  $\lambda = 0$  is a single-soliton solution. It has an energy of  $E = 4\pi\omega_0 c_0$ . Equation (19) corresponds to a  $x$ - $y$  spin system where the continuum limit was taken in one direction.<sup>12</sup> This is consistent with a wide soliton solution,  $c_0/\omega_0 \gg 1$ .

If the continuum limit is taken for all spatial directions, the equations of motion for both Lagrangians (2) and (19) contain spatial derivatives higher than the second. This feature makes Derrick's theorem<sup>7</sup> inapplicable and allows for a large range of Lagrangians which can have soliton solutions. We find, however, the models (2) and (19) to be physically interesting and, in particular, to provide explicit single-soliton solutions for a chosen potential.

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