metals. Extension of this work to other impurities in Al is currently in progress.

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Undamped Lattice Vibrations in Systems with Two Incommensurate Periodicities

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Despite the fact that the Frenkel-Kontorova model, with chain of atoms and sinusoidal potential incommensurate, lacks translational symmetry, the structure factor $S(q,\omega)$ for this model is shown to exhibit always phonon peaks of negligible width.

There has recently been an upsurge in interest in lattices with two incommensurate periodicities. Examples of such systems are charge-density waves incommensurate with the underlying lattice,[1] some superionic conductors in which the mobile ions order in a structure incommensurate with the rest of the lattice,[2] and some thin films which are incommensurate with the substrate.[3] Such systems have no translational symmetry because there exists no nonzero translation under which both periodicities are invariant. Two of us have also shown[4] along with Aubry[5] that a model for such systems, known as the Frenkel-Kontorova model (which consists of a chain of atoms connected by springs, interacting with a sinusoidal potential), exhibits a sharp transition at a critical value of the strength of the sinusoidal potential such that below this critical strength the ground state of an infinite chain incommensurate with the sinusoidal potential is continuously degenerate.[6] This implies the existence of a zero-frequency sliding mode and the possibility of free sliding of one periodicity with respect to the other.

We will show that the dynamical structure factor $S(q, \omega)$ (i.e., the imaginary part of the phonon Green's function for the chain) exhibits sharp phonon peaks of exceedingly small width, as for a system with translational symmetry. Furthermore, because of the existence of a continuously

degenerate ground state in the nonpinned regime, $S(q=0,\omega)$ actually has a peak of the form $\delta(\omega^2)$. Since the electrical conductivity (for charged atoms) is proportional to $i\omega D(q=0,\omega)$, where D is the phonon Green's function, this leads one to speculate on the possible existence of infinite dc conductivity, i.e., the existence of "Fröhlich superconductivity" for charge-density waves, superlubricating properties for incommensurate thin films,[7] and extremely plastic flow of incommensurate layered intercalation compounds.[8] The presence of imperfections will certainly prevent such ideal behavior from occurring, however,[9] and the question of whether anything like this can occur in real incommensurate systems, which are relatively pure, must await further work.

Our method of proof of the smallness of the width of the peaks in $S(q,\omega)$ is similar to the methods used by Anderson, Economou, and Cohen, and Thouless[10] in their studies of impurity localization in lattices. The Frenkel-Kontorova model consists of a chain of atoms connected by springs situated in a sinusoidal potential well and has a potential energy

$$V=\tfrac{1}{2}\alpha\sum_{n=1}^{N}(x_{n+1}-x_n-b)^2-V_0\sum_{n=1}^{N}\cos(2\pi x_n/a), \tag{1}$$

where α is the force constant of a spring, V_0 is the strength of the sinusoidal potential well, b and a are the natural periods of the chain and the sinusoidal potential well, respectively, and x_n is the position of the nth atom. The equation of motion for the lattice phonons is

$$\begin{aligned} m\ddot{U}_n &= -\alpha(2U_n-U_{n+1}-U_{n-1})-V_0(2\pi/a)^2\cos(2\pi\bar{x}_n/a)U_n \\ &= \sum_m K_{nm}U_m, \end{aligned} \tag{2}$$

where K is the dynamical matrix and $\{U_n\}$ are the displacements from the equilibrium positions $\{\bar{x}_n\}$ which satisfy periodic boundary conditions.[4] Then, the Fourier transform of the phonon Green's function satisfies

$$[\omega^2-\omega_0^2(q,\omega^2)]D(q,\omega^2)+V_0\left(\frac{2\pi}{a}\right)^2\sum_l F\left(\frac{2\pi l}{a}\right)D\left(q+\frac{2\pi}{a}l,\omega^2\right)=1, \tag{3}$$

where

$$\omega_0^2(q)=(2\alpha/m)(1-\cos qb) \tag{4}$$

$$D(q,\omega^2)=\sum_{nm}e^{iq(n-m)b}D_{nm}(\omega^2), \tag{5}$$

$$F\left(\frac{2\pi}{a}l\right)=\frac{1}{N}\sum_n\cos\left(\frac{2\pi}{a}\bar{x}_n\right)\exp[i2\pi l(b/a)n], \tag{6}$$

with N the number of atoms in the crystal.

The quantity $F((2\pi/a)l)$ can be found by solving the equilibrium equation, obtained by minimizing Eq. (1), for $\bar{x}_n$ in perturbation theory,[4,11] which to first order gives

$$\bar{x}_n\approx x_1^{(0)}+(n-1)b-\gamma\sin(2\pi/a)[x_1^{(0)}+(n-1)b], \tag{7}$$

where $x_1^{(0)}$ is the zeroth-order position of the first atom in the chain and

$$\gamma=V_0(2\pi/a)[4\alpha\sin^2(\pi b/a)]^{-1}. \tag{8}$$

Perturbation theory was shown in Ref. 4 to give about 1% accuracy for small V_0/α. Using the standard identity

$$e^{iz\sin\varphi}=\sum_{l=-\infty}^{\infty}J_l(z)e^{il\varphi},$$

we find that

$$F\left(\frac{2\pi}{a}l\right)=\frac{1}{2}\exp\left\{i\frac{2\pi}{a}l[b-x_1^{(0)}]\right\}\left[J_{1-l}\left(\frac{2\pi\gamma}{a}\right)+J_{1+l}\left(\frac{2\pi\gamma}{a}\right)\right], \tag{9}$$

which is a rapidly decreasing function of l. Writing down the general term in the perturbation series for $\bar{x}_n$, it is easy to show[4,11] that for $(2\pi/a)\,\gamma<1$, higher-order terms are insignificant and Eq. (11) is sufficient.

Using standard methods[10] the self-energy of $D(q,\omega)$, can be written as a perturbation series whose $(l+1)$th term is

$$\left[V_0\left(\frac{2\pi}{a}\right)^2\right]^{l+1}\sum_{\{n_r\}\neq 0}F_{0n_1}F_{n_1n_2}\cdots F_{n_{l-1},0}\prod_{r=1}^{l}\left[\omega^2-\omega_0^2\left(q+\frac{2\pi}{a}n_r\right)\right]^{-1}, \tag{10}$$

where

$$F_{n,n'}=F((2\pi/a)(n-n')).$$

Since the set of wave vectors $\{(2\pi/a)n\}$ define a reciprocal lattice for one of the periodicities in the problem, we can think of each term in the perturbation series for $\Pi(q,\omega^2)$ as a path in wave-vector space which starts and ends at the point q, without passing this point in any intermediate steps, in which each hop occurs over a distance which is a multiple of $2\pi/a$ (the largest contribution comes from short hops). For any general ω^2 within the phonon band defined by $\omega_0^2(q)$, there will exist some integer p such that

$$\omega_0^2(q+2\pi p/a)=\omega^2 \tag{11}$$

because b/a is an irrational number. Thus, in general there will be terms in the perturbation theory which diverge for almost any value of ω^2. The exception is $\omega^2=\omega_0^2(q)$. Here terms involving $\omega_0^2(q)$ are excluded, by the definition of Π, from the perturbation series.[10] Furthermore, since b/a is irrational, there exists no integer $p\neq 0$ such that

$$\omega_0^2(q+2\pi p/a)=\omega_0^2(q). \tag{12}$$

For the case of a finite lattice these values of ω^2 at which the perturbation series diverges are discrete, and therefore $\Pi(q,\omega^2)$ will have poles along the $\mathrm{Re}\omega^2$ axis. In the thermodynamic limit, the poles coalesce to form a branch cut. For most values of ω^2 the poles that occur in Π for a finite system appear only in very high-order terms in the perturbation series.

We will now argue that these poles have vanishingly small residues.

The $(l+1)$th-order term for Π has a pole at a given value of ω^2 with a residue of the form

$$\left[V_0\left(\frac{2\pi}{a}\right)^2\right]^{l+1}\sum_{\{n_r\}\neq 0}F_{0n_1}\cdots F_{n_{l-1},0}\prod_{\substack{r=1\\ r\neq p}}^{l}\left[\omega^2-\omega_0^2\left(q+\frac{2\pi}{a}n_r\right)\right]^{-1}, \tag{13}$$

where $\omega_0^2[q+(2\pi/a)p]=\omega^2$. The residue is of the order of

$$\beta^{l+1}\prod_{\substack{r=1\\ r\neq p}}^{l}\left\{\Omega^2-\left[1-\cos\left(qb+\frac{2\pi b}{a}n_r\right)\right]\right\}^{-1}, \tag{14}$$

where $\Omega^2=\omega^2(m/2\alpha)$ and $\beta=(V_0/2\alpha)(2\pi/a)^2$. In general, we expect that the mode frequencies will not be shifted by a large amount, and hence we are interested in values of ω^2 close to $\omega_0^2(q)$ for calculating the broadening of the modes. Because b/a is irrational, there are always values of n_r such that $\omega_0^2[q+(2\pi/a)n_r]$ is arbitrarily close in value (but not equal) to $\omega_0^2(q)$. Nevertheless, this does not cause the perturbation theory to diverge because such a denominator always has a numerator of high order in β which keeps the term small if $\beta<1$. We have calculated, on a computer, values $\beta^n/[1-\cos(2\pi/a)bn]$ with n large and equal to values for which the denominator becomes small and have found that these terms become small rapidly as the value of n increases, as long as $\beta<1$. Also, because of the irrational nature of b/a, $qb+(2\pi b/a)n_r$ in Eq. (14), modulo 2π, forms a continuum between 0 and 2π. Thus, we can replace the denominator of Eq. (14) by $\exp[(l-1)I]$, where

$$I=\frac{1}{2\pi}\,\mathrm{P}\int_{-\pi}^{\pi}\ln[\Omega^2-1+\cos\theta]\,d\theta=\ln(\tfrac{1}{2})$$

if $0\leq\Omega^2\leq 2$ and where P denotes the principal part. Thus, Eq. (14) can be approximated by

$$(2\beta)^{l+1}. \tag{15}$$

Similar arguments occur for the higher-order poles. Hence, if $\beta<\frac{1}{2}$, the perturbation series for the residue of Π at ω^2 will certainly converge

(it may also converge for larger values but we cannot say anything about this). Thus, if the Mth-order term is the lowest-order term of Π in which this pole appears, the residue is of order $(2\beta)^M$.

Since M is quite large for general ω, we expect the residue to be negligible. In the thermodynamic limit, these poles coalesce into a branch cut, and the discontinuity across this branch cut must also be negligible. Thus, ImΠ is negligibly small, and hence, the normal-mode frequencies appear in $S(q,\omega)$ with negligibly small width. This can be thought of as a localization in wave-vector space, much like the localization in configuration space found in disordered solids.[10] This result was anticipated by Weisz *et al.*[12] The physical reason for expecting this effect is that although there exists near any main peak of $S(q,\omega)$ a continuum of small peaks arbitrarily close in frequency $\{\omega^2 \approx \omega_0^2[q+(2\pi/a)m]\}$, these peaks produce almost no broadening of a main peak since their intensities are rapidly decreasing functions of M which must be large. The proof of a Bloch theorem for such nearly periodic systems by Dinaburg and Sinai[13] does not address the question of the widths of the phonon peaks.

For $q=0$, $S(q,\omega)$ actually has a δ-function peak at $\omega^2=0$ because it was shown numerically in Ref. 4 that there exists a mode at zero frequency. Thus, we expect that

$$\mathrm{Re}\Pi(q=0,\ \omega^2=0)=0.$$

Although it is difficult to prove this result analytically using Ying's perturbation theory,[11] we can show that ReΠ is zero up to third order in β.

Because denominators containing $\omega_0^2(q=0)$ do not occur in Eq. (12), the perturbation series for $\Pi(q=0,\ \omega^2=0)$ converges. Since this implies that Π has a break in the branch cut along the Reω^2 axis at $\omega^2=0$, $S(q=0,\ \omega)=\mathrm{Im}D(q=0,\ \omega)$ has a peak proportional to $\delta(\omega^2)$.

Our conclusions are valid for $\beta=(V_0/2\alpha)(2\pi/a)^2<0.5$. We have found that for values of β between 0.4 and 0.5 the sliding to nonsliding transition occurs[4] and hence we generally have sliding for values of $\beta<0.5$. For larger values of β, the periodicities are in registry meaning that there are fairly well-defined unit cells (with occasional misfit dislocations), i.e., the system to a good approximation has translational invariance. Hence, we also expect peaks in $S(q,\omega)$ of negligible width in this regime.

Recently Pokrovsky[14] has proven in lowest-order perturbation theory that the present model has an acoustic mode. In the present paper we consider the question of phonon damping, which requires consideration of higher orders in perturbation theory.

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