Theory of the structure and lattice dynamics of incommensurate solids: A classical treatment

Anthony D. Novaco
Lafayette College, Easton, Pennsylvania 18042
and Brookhaven National Laboratory, Upton, New York 11973
(Received 17 December 1979)

A classical theory of the static strains and lattice dynamics for solids possessing incommensurate structures is developed using a spatial Fourier representation of the static strains and a space-time Fourier representation of the dynamical modes. Although the theory is presented for one-dimensional systems, the general technique is not restricted to such systems and can be applied in a straightforward manner to problems in two or three dimensions. A set of coupled, nonlinear equations is derived for the amplitudes and phases of the strains and a controllable sequence of approximations is described for finding the solutions to these equations. Excellent results are obtained using only low-order terms in various truncated expansions even for those cases where the domain walls are quite narrow. It is shown that provided the amplitudes of the dynamical oscillations are small enough, normal modes do exist even in the limit of large static strains. However, these modes are not characterized by a single wave vector but rather have important contributions from density fluctuations of various wavelengths. Strong evidence is given for the energy at zero kelvin of the one-dimensional system being a nonanalytic function of the mean lattice spacing of the type described by Aubry. This means that the pressure is a discontinuous function of the mean spacing with discontinuities existing at rational values of this spacing. The sizes of these discontinuities decrease rapidly as the order of the commensurate state increases. Each commensurate state would thus exist over a finite pressure range and the system will exhibit a "devil's-stair" behavior at zero kelvin.

I. INTRODUCTION

The last several years have witnessed an intensive effort to understand the essential physics of those aperiodic solids which are formed by the aperiodic crystal structures, making the theory of such solids much more complicated than that for the usual periodic system. The incommensurate structures are characterized by some non-symmetry wave vector, they lack the translational and rotational symmetries characteristic of ordinary crystal structures, making the theory of such solids much more complicated than that for the usual periodic system. Examples of such solids are abundant, and the incommensurate structure can involve (either separately or in combination) the electron charge density (eDW), the magnetic density (SDW), or the mass density (MDW) of the solid. The nature of the transition is still a matter of some controversy, with theoretical results showing both continuous and discontinuous transitions. Recent theoretical work has indicated that the transition is, at least in one dimension and zero kelvin, a continuous transition with an unusual nonanalytic nature described as a "devil's stair." Our results show that this devil's stair (which we shall describe in detail later) is the correct description in the absence of thermal and quantum fluctuations.

A model which has been used extensively in the theoretical study of the IC transition is the Frenkel-Kontorova model which consists of a linear chain of point masses connected by springs and subject to an external sinusoidal potential. This "sine-Gordon" chain was examined by Frank and van der Merwe in the long-wavelength or continuum approximation which reduces the problem to solving the sine-Gordon equation. The transition was found to be continuous in this limit. Later studies by Ying indicated that the IC transition in the discrete lattice problem was discontinuous or first order. Recent work by Theorod'orou and Rice indicates that the results of Ying were generated by the approximations used, and that even in the discrete case the transition is continuous. Their results are consistent with the findings of Aubry. Aubry found that the transition appears continuous, but consists of an infinite number of closely spaced transitions, one at each commensurate value of the mean lattice constant. Most of these transitions produce effects which are infinitesimally small and these small effects "smooth" out at finite temperature with the lowest-order commensurate phases being the most stable. At high temperature, the incommensurate phase dominates the phase diagram. This is the model which we chose as a test case for our theory. It is clear that the study of a system with such a complicated behavior requires a very carefully con-
structed theory whose approximations can be carefully controlled.

Many of the techniques which are used to study the sine-Gordon chain rely heavily upon its simple structure or one-dimensional character. Such techniques cannot be extended to more complicated models nor to systems in higher dimensions in any obvious manner. We propose a new approach to the statics and dynamics of this problem which is, in principle, not restricted to either a one-dimensional system nor to a simple sinusoidal potential. Furthermore, many of the features of this technique appear to be applicable to models which involve realistic potentials and/or quantum effects. Although the method is exact in principle, approximations are required to obtain numerical results. However, the errors made by these approximations can be made arbitrarily small and calculated results compare favorably with the exact numerical simulations of Sacco and Sokoloff. The structure of the general equations is useful in discussing general properties of the system and we can prove certain exact results based upon their functional form.

In Sec. II we describe the equations for the static strains and discuss some of the general properties of the static solutions. In Sec. III, we show how to describe the dynamics of the chain and derive the equations for the "normal modes" of the system. These modes are shown to exist provided the amplitudes of the dynamical oscillations are small enough. In Sec. IV we compare the numerical results of the above theory to the numerical simulations referenced above and show that the agreement is excellent. The solutions are then examined in the vicinity of low-order commensurate states and they are found to demonstrate the unusual properties discussed by Aubry.

II. STATIC STRAINS

The structure of the classical linear chain of coupled particles (atoms) subjected to a periodic external potential field (substrate) is determined by a delicate balance between interchain forces and chain-substrate forces. When the period of the chain and that of the substrate are incommensurate (that is, their ratio is an irrational number) this problem becomes quite complicated. Even for a high-order commensurate phase (rational ratio), the problem is not simple since there are a large number of atoms per unit cell. There is little difference (both physically and mathematically) between the high-order commensurate phases and the incommensurate phase. In fact, the latter is the limit, as the size of the unit cell goes to infinity, of a sequence of commensurate phases.

When the periods of the two lattices are incommensurate, the contributions to the energy due to the chain-substrate interaction must be treated with great care since the two lattices move "in" and "out" of phase with each other in a complicated way as one moves along the chain. Approximations which rely upon the displacement of an atom in the chain relative to some chosen lattice site on the substrate being "small" will not properly describe the energy contributions in the region of the domain walls since many particles in this wall will be near the maximum in the substrate potential not near the bottom of the well. Even near the transition, when large domains of the system are nearly in registry with the substrate, the domain-wall energy and the wall-crossing energy may not be properly treated and these terms are important in the determination of the physics of the transition. Approximations which rely upon the displacement of an atom in the chain from a lattice site of the undistorted lattice being small also cannot properly describe the situation near the transition since here the distortions can be quite large. In fact, these distortions diverge if a simple perturbation theory is used to describe the approach to the registered phase. To avoid these problems, we transform the entire problem into momentum or wave-vector space and write a set of coupled, nonlinear equations for both the space and the space-time Fourier amplitudes. These equations are exact and from their general form one can prove that there are certain characteristics that the system must possess. To obtain numerical solutions for a particular case, approximations must be made in the treatment of these amplitudes and their coupling. However, the solutions to the approximate equations are "well behaved" and do not have any of the singularities associated with some models which use real-space approximations. The low-order equations are quite tractable and generate excellent results. The higher-order equations are manageable and can, in principle, give results which are arbitrarily close to the exact result.

The sine-Gordon chain which we examine is a linear chain of atoms with mass \( \mu \), each atom connected to its nearest neighbor by a spring whose spring constant is \( k \) and whose unstretched length is \( c \). The substrate subjects the chain to a periodic potential whose period is \( b \) but whose shape is otherwise arbitrary. The entire chain of \( N \) atoms has a length of \( N \) times \( a \), where \( a \) is the average or mean lattice parameter, and the chain is subject to periodic boundary conditions with \( N \rightarrow \infty \) in the usual way. The equilibrium positions at zero kelvin are determined by minimizing the total energy of the system, subject to the above boundary.
conditions. The equations for the incommensurate system are obtained by taking the limit as $N \to \infty$ with $a/b$ an irrational number. The substrate and chain lie along the $x$ axis and the substrate potential $U(x)$ is written as a Fourier series with

$$U(x) = \sum \tilde{U}_G \exp[iG(x - \Delta)], \quad (1)$$

where $\tilde{U}_G$ is the Fourier amplitude associated with $G$, a reciprocal-lattice vector of the substrate lattice, and the sum is over all $G \neq 0$. The $\tilde{U}_G$ are real and symmetric in $G$. The parameter $\Delta$ represents the displacement of some chosen inversion symmetry point of the substrate relative to the origin. An atom of the undistorted chain is placed at the origin, and varying $\Delta$ slides the substrate relative to the chain. If $R_j$ represents a lattice vector for the chain, then $u_j = x_j - R_j$ gives the displacement of the $j$th atom from its ideal position.

If $\{q_m\}$ represents the set of equivalent $G_m$, then the above mapping takes a finite set of equivalent $G_m$. In this case, only a finite number of terms are needed in the sum in Eq. (3). If the $\{q_m\}$ and $\{R_j\}$ are incommensurate, then the above mapping is one to one for all $q_m$ and $G_m$ and Eq. (3) contains an infinite sum of terms.

The first step is to minimize $\Phi$ as a function of $\langle u_j \rangle$ and rewrite the entire expression in terms of the $\tilde{u}_m$. For those cases where $\{q_m\}$ does not contain zone-boundary terms, one finds that

$$\mu \omega_m^2 \tilde{u}_m = \sum G \tilde{U}_G \exp[-i(G - q_m)R_j] \times \frac{1}{N} \sum \exp[iG \sum \tilde{R}_n \sin(qR_j - \theta_n)], \quad (4)$$

where

$$\Omega_g = G \Delta \quad (5a)$$

and

$$\omega_m = \{2(k/\mu)[1 - \cos(q_m n)]\}^{1/2} \quad (5b)$$

is the vibrational spectrum for the undistorted linear chain. Equation (4) holds true for incommensurate states and commensurate states with an odd number of particles in a unit cell. Appendix A shows how to treat those cases (even number of particles per unit cell) where zone-boundary modes are needed to describe the distortions. The summation over $j$ in Eq. (4) can be carried out explicitly by first expanding the last exponential term in Eq. (4) and the summations over the real-space lattice sites can be carried out explicitly. As result of these manipulations we find

$$\mu \omega_m^2 \tilde{u}_m = \sum G \tilde{U}_G \sum_{J_{-v_1}(G \tilde{R}_1) \cdots J_{-v_n}(G \tilde{R}_n)} \exp[i(G - q_m + v_1 \theta_1 + \cdots + v_n \theta_n)] \Delta_+ (G - q_m + v_1 q_1 + \cdots + v_n q_n), \quad (7)$$

where $\Delta_+$ is the periodic Kronecker delta with period $\tau$. If the system is in a commensurate phase, then the products and sums in Eq. (7) contain $n$ terms where $n$ is finite and equal to the number of atoms in the commensurate unit cell minus one. If the system is incommensurate then the number of atoms in the unit cell $\rightarrow \infty$ and $n \to \infty$. Formally, Eq. (7) applied to the incommensurate case means an infinite number of terms in Eq. (3) and the replacement of the periodic Kronecker delta in Eq. (3) by the ordinary Kronecker delta. This requires that the $q_m$ are replaced by the equivalent $G_m$ in the arg-
ument of the delta symbol. For the purposes of obtaining numerical solutions to the above equations, Eq. (3) must then be truncated at a finite (although perhaps large) number of terms and the Bessel-function expansion must be truncated in some manner. To treat the various products of Bessel functions, we reorder the terms in Eq. (7) and classify all terms by the “order” of the product, the order being defined by

$$\nu = \sum_{j=1}^{\infty} |\nu_j|.$$  (8)

This is a much more efficient way of generating the important coupling terms than a simple truncation in each summation over \(\nu\). To solve Eq. (7), we first introduce the set of real functions \(F_m\) and \(F'_m\) through the definition

$$\mu \omega^2 \tilde{u}_m = F^R_m - iF'_m,$$  (9)

where \(F^R_m\) and \(F'_m\) are evaluated through comparison to Eq. (7). We now introduce the derivatives of these functions with respect to the \(\bar{n}_i\) and \(\theta_i\) parameters defining the matrices

$$\begin{align*}
C^m_{n,t} &= \frac{\partial}{\partial \bar{n}_t} F^R_m, \\
C^m_{n,i} &= \frac{\partial}{\partial \theta_i} F^R_m, \\
D^R_m &= \frac{\partial}{\partial \bar{n}_t} F'_m, \\
D^R_m &= \frac{\partial}{\partial \bar{n}_i} F'_m,
\end{align*}$$  (10a-10d)

and write the \(F\) functions in a Taylor-series expansion about some chosen \(\{\bar{n}_m, \theta_m\}\) keeping only the linear terms. Equation (7) then becomes a set of coupled equations which can be rewritten as

$$\begin{align*}
\mu \omega^2 \tilde{u}_m &= C^m_{n,t} \tilde{u}_t - D^R_{n,t} \theta_t \\
&= F^R_m(\bar{\rho}_m, \theta^0) - C^R_m \bar{n}_t - D^R_{m,t} \theta_t, \\
- C^R_m \bar{n}_i - D^R_{m,i} \theta_i &= F'_m(\bar{\rho}_m, \theta^0) - C^f_m \bar{n}_i - D^f_{m,i} \theta_i,
\end{align*}$$  (11a-11b)

where the Einstein summation convention is used to indicate the summations over indices, and the \(C\) and \(D\) matrices are evaluated at \(\{\bar{n}_m, \theta_m\}\). The iteration of Eqs. (11) is essentially a multidimensional Newton’s-rule technique for solving Eq. (7), and in many cases the iterations converge very quickly starting from \(u^0_m = \theta_m^0 = 0\). For those cases where convergence from zero strain is poor, solutions are obtained by starting from the solutions of Eq. (7) at nearby values of \(a\) and/or \(U_a\). Thus it is possible to bootstrap the solutions from weak coupling to strong coupling and find the solutions at any value of \(a\) or \(U_a\). Once the amplitudes and phases have been calculated, it is straightforward to evaluate the energy as a function of the mean lattice constant.

The energy calculation is carried out using the same Bessel-function expansion used to generate Eq. (7). Writing \(\Phi\) in terms of the \(u_m\) we have

$$\frac{1}{N} \Phi = \frac{1}{2} k d^2 + \frac{1}{2} \sum_{m} \mu \omega^2 \bar{u}_m^2 + \sum_{n=1}^{\infty} \sum_{\nu=1}^{\infty} \sum_{\gamma=1}^{\infty} J_{\nu} G_{\gamma} J_{\nu} G_{\gamma} \left( \cos(\theta_\nu + \nu \theta_\gamma + \cdots + \nu \theta_\nu) \times \Delta_\nu (G + \nu \theta_\gamma + \cdots + \nu \theta_\nu) \right).$$  (12)

The imaginary part generated by the complex exponential term is zero (as it must be) by the symmetry properties of the \(u_m\). In writing Eq. (12), it has been assumed that zone-boundary terms are not included. For those cases with a commensurate unit cell having an even number of particles, this wave vector must be included and we again refer the reader to Appendix A for the treatment of that case.

The structure of the equations for both the strain amplitudes and the energy terms can be used to demonstrate some properties of the exact solutions. For example, it is easily shown that the energy of the static solution is independent of \(\Delta\) for incommensurate states. This property of the incommensurate state shows that the \(\Delta = 0\) solution (which means all \(\theta_m = 0\)) is the lowest-energy solution, and this simplifies the actual calculation of these energies. The transformation that generates the new strain amplitudes and phases \(\{u'_m, \theta'_m\}\) under \(\Delta' = \Delta + \delta\) is given by

$$\begin{align*}
\theta'_m &= \theta_m + G m \delta, \\
\bar{u}'_m &= \bar{u}_m.
\end{align*}$$  (13a-13b)

These equations show that \(\bar{u}_m\) is invariant under the translation of the substrate, and shifting one lattice with respect to the other results in a change only in the phases of the strain amplitudes and not their magnitude. This property of the system guarantees that \(\Phi\) is invariant to changes in \(\Delta\) as can be proven by insertion of Eqs. (13) into Eq. (12). It is thus possible to slide the film over the substrate without energy cost and this implies the existence of the zero-frequency mode (Goldstone boson) which has been called the sliding mode. The proof of energy invariance fails for commensurate states because a given \(q_m\) can be mapped into many \(G\) vectors. Note that the movement of one lattice
with respect to the other is not the equivalent to a simple translation of the chain relative to the substrate, but includes both a shift and internal rearrangement of atoms.42 This can be seen by inserting Eqs. (13) into Eq. (3). Nevertheless, the difference between the incommensurate state and a high-order commensurate state with nearly the same mean lattice parameter involves only the manner in which the very-high-order Bessel functions contribute to both the strain wave amplitudes and the energy. Therefore there can be little difference between the structure and energy of the high-order commensurate phase and an incommensurate phase with essentially the same mean lattice constant.31

Finally, it should be noted that our statements and results for the incommensurate system and the IC transition hold true (a) only for those systems with periodic boundary conditions and (b) when the expansion in Eq. (3) converges properly.55 The periodic boundary conditions exclude systems with free ends and thus exclude edge-pinning effects.43 The physical consequences of the restriction on convergence we have not yet fully explored. However, we expect that this mathematical constraint places two related restrictions on the substrate potential. This potential should not have any "sharp" breaks nor should it be so strong as to produce a "defectable" system.5 Throughout the rest of this paper, we shall assume that we are dealing with such a system.

III. DYNAMICAL MODES

The motions of the atoms in a periodic lattice are described in terms of normal modes, each mode being characterized by a wave vector \( q \) and representing a density wave with this wave vector. Since the system being studied is aperiodic, \( q \) will no longer be a well-defined label for a normal mode and each normal mode will consist of several coupled density waves of various \( q \) values. Furthermore, if the amplitude of the dynamical oscillation is not small enough, the normal modes will couple strongly and may not exist as well-defined characteristic motions.

We begin by writing \( H \), the Hamiltonian for the system, simply by adding the momentum terms to the potential energy of Eq. (2). We now have

\[
H = \sum_j \frac{1}{2} P_j^2 + \Phi.
\]

We first introduce \( A_q(t) \) and \( P_q(t) \), the time-dependent spatial Fourier transforms of \( u_j \) and \( p_j \) and then rewrite \( H \) in terms of these transforms. Since the transformation is canonical, we can use the \( A_q \) and \( P_q \) as our new coordinates and momenta. Then we obtain the dynamical equations for \( A_q \) and \( P_q \) from Hamilton's equations. To solve these equations, we introduce the time Fourier transform of \( A_q \) with \( A_q^0 \) and \( \theta_q^0 \) being, respectively, the amplitude and phase of the component having frequency \( \omega_q \). The \( u_j \) can now be written as

\[
u_j = \sum_q A_q^0 \sin(q R_j - \omega_q t - \theta_q^0), \tag{15}\]

where the sum over \( q \) is over all wave vectors within the first Brillouin zone. The frequencies \( \omega_q \) are labeled such that \( \omega_0 = 0 \) and \( \omega_{\pm q} = -\omega_q \). The \( A_q^0 \) and \( \theta_q^0 \) are both real and both antisymmetric in the simultaneous inversion of \( q \) and \( \theta \). The \( A_q^0 \) term in Eq. (15) is the analog of the \( \tilde{u}_m \) in the purely static case, but it is now determined along with the finite frequency amplitudes and can be affected by them. The equations for the \( A_q^0 \) are obtained in much the same way as the equations for the \( \tilde{u}_m \) were obtained in Sec. II. Following the development of the static case we find

\[
(\omega_q^2 - \omega_n^2) A_q^0 = \frac{1}{\mu} \sum_{\ell} G_{\nu,\ell} \sum_{\ell_0} \cdots \sum_{\nu_0} \{ J_{\nu_1} (G A_{\ell_1}^0) \cdots J_{\nu_n} (G A_{\ell_0}^0) \} \exp(\Theta_{\ell} - \Theta_{\ell_0}^0 + \nu_1 \theta_{\ell_1}^0 + \cdots + \nu_n \theta_{\ell_0}^0) 
\times \Delta_{\nu} (G - q + \nu_1 \ell_1 + \cdots + \nu_n \ell_0) \delta(\omega_q - \nu_1 \omega_{\ell_1} - \cdots - \nu_n \omega_{\ell_0}), \tag{16}\]

where the number of terms in the product of Bessel functions is the number of \( q \) vectors times the number of frequency values needed for a complete description. For small values of \( A_q^0 (\sigma = 0) \), the above equation takes the form of an eigenvalue equation even if the static strains (the \( \sigma = 0 \) terms) are quite large. In this limit the static and dynamical amplitudes decouple into two sets of equations. The static equations reduce to those of the last section and the dynamical equations take the "standard" form of an eigenvalue problem for a generalized dynamical matrix. For the incommensurate case, this dynamical matrix is of infinite order, but the off-diagonal elements decrease rapidly as one "moves" away from the main diagonal.

The frequencies and amplitudes of the incommensurate state are invariant to a translation of the substrate relative to the chain, this translation causing a shifting of phases. The proof is virtually identical to the corresponding proof for the static \( \tilde{u}_m \).

It can be seen that Eq. (16) does not have the
form needed for normal modes since motion with frequency $\pm \omega$ generates higher harmonics $\pm 2\omega$, $\pm 3\omega$, etc. However, if we assume that the $A^o_{\nu}$ are arbitrarily small for $\sigma \neq 0$, then we can show that the equations for these $A^o_{\nu}$ have the usual eigenvalue problem form and the $A^o_{\nu}$ are just the $\bar{u}_n$ of Sec. II. Only in this limit do normal modes exist in the usual sense and the static problem decouples from the dynamical problem. To show this we note that $J\nu(x) \propto x^x$ as $x \to 0$, and in the limit of small dynamical oscillations we can ignore all $J\nu(G\bar{u}_n^*)$ for $\sigma \neq 0$ except the following:

(a) In the equations for the dynamical amplitudes we must include those terms where $\sigma \neq 0$ but where one $\nu_\sigma$ equals $+1$ or $-1$ and all the other $\nu_\sigma = 0$.

(b) In the equations for the static amplitudes we need only those $\sigma \neq 0$ terms where $\nu_\sigma = 0$.

Those terms in the equations for the dynamical amplitudes where $\sigma \neq 0$ but all $\nu_\sigma = 0$ sum to zero because of the symmetrical nature of $\bar{u}_n$ to the $G \to -G$ transformation. Since $J\nu(0) = 1$, the equations for $A^o_{\nu}$ are identical to those for the $\bar{u}_n$ as long as the dynamical oscillations are very small, and thus we have $A^o_{\nu} = \bar{u}_n$. After some reduction, the remaining terms for the dynamical $A^o_{\nu}$ can be put into the form of an eigenvalue equation for a dynamical matrix. Using the summation convention, the form of the equations is found to be

$$D_{\nu m}A^o_{\nu m} = \omega^2 A^o_{\nu m},$$

where we have defined the dynamical matrix $D_{\nu m}$ to be

$$D_{\nu m} = \frac{1}{\mu} \sum_r \alpha^2 \beta_{\nu m} \sum_{r_1} \cdots \sum_{r_n} \left[ J_{\nu r_1}(G\bar{u}_1) \cdots J_{\nu r_n}(G\bar{u}_n) \right] \exp \left\{-i[\Omega_\nu - (\theta_{\nu m} - \theta_{\nu m}) + \nu_1 q_1 + \cdots + \nu_1 q_1] \right\} \times \Delta_\nu \left[ \Omega - (q_m - q_m) + \nu_1 q_1 + \cdots + \nu_1 q_1 \right].$$

(17)

In the incommensurate case the mapping from $q_m$ to $G_m$ is the same as in the static case. For the commensurate case the mapping is $q_m = q + G_1 + \tau_1$, where $q$ is a wave vector in the range $-q_{2n}$ to $+q_{2n}$ and $q_m$ is one-half the smallest $q_i$ such that $q_{2n} - q_m = G_1 + \tau_1$. Thus for the incommensurate case Eq. (17) is a single matrix equation of "infinite" order while for the commensurate case it is block diagonal and decomposes into an infinite set of matrix equations, each member of the set labeled by $q$ and being of finite order. The $q_{2n}$ are the zone-boundary modes for the unit cell of the commensurate state.

The dynamical amplitudes in Eq. (16) contain one $q$ vector not included in the static amplitudes given by Eq. (7), this being $q = 0$. Because of this, there appears in Eq. (16) a solution for the incommensurate case having $\omega_\sigma = 0$ but which does not appear directly in Eq. (7). This is the zero-frequency phason mode which is the Goldston boson guaranteed by the invariance of the energy of the incommensurate state to translations of the substrate by $\Delta$. If one describes the motion of the chain with respect to the substrate, the continuous transformation which leaves the energy of the incommensurate ground-state invariant can be obtained from Eq. (13) and it is given by

$$u_j = \Delta - i \sum_n \bar{u}_n \exp[iG_n(R_j + \Delta)].$$

(19)

The substrate is now fixed and the chain particles are moved to the right by an average displacement of $\Delta$. The $\{\bar{u}_n\}$ is the solution to Eq. (7) for $\Delta = 0$. This transformation consists of an average displacement and an internal rearrangement of atoms corresponding to the movement of the domain walls. It is straightforward to show that the $A^o_{\nu}$ defined thru Eq. (19) explicitly solve Eq. (16) provided the state is incommensurate and $\omega_\sigma = 0$. Thus the dynamical matrix given by Eq. (18) will have a zero eigenvalue for any incommensurate state.

IV. THE DOMAIN-WALL STRUCTURE AND ITS ENERGY

The advantage of using the Bessel-function expansion can be seen by examining the solutions for $\bar{u}_n$ in the lowest-order equations where only the $J\nu$ terms appear on the right-hand side of Eq. (7). In this approximation, there is no coupling between harmonics and if only the lowest-order expansion is used for the substrate potential we have

$$\mu \omega^2 \bar{u}_1 = G_1 \bar{J}_0(G\bar{u}_1).$$

(20)

As $a = b$, $\tau_1 = G_1$, $\omega_\sigma = 0$, and $G\bar{u}_1 - z_1$, the first root of $J_0$. In perturbation theory one would find $x_1 \to \infty$ in this same limit, yet the amplitudes of the waves saturate even in the lowest order of the nonlinear theory. The first zero of $J_0$ is about 2.4, so one finds that in this approximation the maximum amplitude is $2.4/2\pi$ in units of $a$. The actual value of the maximum amplitude is, as we shall see later, $1/2\pi$. Although the lowest-order approximation is not very good quantitatively as $a \to b$, it does have the proper qualitative behavior. To obtain better quantitative results in this limit we must
obviously include higher-order terms. Similar results are found as one approaches any commensurate ratio of \( a \) to \( b \).

The zero kelvin energy of the Frankel-Kontonova model (the only nonzero \( \mathcal{U}_c \) are \( \mathcal{U}_{0} \) and \( \mathcal{U}_{-a} \)) has been calculated quite accurately by Sacco and Sokoloff for various \( a/b \) ratios via a numerical solution to the real-space difference equations for the equilibrium positions of the particles. Following Frank and van der Merwe, they define the parameter \( l_0 \) where in our notation

\[
l_0 = b(kb^2/8Uc_{1})^{1/2}.
\] (21)

The \( l_0 \) parameter determines the relative strength of the intrachain and chain-substrate forces and is, in the continuum approximation, the size of the domain wall. The mass-density wave energy depends only on \( l_0 \) and this is what was calculated by Sacco and Sokoloff. The uniform strain term \( -\mathcal{W}Nk\alpha^2 \) must be added to this strain energy to obtain the total energy. Table I contains a comparison of the mass-density wave energy calculated via Eq. (12) and that calculated by Sacco and Sokoloff. This comparison is made at several \( \alpha/b \) ratios for an \( l_0/b \) value of 4, a "strongly" substrate-coupled system. In calculating the strain amplitudes and the corresponding energy, the equations of Sec. II were reduced via the method described in Appendix B. The agreement between our harmonic-coupling calculation and the Sacco-Sokoloff results is very good even though the harmonic-coupling calculation was truncated at moderately low orders.

The structure of the incommensurate solid near registry \((\alpha = \beta)\) is described in the continuum approximation by large regions where the particles in the chain are locked into the substrate potential wells with these regions separated by narrow regions or domain walls. At the domain walls, there is a poor match between the position of the atoms and the substrate potential wells. This structure is expected to be the same in the discrete lattice problem and it is possible to check the calculated Fourier amplitudes to see if the anharmonic calculation is producing a reasonable picture of the system near registry. In Fig. 1 we show a schematic plot of the displacement of the atoms near registry and an "idealized" displacement for domain walls whose width is infinitesimally small. This sharp domain-wall limit is convenient to use, since the Fourier amplitudes can be calculated analytically and are given by

\[
\tilde{u}_n = \left(\frac{(-1)^n}{2\pi Nk}\right) b_n \quad (n \neq 0),
\] (22a)

\[
u_j = \sum_{n=-\infty}^\infty \tilde{u}_n \sin\left(\frac{2\pi n}{b} j nR\right).
\] (22b)

The Fourier amplitudes of the continuum prediction will differ from Eq. (22) only in the higher-order terms, so we can expect our calculation to agree with these equations for the lowest values of \( n \). Table II compares the harmonic-coupling calculation for a chain near registry to the values obtained from the equations above. The agreement is very good with the amplitudes calculated from Eq. (7) decreasing faster than those of Eq. (22). This is to be expected since the actual system will have a finite domain-wall width similar to that predicted by the continuum limit.

The structure of the domain walls near the registry-deregistry transition appears to be given reasonably well by the continuum limit. To see why this is the case, it is important to remember that Eq. (22) provides an upper bound to the Fourier amplitudes, and that the actual amplitudes will decrease faster than \( 1/n \) for finite-size domain walls.

<table>
<thead>
<tr>
<th>( a/b )</th>
<th>( E^a )</th>
<th>( m )</th>
<th>( \nu = 0 )</th>
<th>( \nu = 1 )</th>
<th>( \nu = 2 )</th>
<th>( \nu = 4 )</th>
<th>( \nu = 9 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.601</td>
<td>-0.04334</td>
<td>2</td>
<td>-0.04240</td>
<td>-0.04317</td>
<td>-0.04317</td>
<td>-0.04317</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>-0.04321</td>
<td>-0.04322</td>
<td>-0.04322</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6</td>
<td>-0.04320</td>
<td>-0.04326</td>
<td>-0.04329</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.80</td>
<td>-0.10906</td>
<td>2</td>
<td>-0.10844</td>
<td>-0.10894</td>
<td>-0.10906</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.95</td>
<td>-0.57535</td>
<td>4</td>
<td>-0.3894</td>
<td>-0.5428</td>
<td>-0.5482</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6</td>
<td>-0.3888</td>
<td>-0.5675</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>8</td>
<td>-0.3888</td>
<td>-0.5729</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>-0.3985</td>
<td>-0.5746</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^a\)Taken from Ref. 43.

\(^b\)Calculated from Eq. (12).
FIG. 1. Comparison between displacements for domain walls of zero width (---) versus that for a more realistic case (---). The long-wavelength portion of the Fourier transforms of both cases are similar. The zero-width case has strain amplitudes given by Eq. (22a).

Furthermore, as \(a \rightarrow b\), the primary wave vector \(q_i\) where
\[
q_i = 2\pi(1/b - 1/a)
\]  
(23)
goes to zero as \(a \rightarrow b\). Since in this limit, \(q_n = nq_i\) \((n = \pm 1, \pm 2, \ldots)\), the region in wave-vector space needed to describe the strains associated with the domain walls collapses to zero but becomes highly dense with "relevant" wave vectors. In this limit, we can expect also to replace \(\omega_q\) by \(cq\) where \(c\) is the sound velocity. But if \(\omega_q\) is replaced by \(cq\), then the amplitudes are just those generated by the sine-Gordon equation. At what value of \(q_n\) can we expect to see significant effects due to the discrete lattice we have yet to examine in detail.

We have also examined the domain-wall structure near the \(a = \frac{1}{2}b\) commensurate structure. Near any incommensurate-commensurate transition, the relevant \(q\) vectors will be in one of two distinct sets. There will be the set of long-wavelength distortions associated with the domain-wall structure and another set of distortions with wave vectors close to those that describe structure of the commensurate unit cell. The continuum limit might be expected to properly describe the long-wavelength distortions but will not properly describe the structure of the commensurate state. This is certainly the case near the \(2a = b\) transition where the long-wavelength amplitudes approached those given by Eq. (28). However, it is necessary to be much closer to the transition before this limiting behavior for the long-wavelength \(q\) vectors is found.

FIG. 2. Total energy versus \(a/b\) for \(l_0 = 4b\) and \(c = b\). On the scale shown, the curve appears to be smooth and without breaks. This curve is for a calculation using 6th-order harmonics and 4th-order Bessel expansion.

### V. THE DEVIL'S STAIR

The results of Aubry suggest that at zero kelvin the classical linear chain is always locked into some commensurate wave vector, although these states could be very-high-order commensurate states which would be difficult to distinguish from an incommensurate state. As the pressure is changed, one should see various ranges of pressure where the system is locked into some commensurate wave vector. There will be, therefore, some range in pressure over which a given commensurate state is stable and these regions become progressively smaller as the order of the state increases. For high-order states these regions are expected to be very small and experimentally undetectable. Figure 2 shows the total (reduced) energy as a function of \(a/b\) with a smooth line drawn between the calculated points. The (one-dimensional) pressure is (proportional to) the negative of the slope of this line and the break in the slope

### TABLE II. Ratio of the MDW static amplitudes calculated from Eq. (7) to those given by Eq. (22). The calculation is for \(l_0 = 4b\) and \(a = 0.98b\). The order of the harmonic coupling, \(v\), is 4 and the order of the harmonic expansion is 10.

<table>
<thead>
<tr>
<th>(m)</th>
<th>(\pm 1)</th>
<th>(\pm 2)</th>
<th>(\pm 3)</th>
<th>(\pm 4)</th>
<th>(\pm 5)</th>
<th>(\pm 6)</th>
<th>(\pm 7)</th>
<th>(\pm 8)</th>
<th>(\pm 9)</th>
<th>(\pm 10)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{(-1)^m}{b} p_m)</td>
<td>0.999</td>
<td>0.933</td>
<td>0.883</td>
<td>0.745</td>
<td>0.623</td>
<td>0.488</td>
<td>0.377</td>
<td>0.284</td>
<td>0.208</td>
<td>0.152</td>
</tr>
</tbody>
</table>
at $a=b$ is just the first step in the devil's stair. The $a=b$ registered phase is stable from zero pressure to some critical pressure. We define a reduced pressure $P$ by

$$P = -\frac{\partial (\phi/2NU_{c})}{\partial (a/b)}$$

(24)

and let $P_o$ be the corresponding reduced critical pressure. For $P > P_o$, the mean lattice constant decreases in a way that looks smooth on the scale of Fig. 2. However, if an examination is made of the energy versus $a/b$ curve on a finer scale, such as in Figs. 3(a) and 3(b), there appear kinks in the curve indicating that there exists a difference between left and right derivatives of the energy curve at rational values of $a/b$. This implies that a commensurate phase is stable over a finite range in pressure, the lower pressure being determined by the right derivative and the upper pressure being determined by the left derivative. Note that this range in pressure is smaller for the $\frac{5}{2}$ state shown in Fig. 3(b) than for the $\frac{3}{2}$ state shown in Fig. 3(a). The pressure range for very-high-order commensurate states is effectively of zero width as can be seen from the smoothness of the curves in Fig. 3 to the right and to the left of the main kink. To calculate the pressure ranges for these high-order states would require many more terms in both the harmonic and the Bessel-function expansions. However, in general this procedure is computationally difficult and is probably only practical for the low-order commensurate phases.

The values of $\Delta P$ were calculated by using linear least-squares fits to the left and to the right of the commensurate value of $a/b$. The difference in the slopes gives $\Delta P$ and the uncertainty in $\Delta P$ is calculated from the uncertainty in each slope. The correlation coefficient for each linear fit was 1.0000, indicating a high degree of confidence in the validity of the linear fit. Each fit used eleven data points spaced evenly along the lines shown above, and included the commensurate value in the fit. The accuracy of the calculated energy as one approaches some commensurate state is limited, in the final analysis, by the order of the truncations used. These truncations tend to round the energy curve so that the kinks actually appear as sharp bends. However, the energy of the commensurate state can be calculated directly so it is only necessary to obtain convergence at several $a/b$ values near the state of interest and then interpolate using the commensurate-value energy. This is shown in Fig. 4 where the calculated energy is shown near $a=b$ where this effect is most apparent. Note how the rounding due to the truncation is decreased by increasing the number of terms in the harmonic expansion. However, very close to $a=b$, the curves for the low-order harmonic expansion and the higher-order cross in violation of the variational principle. This phenomena is caused by the truncation of the Bessel-function expansion at fourth order. To obtain better calculated values it is necessary to increase the number of terms in
These curves show the effects of truncation in the number of terms of both the harmonic and Bessel-function expansions. The solid line is the expected exact solution, and the other curves are for 4th-order Bessel expansions with 6th-order (---) and 15th-order (----) harmonic expansions. Note the expanded scale for \( a/b \).

both expansions. Nevertheless, with the energy of the \( a = b \) state known it is “apparent” that the calculation is converging to the solid line. The slope of the solid line gives \( P_0 \). For higher-order commensurate states it is necessary to probe much nearer to the state to see this rounding, which is why the curves in both Figs. 2 and 3 appear to be composed of true straight lines with different slopes. In one dimension, the results of Aubry suggest that the energy curve is continuous. In two and three dimensions, where one does not have similar results, it may only be possible to place limits on the first-order character of the transition. However, these limits can be carefully examined by increasing the order of the calculations to obtain the desired accuracy.

VI. PHONONS, PHASONS, AND SOLITONS

The modes of the incommensurate lattice are not characterized by a single wave vector but, as we have seen, are composed of several coupled density waves having different wave vectors. For a commensurate lattice, a single wave vector can be defined for a given mode provided this wave vector is restricted to a region equal to the range of the original Brillouin zone divided by the number of atoms in the unit cell. This limited range can be viewed as a result of the coupling of the wave vector designated to define the mode to its higher harmonics. The only difference between the commensurate and the incommensurate states is the finite number of coupled wave vectors in the first case and the infinite number in the latter. However, for any given mode of the incommensurate state, there will be a relatively small set of wave vectors which produce the major contributions to the structure of the mode. Thus it is reasonable to expect to find the dynamical structure of an incommensurate state closely resembling that of “nearby” commensurate states, provided both are described in a way which does not distinguish between commensurate and incommensurate states in some explicit fashion. In Fig. 5 we show the frequency spectrum for the undistorted linear chain and that for the 1:1 registered phase. In the language of Sec. III, these lines represent contours in \( \omega vs q \) space where \( \Delta_v^0 \) has “large” values (of course, for these two cases \( \Delta_v^0 \) is either one or zero). These contours can be plotted for any value of \( a/b \) and are the obvious way in which to compare the incommensurate and the commensurate dynamics. Figure 6 shows contours for significant \( \Delta_v^0 \) values in \( \omega vs q \) space for the (commensurate) case of \( a/b = 8/9 \). The criterion chosen for the drawing of these contours is that the magnitude of \( \Delta_v^0 \) has a value of at least 0.25 times the magnitude of the largest \( \Delta_v^0 \) with the same value of \( a \). To generate these \( \Delta_v^0 \) values, a 9\( \times \)9 dynamical matrix...
was constructed which includes all terms up to order 4 in the harmonic amplitude coupling. Values of \( qa \) (about 150) were chosen at random between \(-\pi\) and \(\pi\), and for each value of \( a \) the \((\omega, q)\) positions of the \( A^0_s \) satisfying the above criterion were plotted. These contours then represent the most significant values of the space-time Fourier amplitudes for the system, and the density of points along a contour is a measure of the density of \( A^0_s \) values at some point in \( \omega q \) space. These contours also represent the major contributions to \( S(Q, \omega) \), the dynamical-structure factor. In Fig. 7 we show the same plot for the (incommensurate) case of \( a/b = 0.87 \). These contours were generated by using a 15 x 15 dynamical matrix centered about values of \( qa \) equal to 0, \(+\pi\), and 48 randomly chosen values between \(-\pi\) and \(\pi\). Note how similar the plots in Figs. 6 and 7 are, although the contours for the commensurate case are sharper and better defined. Furthermore, the commensurate case has a definite gap at zero \( q \) while the incommensurate case shows a branch which goes to zero. Finally, the various gaps in the commensurate case are true gaps with a zero density of modes within the gap. In the incommensurate case there exists modes inside these gap regions, although the density of these modes is very low and may be too small to measure.

The mode structure of the incommensurate state was studied in the continuum limit by Sutherland. It was found that, in this limit, the spectrum separates into two branches. The upper branch represents renormalized phonons and the lower one represents the collective motion of the domain walls. It is of obvious interest to examine the modes shown in Fig. (7) to see if these branches represent a dynamical structure similar to that found for the continuum limit.

We begin with Eq. (19) which describes the motion of the atoms of the incommensurate chain which leaves the ground-state energy invariant. Figure 8 shows the position of the domain walls for \( a/b = 0.98, l_0 = 4 \), and \( \Delta \) ranging from zero to \( b \). Note that the motion of the atoms across the substrate is accomplished solely by the motion of the domain walls as they lift atoms from one potential well and deposit them in the next. Because the domain walls shown correspond to an extra atom per wall, the domain walls move in the same direction as the atoms. Domain walls corresponding to a missing atom \((a > b)\) move in the direction opposite to the motion of the atoms. Since \( \Delta \) does not vary along the chain, the domain walls move uniformly to the right or left. To produce a collective oscillation of domain walls, all we need to do is vary \( \Delta \) throughout the chain in some wavelike fashion.
We first extract from Eq. (19) the \( A^m_n \) values of the zero-frequency phason. This is done by rewriting this equation using a power-series expansion in \( a \) and retaining the dominant terms in the limit as \( a \to 0 \). In this limit we find

\[
U_j = \alpha (1 + \sum_{n=0}^\infty \tilde{\alpha}_n \exp(iG_n R_j)),
\]

so that by inspection we can write the eigenvectors of the phason mode as

\[
A^m_n \propto \begin{cases} 
1, & n = 0 \\
G_n \tilde{\alpha}_n, & n \neq 0
\end{cases}
\]

for \( a \) such that \( \omega_a = 0 \). This is, in fact, precisely the eigenvector generated numerically for the "zero"-frequency mode upon the diagonalization of \( D_{q1q2} \). To generate the very-low-frequency modes we shall assume the simplest wavelike variation for \( \Delta \), namely,

\[
\Delta = \delta \sin(qR_j - \omega t).
\]

We will call these modes the phason modes. To obtain the \( A^m_n \) for these modes we again use a power-series expansion in \( \Delta \) and retain the leading terms. We find for such modes that

\[
u_j = \langle u_j \rangle + \sum_{n} A^m_n \sin[G_n + q]R_j - \omega t,
\]

where \( A^m_n \) is still given by Eq. (26) but now \( \omega_a \neq 0 \). An examination of the very-low frequency modes (\( \omega_a < 0.02 \omega_0 \), where \( \omega_0 \) is the zone-boundary frequency of the undistorted chain) for \( a/b = 0.87 \) showed that the eigenvectors do have this behavior, but that the components of the eigenvectors deviate strongly from this form as \( \omega_a \) increases. Table III shows some sample values for \( A^m_n \). The modes for those frequencies between about 0.4 and 0.8 \( \omega_0 \) are essentially a single-wave-vector density wave with "small" corrections. These are renormalized "acoustical" phonons. Near \( \omega_0 \), the modes are strongly coupled density waves but they have essentially the same structure as the corresponding modes in the commensurate case and are intracell vibrations superimposed upon a longer-wavelength density wave. These are, therefore, best described as renormalized "optic" phonons. Whether all of these modes are solitons in the strictest sense of the term is not yet clear, but it is most likely true for the long-wavelength modes since their motion should be well characterized by the sine-Gordon equation.

### VII. Discussion

The results of the previous sections show that the theory presented for the statics and dynamics

| \( \omega_a \) dynamic amplitudes (eigenvectors) for \( \omega_a = 0.012 \omega_0 \) |
|---|---|---|---|---|---|
| \( \alpha \) | 1 | 0.0304 | -0.0125 | 0.0108 |
| \( \beta \) | 1 | 0.0304 | -0.0126 | 0.0108 |
| \( \gamma \) | 1 | 0.0291 | -0.0100 | 0.0032 |

TABLE III. MDW dynamic amplitudes (eigenvectors) for \( l_0 = 4b \) and \( a = 0.87b \). The incommensurate phase equations were used to calculate \( A^m_n \). The harmonic expansion was carried out to 15th order and the harmonic coupling was included up to 4th order. The eigenvectors have 31 components, but only the lowest 5 are shown. Row (1) lists the values given by Eq. (26), row (2) lists \( A^m_n \) for \( \omega_a = 0 \), and row (3) lists \( A^m_n \) for \( \omega_a = 0.012 \omega_0 \). The \( A^m_n \) are not normalized to unity.
of the incommensurate state and the IC transition gives very good results even for a relatively low-order calculation. The ability of the theory to treat incommensurate and commensurate phases within the same formalism is a definite advantage when examining the physics of the IC transition. Since the accuracy of the calculation can be improved by simply increasing the order of the calculation, phenomena such as the devil’s stair can be examined with great care. The extensions of this calculation to treat more complicated potentials and to treat systems of higher dimensionality are, in principle, straightforward. Work is now in progress on such extensions and it is hoped that the results will shed some light on those experiments with monolayer films in which the IC transition is observed. It will also be possible to examine the validity of the simple models used to treat these systems.

Some of the questions that still need to be examined in the one-dimensional systems involve the effects of the shape of the substrate potential (that is, higher-order coefficients in the substrate potential), quantum effects, and the effects of finite temperatures. We would expect changes in the shape of the substrate potential will stabilize some commensurate states and destabilize others. If so, then the pressure range over which some phases exist will increase while other phases will exist over smaller regions in pressure. We would not expect a radical change in the physics of the IC transition. Finite temperatures should smooth out the smallest steps in the devil’s stair and reduce the size of the larger ones. The finite temperature extension of the theory presented is complementary to the transform matrix method for obtaining the thermodynamic functions of the system since that technique works best at “high” temperatures and our theory would work best at “low” temperatures. Work is also in progress on the quantum theory of the one-dimensional chain. One of the more intriguing questions is the extent to which the devil’s stair survives when the various effects discussed above are included. It is also not known if the devil’s stair is complete for smooth substrate potentials of the type which we have used.

ACKNOWLEDGMENTS

The author would like to express his appreciation to V. J. Emery, J. D. Axe, T. M. Rice, and especially to J. P. McTague for very stimulating and helpful discussions. He would also like to thank J. B. Sokoloff for providing unpublished numerical results. This work was supported in part by the National Science Foundation under Grant DMR75-15630-A01. Work at Brookhaven was supported in part by the Division of Basic Energy Sciences, U. S. Department of Energy, under Contract No. EY-76-C-02-0016.

APPENDIX A: MASS-DENSITY WAVES WITH ZONE-BOUNDARY MODES

A zone-boundary mode requires special treatment in the mass-density-wave calculation since \( q_m \) and \(-q_m\) are equivalent wave vectors in this case. This equivalence means \( \theta_m \) and \( -\theta_m \) in Eq. (3) are not independent parameters but rather the product \( u_m \sin \theta_m \) is the proper measure of the amplitude of the zone-boundary MDW. We begin by rewriting Eq. (3) in complex notation. If we now sum this equation over \( \pm m \) for \( q + q_{ZB} \) and include only one zone-boundary term, then our expansion includes only inequivalent wave vectors. The result for \( \langle u \rangle \) now looks like

\[
\langle u \rangle = -i \sum_m \tilde{u}_m \exp[i(q_m R - \theta_m)]
\]

\[
- i \tilde{u}_{2ZB} \exp[i(q_{ZB} R - \theta_{ZB})].
\] (A1)

Since \( \langle u \rangle \) must be real, one finds \( \theta_{ZB} = \pm \pi/2 \). The minimization of \( \Phi \) again leads to Eq. (4) for all \( q \) in the set, however this set includes only \( q_{ZB} \) not \(-q_{ZB}\). The Bessel-function expansion then leads to Eq. (7) for the MDW amplitude and to Eq. (12) for the energy. However, \( \theta_{ZB} \) is fixed at \( \pm \pi/2 \) in both cases. The loss of this degree of freedom is matched by a corresponding reduction in the number of independent equations in Eq. (7). This can be seen by writing Eq. (7) in the form

\[
\mu \omega_m^2 \tilde{u}_m \exp(-i\theta_m) = \sum_q G\tilde{u}_q \sum_{n_1} \sum_{q_1} J_{n_1}(G\tilde{u}_q) \sum_{n_2} J_{n_2}(G\tilde{u}_q) \exp[-i(G + \nu_1 q_1 + \cdots + \nu_n q_n)]
\]

\[
- \Delta_x (G - q_m + \nu_1 q_1 + \cdots + \nu_n q_n).
\] (A2)

If \( q_m \) is now set equal to \( q_{ZB} \), the real part of the left-hand side of Eq. (A2) is obviously zero since \( \theta_{ZB} = \pm \pi/2 \). The real part of the right-hand side of Eq. (A2) can also be shown to be identically zero by using \( q_{ZB} = -q_{ZB} + \tau \) and the symmetry properties of the Bessel functions under simultaneous changes in the sign of the argument and the sign of the order. The imaginary part of Eq. (A2) gives the value of
There are corresponding modifications in the definitions of the matrices defined by Eqs. (10).

**APPENDIX B: CONTRACTION OF EQUATIONS FOR MDW AMPLITUDES AND ENERGY**

Except for $\mathbf{\delta}_{2B}$, both $\mathbf{\delta}_m$ and $\mathbf{\theta}_m$ are antisymmetric in $m$, and it is possible to contract the various equations in which they appear. This significantly reduces the computational effort required to evaluate the various terms in these equations. The contraction process relies upon the following property of Bessel functions:

$$J_{\nu}(z_1 + z_2) = \sum_{\nu'} J_{\nu'}(z_1) J_{\nu'}(z_2). \quad (B1)$$

All the equations involving products of Bessel functions have the following general form:

$$\sum_{\nu} \sum_{\nu'} \left( \mathbf{G}_{\nu_m} \right) \left( \mathbf{G}_{\nu_{-m}} \right) \times \text{funct}(\cdots + \nu_m\mathbf{\theta}_m + \nu_{-m}\mathbf{\theta}_{-m}\cdots) \times \Delta_{\nu}(\cdots + \nu_m\mathbf{\theta}_m + \nu_{-m}\mathbf{\theta}_{-m}\cdots), \quad (B2)$$

where funct represents one of the trigonometric functions. Defining $\nu = \nu_m - \nu_{-m}$ and using the antisymmetric properties of $\mathbf{\delta}_m$ and $\mathbf{\theta}_m$ we can rewrite Eq. (B2) as

$$\sum_{\nu} \sum_{\nu'} \left( \mathbf{G}_{\nu_m} \right) \left( \mathbf{G}_{\nu_{-m}} \right) \text{funct}(\cdots + \nu_m\mathbf{\theta}_m \cdots) \times \Delta_{\nu}(\cdots + \nu_m\mathbf{\theta}_m \cdots) \quad (B3)$$

which then becomes

$$\sum_{\nu} \left( \mathbf{2G}_{\nu_m} \right) \text{funct}(\cdots + \nu_m\mathbf{\theta}_m \cdots) \Delta_{\nu}(\cdots + \nu_m\mathbf{\theta}_m \cdots)$$

once Eq. (B1) is used. This procedure eliminates $\mathbf{\delta}_m$ and $\mathbf{\theta}_m$ from the equations and thus reduces by one-half the number of products that need to be evaluated in Eq. (7). This reduction in the number of terms in the products of Bessel functions greatly reduces the number of terms in the summations needed for a given order of $\nu > 0$. 

---

*Permanent address.


THEORY OF THE STRUCTURE AND LATTICE DYNAMICS OF...

2217, 3611 (1978).
43 J. E. Sacco and J. B. Sokoloff, Phys. Rev. B 18, 6649 (1979) and private communications.
55 The shape of the substrate potential must possess a certain degree of “smoothness” so that the various expansions are absolutely convergent.
56 This causes a problem with the zone-boundary mode which is discussed in Appendix A.