

Some Exact Results for One-Dimensional Models of Solids*

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(Received 16 July 1973)

Exact results are presented for one-dimensional models of a band problem, an elastic solid, and a classical relativistic field theory with broken symmetry.

In this paper we wish to report on a series of recent model calculations in one dimension. Although related mathematically, the models provide insight into a number of physical phenomena: band structure, phonon spectra, and relativistic field theory. The results contain both the expected and the unexpected.

Let us begin with the Schrödinger equation in one dimension, and ask first: For what potentials will we have reflectionless transmission at all energies? This question has been answered by Kay and Moses,¹ and if we require exactly one bound state, they find the potential to be essentially unique:

$$V(x) = -g/\cosh^2(x/r), \quad (1)$$

with

$$g = 2/r^2.$$

Now let us consider a lattice of such potentials. If the lattice constant is b , then the potential $U(x)$ will be given by the lattice sum,

$$U(x) = \sum_{n=-\infty}^{+\infty} V(x - nb). \quad (2)$$

We now ask the question: Will any aspect of perfect transmission persist in the lattice problem? The answer we find is affirmative; the band problem will be characterized by only two bands! This result might be surprising to solid-state physicists, although it is known in mathematics from a study of Hill's equation.² In fact, given the existence of exactly two bands, one proves that the potential must be an elliptic function.

Let us now perform the lattice sum indicated by Eqs. (1) and (2). Using a well-known expansion of the Weierstrass elliptic function $P(z)$ with periods ω_1, ω_2 (see Whittaker and Watson³), we have

$$U(x) = g \left(\frac{2\Omega}{\pi} \right)^2 P(z) + E_0, \quad (3)$$

where

$$r = 2\Omega, \quad b = 2\omega_2, \quad \omega_1 = i\Omega\pi, \quad z = x + i\omega_1 = x - \Omega\pi;$$

$$E_0 = -g \left(\frac{\pi}{2\omega_1} \right)^2 \left[\frac{1}{3} + \sum_{n=-\infty}^{+\infty} \text{cosec}^2 \left(\frac{n\pi\omega_2}{\omega_1} \right) \right].$$

Thus, using the relation between g and r , the Schrödinger equation for the wave function ψ becomes (subscripts indicate differentiation)

$$\psi_{xx} = [2P(z) + E_0 - E] \psi; \quad (4)$$

this is simply Lamé's equation³

$$\psi_{xx} = [n(n+1)P(z) + B] \psi,$$

with $n=1$. We defer discussion of the band structure until later, simply noting that periodic solutions of Lamé's equation occur in $n+1$ bands for n integer.² Thus the band problem of Eq. (4) has exactly two bands (henceforth to be called valence and conduction, respectively), instead of the usual infinity of bands.

How then do the usual simple "physical" arguments, as given in the elementary textbooks,^{4,5} for band gaps at each zone boundary go wrong? First, although our potential $U(x)$ can be made arbitrarily weak, it does not depend linearly upon a coupling constant, as in perturbation theory. But even these perturbation arguments may be rigorously justified only in the instance that $U(x)$ can be represented by a finite Fourier series.²

On the other hand, we may obtain an understanding from the following simple consideration: The potential $V(x)$ of an isolated site has one bound state and no reflection. Thus, if we imagine these atomic potentials strung together with a very large lattice constant so there is essentially no overlap, then, since there is no reflection from an isolated site, there is no Bragg reflection and hence only one band. The other band will arise from overlap of the bound states, and hence will be nearly degenerate in our limit of large lattice constant.

This argument is certainly not rigorous, but simply offered to supply a feel for the phenomena. It is a reasonable picture, since the size of the valence band gaps depends upon the reflection coefficient rather than overlap, in contrast to conduction band gaps.

We now turn to another problem, seemingly unrelated, which is the sine Gordon equation. This is a classical scalar field $\phi(x, t)$ in one space dimension. The Hamilton density is taken to be

$$\mathcal{H}C = \frac{1}{2} [\phi_t^2 + \phi_x^2 + 4m^2 \sin^2(\frac{1}{2}\phi)]. \quad (5)$$

This system and its higher-dimensional counterparts have arisen in such diverse physical situations as the Josephson effect, dislocation theory, and relativistic field theory. Such wide application might best be understood by remarking that Eq. (5) is the simplest example of an interaction periodic in the field. Thus, our system bears the same relation to a general periodic interaction as does Mathieu's equation to the general Hill equation. In addition to small-amplitude oscillations satisfying, in first approximation, the Klein-Gordon equation, and in second approximation a $\lambda\phi^4$ interaction, the system has static solutions corresponding to a kink or an antikink,

$$\phi^0(x) = 4 \tan^{-1} e^{\pm m(x-a)}. \quad (6)$$

Further, these kinks are completely transparent to small-amplitude oscillations.

We now wish to consider static solutions with a finite density of kinks (or antikinks), i.e., a kink crystal. The equation of motion for the ϕ field, as derived from the Hamiltonian, is

$$\phi_{xx} - \phi_{tt} = m^2 \sin\phi. \quad (7)$$

Thus, a static solution will satisfy

$$\phi_{xx}^0 = m^2 \sin\phi^0. \quad (8)$$

This equation may be transformed into the equation of motion of a pendulum,⁶ and may thus be integrated in the same way to yield

$$F\left[\frac{\phi^0}{2} \middle| -\left(\frac{2m}{\beta}\right)^2\right] = \frac{\beta x}{2}. \quad (9)$$

F is the incomplete elliptic integral; $\phi_x^0(0) = \beta$, $\phi^0(0) = 0$, fixing the location and spacing of the lattice.

We now consider small oscillations about the static solution, i.e., $\phi(x, t) = \phi^0(x) + \psi(x, t)$. Then ψ satisfies the equation

$$\psi_{tt} - \psi_{xx} + m^2 \cos\phi^0 \psi = 0. \quad (10a)$$

If we set $\psi(x, t) = \psi(x)e^{-i\omega t}$, then

$$\psi_{xx} + (\omega^2 - m^2 \cos\phi^0)\psi = 0. \quad (10b)$$

After a change of variables, and substitution of Eq. (9) for ϕ^0 , we find

$$\psi_{\alpha\alpha} = \left[2\mu \operatorname{sn}^2\left(\frac{\alpha}{\mu}\right) - \mu \left(1 + \frac{\omega^2}{m^2}\right) \right] \psi, \quad (11)$$

where

$$\alpha = [xm/(\mu)^{1/2}] - K(\mu), \quad \mu = 4m^2/(\beta^2 + 4m^2), \\ \operatorname{sn}(\alpha/\mu), \operatorname{cn}(\alpha/\mu), \operatorname{dn}(\alpha/\mu)$$

are the Jacobi elliptic functions with parameter

μ ; $K(\mu)$ is the complete elliptic integral of the first kind with parameter μ . We have transformed to positive parameter and hence to a real modulus.

We note that the relation of β (and thus μ) to the lattice constant b is given by

$$b = 2(\mu)^{1/2}K(\mu). \quad (12)$$

We now observe that this is an alternate form for Lamé's equation, again with $n=1$. The solutions are³

$$\psi(\alpha; \alpha_0) = \frac{H(\alpha + \alpha_0)}{\Theta(\alpha)} e^{-\alpha Z(\alpha_0)}, \quad (13)$$

and ω will be determined from

$$\mu \left(1 + \frac{\omega^2}{m^2}\right) = 1 + \mu \operatorname{cn}^2\left(\frac{\alpha_0}{\mu}\right) \equiv A \quad (14)$$

and the requirement that $Z(\alpha_0)$ be purely imaginary. H , Θ , and Z are Jacobi's eta, theta, and zeta functions with parameter μ .

The usual wave vector k will be determined from the equation

$$e^{-ibk} = -e^{-2kZ(\alpha_0)}, \quad (15)$$

and is necessarily real. Thus Eqs. (14) and (15) together determine the band structure of Eq. (4). We distinguish two cases.

Case 1: valence band. Let $\alpha_0 = K + ia$; then

$$A = 1 - \mu\mu_1 \frac{\operatorname{sn}^2(a/\mu_1)}{\operatorname{dn}^2(a/\mu_1)}, \quad (16a)$$

where $\mu_1 + \mu = 1$.

Case 2: conduction band. Let $\alpha_0 = ia$; then

$$A = 1 + \frac{\mu}{\operatorname{cn}^2(a/\mu_1)}. \quad (16b)$$

In both cases, a is restricted to lie between $\pm K(\mu_1)$. Thus the valence band lies within $m^2\mu_1/\mu \geq \omega^2 \geq 0$, and the conduction band above $\omega^2 \geq m^2/\mu$. The band gap is $m^2/\mu \geq \omega^2 \geq m^2\mu_1/\mu$.

Figure 1 shows the energy as a function of wave vector for a particular value of the lattice constant b comparable to a single kink width. The actual value is $\mu = \frac{1}{2}$, $bm = 2.61$. This figure is appropriate to a band problem.

Figure 2 shows frequency as a function of wave vector for the same parameters as Fig. 1.

As has been noted,⁷ the sine Gordon equation serves as a very interesting model of a relativistic field. Upon analyzing small oscillations about a single kink, it is found that the bound state in fact corresponds to a rigid translation of the kink. Thus, the valence band in fact is made of correlated translations of the individual kinks, and is properly identified as the phonon mode of our original kink crystal (or, if one wishes, the Gold-

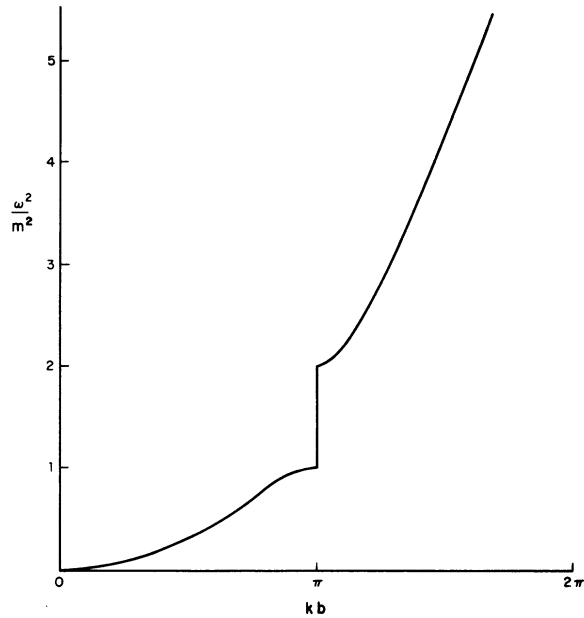


FIG. 1. Energy is shown as a function of wave vector for the band problem when the lattice constant b is $2.61/m$.

stone bosons associated with broken translational invariance). This phonon mode is shown as the lowest dispersion curve of Fig. 2. The remaining conduction band corresponds to renormalized Klein-Gordon bosons.

Thus, to summarize our reinterpretation of the problem as an elastic solid, we have determined the phonon modes of a one-dimensional crystal in the harmonic approximation. The harmonic approximation is appropriate for a classical problem. But we have included interactions between all particles, not just near neighbors, since the interaction is exponential for large distances.

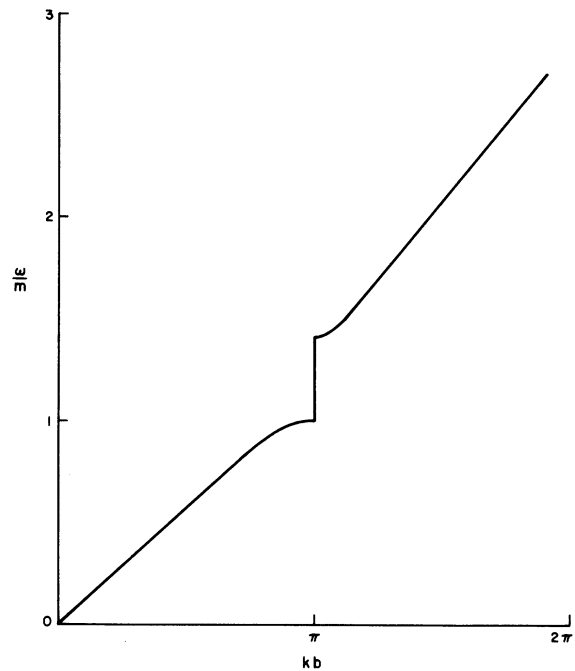


FIG. 2. Phonon frequency ω is shown as a function of wave vector for the same lattice constant as Fig. 1.

And, of even greater interest, our particles making up the crystal are not points, but extended polarizable bodies, as are real atoms and molecules. Thus, our interaction is not given by a simple two-body potential.

As might be expected, at finite temperatures there is no long-range crystalline order, since the interaction is essentially exponential at large distances. In fact, all thermodynamic properties of the sine Gordon equation can be evaluated by functional integral methods, and will be presented in a subsequent publication.

*Work supported in part by National Science Foundation under Grant No. GP38905.

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