Change in sound velocity due to sliding charge-density waves

G. W. Lehman
Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506-0055
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The Coppersmith-Varma model [Phys. Rev. B 30, 3566 (1984)] has been solved for arbitrary lattice distortions to calculate the shift in sound velocity due to sliding charge-density waves. If the coupling strength g_0 is large enough, it is found that the sound velocity goes to zero in the one-dimensional case. A table of these results is presented. The flexure-wave sound velocity c_F in a thin plate is also derived from this model in the weak-coupling limit $g_0 \ll 1$. The relative shift $\Delta c_F / c_F$ is orders of magnitude smaller that the few percent found experimentally by Brill and Roark [Phys. Rev. Lett. 53, 846 (1984)] for thin crystals of TaS_3.

I. INTRODUCTION

Sliding charge-density waves (CDW's) strongly affect electronic properties. When electric fields larger than a threshold field, E_T, are applied, CDW's become depinned and carry current (cf. Monceau *et al.*[1] and Fleming *et al.*[2]). Recent experiments by Brill and Roark[3] (BR) and Brill[4] show that Young's modulus for TaS_3 decreases by a few percent when fields above threshold are applied. Coppersmith and Varma[5] (CV) have solved a one-dimensional model in the double limit of weak distortion of the lattice and no distortion of the CDW. They find that bulk acoustic phonons have a small decrease in velocity, c, proportional to the CDW drift velocity, v, for fields above threshold. CV find $\Delta c/c \sim -10^{-5}$. The measurements of BR were done with a vibrating-reed apparatus in which changes in the resonant frequency of a thin crystal (3 μm) are measured. Since the speed of propagation of a flexural vibration, c_F, is much less than the speed of a bulk acoustic phonon, c_B ($c_F \sim aqc_B$, where a and q are sample thickness and wave vector, respectively), it is not clear how the CV result would be modified for flexure waves. Consequently, in this paper we reformulate the CV work into a continuum model with boundary conditions appropriate to the vibrating-reed experiment of BR. Important reviews of CDW's relevant to this work have been presented by Toombs[6] and Gruner and Zettl.[7]

A derivation of the CV model is presented in Sec. II and a complete discussion of the one-dimensional continuum version of this model is presented in Sec. III for arbitrary coupling strengths between the CDW and atomic displacements. If the coupling is strong enough the sound velocity can go to zero in this model.

In Sec. IV flexure waves in a thin-plate geometry and Rayleigh waves in a thick-plate geometry are investigated using our continuum approximation to the CV model in the weak-coupling limit.

In Sec. V the predictions of our CV-model calculation of Sec. IV in the weak-coupling limit are compared with the experimental results of BR.

II. DERIVATION OF THE CV MODEL

The CV model is based on the work of Fukuyama and Lee[8] (FL) and Lee and Rice.[9] Other papers relevant to this FL model are those of Sneddon *et al.*,[10] Sneddon,[11] and Fisher.[12]

Using FL, one can write an equation of motion for the nth ion of mass M_n located at $\mathbf{R}_n(t)$, t being the time, as

$$M_n \frac{d^2\mathbf{R}_n}{dt^2} = \mathbf{F}_n^0 + e \int d^3r\, \rho_{\rm CDW}(\mathbf{r};t)(\mathbf{r}-\mathbf{R}_n)/|\mathbf{r}-\mathbf{R}_n|^3 . \tag{1}$$

The term $\mathbf{F}_n^0$ describes the restoring force in the absence of a CDW, while the last term is the restoring force associated with a CDW and e is the electronic charge. The CDW charge density, $\rho_{\rm CDW}$, obeys

$$\rho_{\rm CDW}(\mathbf{r};t) = \rho_0 \cos(\mathbf{Q}\cdot\mathbf{r}+\Phi) , \tag{2}$$

where the phase $\Phi(\mathbf{r},t)$ satisfies

$$\lambda_0 \frac{d\Phi}{dt} = D\nabla^2\Phi + \sum_n V_{nI}(\mathbf{r})\rho_0 \sin(\mathbf{Q}\cdot\mathbf{r}+\Phi) + e^* E_c . \tag{3}$$

In Eq. (2), $\mathbf{Q}$ describes the CDW direction, $|Q| = 2k_F$, k_F being the Fermi wave vector. In Eq. (3), the λ_0 parameter is a damping parameter, D is a diffusion coefficient, V_{nI} denotes a pinning potential due to an impurity at $\mathbf{R}_n$, e^* is an effective charge of the CDW, and E_c is the electric field strength.

The zeroth-order solution to Eq. (3) for Φ is given by

$$\Phi(\mathbf{r},t) = w_v t , \tag{4}$$

where

$$w_v = e^* E_c/\lambda_0 = Qv , \tag{5}$$

where v is the CDW drift velocity.

The discussion in this paper is limited to the zeroth-order solution for Φ which is valid for large v. Hence, the substitution of Eq. (4) into Eq. (2) leads to the Coppersmith-Varma model

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$$M_n \frac{d^2\mathbf{R}_n}{dt^2} = \mathbf{F}_n^0 + V_0 \mathbf{Q} \sin(\mathbf{Q}\cdot\mathbf{R}_n + w_v t) \;, \quad (1')$$

where the potential-energy parameter V_0 is given by

$$V_0 = e\rho_0/Q^2 \;. \quad (6)$$

It appears that Φ in Eqs. (2) and (3) may depend upon the CDW velocity v in a rapidly varying fashion when v approaches threshold. This is quite apparent in a recently investigated model calculation presented by Sneddon.[13]

III. ONE-DIMENSIONAL CV MODEL

In the long-wavelength limit, Eq. (1′) for a one-dimensional sample with a sliding CDW in the z direction is

$$\frac{\partial^2 u(z;t)}{\partial t^2} = c_L^2 \frac{\partial^2 u(z;t)}{\partial z^2} + \frac{V_0 Q}{M} \sin[Q(z+u)+w_v t] \;, \quad (7)$$

where c_L is the longitudinal sound velocity and $u(z;t)$ denotes the displacement of an ion mass M located at the point z at time t.

Following CV's analysis, let $u = u_0 + u_1$, where u_0 is the *dynamic equilibrium* solution to Eq. (7) and u_1 describes the excitation spectrum about the *dynamic equilibrium* u_0.

A. Dynamic equilibrium solution u_0

The dynamic equilibrium solution, $u_0(z;t)$, is obviously a periodic solution of Eq. (7) with respect to the variable

$$\theta = Qz + w_v t \;. \quad (8)$$

Setting

$$Qu_0(z;t) = h(\theta) \;, \quad (9)$$

one finds that

$$h''(\theta) = -g_1 \sin(h+\theta) \;, \quad (10)$$

where

$$g_1 = V_0/[M(c_L^2 - v^2)] \;. \quad (11)$$

(In TaS_3, $v \sim 10$ cm/sec so $v \ll c_L$ and $g_1 \cong g_0 = V_0/Mc_L^2$.) From Whittaker and Watson[14] (WW), one finds that the solution to Eq. (10) can be expressed in terms of elliptic functions. Moreover, from WW's analysis, one readily finds that

$$h(\theta) = 4 \sum_{n=1}^{\infty} q_0^n \sin(n\theta)/[n(1+q_0^{2n})] \;. \quad (12)$$

(The notation q_0 is used rather than the customary q to avoid confusion with our use of q as a wave vector later on.) The parameter q_0 is related to our coupling constant g_1 in a simple manner, i.e.,

$$g_1 = 4q_0 \left[\sum_{n=0}^{\infty} q_0^{n(n+1)} \right]^4 \quad (13)$$

for any $0 < q_0 < 1$. A Newton-Raphson procedure allows one to obtain q_0 quite simply for a *fixed* g_1 from Eq. (13) as was done in our numerical calculations. Our machine calculations show numerically that Eq. (12) is a solution of Eq. (10) which is periodic in θ as required.

As a further check, one should note that the proper solution of h, correct to terms linear in g_1, is

$$h \cong 4q_0 \sin(\theta) \cong g_1 \sin(\theta) \;, \quad (14)$$

which agrees with CV's analysis for small g_1 in the long-wavelength limit.

B. Vibrational spectrum

Expanding $u(z;t)$ about u_0 gives a linear wave equation for u_1, the vibrational amplitude for the excitation spectrum of our one-dimensional system. One easily finds that

$$\frac{\partial^2 u_1}{\partial t^2} = c_L^2 \frac{\partial^2 u_1}{\partial z^2} + \frac{V_0 Q^2}{M} \cos(\theta+h) u_1 \;, \quad (15)$$

with θ and $h(\theta)$ given by Eqs. (8) and (12), respectively.

In order to solve Eq. (15) for the excitation spectrum for arbitrary values of the coupling parameter, V_0/Mc_L^2, we need to find a Fourier series representation for $\cos(\theta+h)$. WW in their chapter on Jacobian elliptic functions provide us with just such an expansion, first derived by Jacobi himself. Since the connection is a bit obtuse, one must first note that

$$\cos(\theta+h) = 1 - 2[\mathrm{sn}(K\theta/\pi)]^2 \quad (16)$$

$$= C_0 + \sum_{n=1}^{\infty} D_n \cos(n\theta) \;, \quad (17)$$

where

$$C_0 = 1 - \sum_{n=1}^{\infty} D_n, \;\; D_n = 4nq_0^n/[g_1(1-q_0^{2n})] \;. \quad (18)$$

The parameter q_0 as mentioned before is related to g_1 by Eq. (13). K and sn in Eq. (16) are standard WW symbols for an elliptic integral and function, respectively. Our machine calculations verify directly the remarkable relationship between Eqs. (16) and (17) using the Fourier series for $h(\theta)$, Eq. (12).

To get the excitation spectrum from Eq. (15), one can follow CV and expand u_1 in a double Fourier integral

$$u_1(z;t) = \int dw \int dq \exp(iqz - iwt) A(q,w) \quad (19)$$

using Eq. (17) for $\cos(\theta+h)$. Noting that $D_0 = 0$ if $n=0$ is included in its definition, one gets

$$[(c_L q)^2 - w^2 - V_0 Q^2 C_0/M] A(q,w) = (V_0 Q^2 C_0/2M) \sum_{n'=-\infty}^{\infty} D_{|n'|} A_{n'}(q,w) \;, \quad (20)$$

where

$$A_n(q,w) = A(q+nQ, w-nw_v) \;. \quad (21)$$

Using the definition of A_n, one can get a set of equations which fix $w(q)$ from Eq. (20). Now,

$$A_{n'}(q+nQ, w-nw_v) = A_{n+n'}(q,w) \;,$$

so that, after a shift of index in the sum generated from Eqs. (20) and (21), one can write

$$[c_L^2(q+nQ)^2-(w-nw_v)^2-V_0Q^2/C_0M]A_n =(V_0Q^2/2M)\sum_{n'=-\infty}^{\infty} D_{|n-n'|}A_{n'}\,, \quad (22)$$

for all integer n.

To solve Eq. (22) for $|q|<Q/2$ and $w<w_v/2$, set

$$A_n=(g_0/2)A_0G_nB_n,\quad n\neq 0 \quad (23)$$

where

$$G_n=[(n+q/Q)^2-(qc/Q-nv)^2/c_L{}^2-g_0C_0]^{-1} \quad (24)$$

is a Green's function and

$$g_0=V_0/Mc_L^2 \quad (25)$$

is g_1 when the CDW drift velocity v is zero.

Next, let

$$w=qc\,, \quad (26)$$

where c is the sound velocity. When Eqs. (23)–(25) are substituted into Eq. (22), one finds that the sound velocity $c(q)$ is fixed by setting the coefficient of A_0 equal to *zero*. This results in the following equation:

$$(c/c_L)^2=1-g_0(Q/q)^2 \times\left[C_0+(g_0/4)\sum_{n\neq 0}^{\infty} D_{|n|}G_nB_n\right]. \quad (27)$$

The coefficients B_n in Eq. (27) now satisfy a set of linear equations:

$$B_n-(g_0/2)\sum_{n'\neq 0}^{\infty} D_{|n-n'|}G_{n'}B_{n'}=D_{|n|}\,. \quad (28)$$

The term $n=0$ is obviously excluded from Eq. (28). When $q=0$, $G_n=G_n^0$, where

$$G_n^0=[n^2(1-v^2/c_L^2)-g_0C_0]^{-1} \quad (29)$$

and $B_n=B_n^0=B_{-n}^0$ satisfies

$$B_n^0-(g_0/2)\sum_{n'=1}^{\infty}(D_{|n-n'|}+D_{n+n'})G_{n'}^0B_{n'}^0=D_n\,, \quad (30)$$

for $n=1,2,\ldots$. The quantity in the large parenthesis of Eq. (27) must vanish for $q=0$, so that

$$C_0+(g_0/2)\sum_{n=1}^{\infty} D_nG_n^0B_n^0=0\,. \quad (31)$$

Our machine solutions of Eq. (30) for B_n^0 show that Eq. (31) is satisfied numerically if enough terms are included. Numerical computations include the range $0<g_0=V_0/Mc_L^2<5$. When $g_0=5$, one must include about 40 terms in Eqs. (30) and (31) for convergence, i.e., one part in 10^{15}.

When $g_0\ll 1$, $C_0=-2q_0$, and only B_1 and B_{-1} need be retained. A short computation shows that

$$c/c_L=1-g_0^2(1+2v/c_L)+O(q/Q)^2\,, \quad (32)$$

which is essentially the result obtained by CV for $q/Q\ll 1$.

For larger values of the coupling constant g_0, one must solve Eq. (28) for the B_n's and substitute them into Eq. (27) to get $c(q)$ as a function of q. From a computational standpoint, one would like to rewrite Eqs. (27) and (28) so that the factor $(Q/q)^2$ preceding the term in large parentheses in Eq. (27) cancels out as it must. This can be done by rewriting G_n in three parts as

$$G_n=G_n^0+(q/Q)G_n^{(1)}+(q/Q)^2G_n^{(2)}\,, \quad (33)$$

where G_n^0 is given by Eq. (29) and is independent of q. $G_n^{(2)}$ as well as G_n^0 are symmetric to the interchange of n and $-n$. On the other hand, $G_n^{(1)}$ is antisymmetric when n is replaced by $-n$. After a bit of algebra, one finds that

$$G_n^{(1)}=-2n(1+vc/c_L^2)W_n \quad (34)$$

and

$$G_n^{(2)}=-G_n^0W_n\{[(q/Q)^2R_L-Z_n]R_L-Y_n\}\,, \quad (35)$$

where

$$R_L=1-(c/c_L)^2,\quad Z_n=(G_n^0)^{-1}\,,\qquad Y_n=4n^2(1+vc/c_L^2)^{-1}\,, \quad (36)$$

and

$$W_n=\{[Z_n+(q/Q)^2R_L]^2-(q/Q)^2Y_n\}^{-1}\,. \quad (37)$$

When Eq. (30) is substituted into Eqs. (27) and (28), one can factor out a term proportional to Eq. (31) which *vanishes*. After a bit of algebra, one finds that the equation for the sound velocity c given by Eq. (27) can be written as

$$(c/c_L)^2=1-(g_0^2/2)\sum_{n=1}^{\infty} D_n(G_n^{(2)}B_n^0+G_n^{(1)}B_n^{(1)}+G_n^eB_n^{(2)})\,, \quad (38)$$

where

$$B_n^{(k)}-(g_0/2)\sum_{n'=1}^{\infty}[D_{|n-n'|}+(-1)^kD_{n+n'}]G_{n'}^eB_{n'}^{(k)}-(g_0/2)(q/Q)^{2(2-k)}\sum_{n'=1}^{\infty}[D_{|n-n'|}+(-1)^kD_{n+n'}]G_{n'}^{(1)}B_{n'}^{(3-k)} =g_0\sum_{n'=1}^{\infty}[D_{|n-n'|}+(-1)^kD_{n+n'}]G_{n'}^{(k)}B_{n'}^0\,, \quad (39)$$

$$G_n^e=G_n^0+(q/Q)^2G_n^{(2)}\,, \quad (40)$$

and $k=1$ or 2. B_n^0 is given by solving Eq. (30).

Sound velocities for our one-dimensional CV model are given in Table I as a function of q/Q and v/c_L for various values of $g_0=V_0/Mc_L^2$. One should note that the sound velocity c decreases as the coupling parameter increases, going to zero if g_0 is large enough. $g_0 \sim 0.1$ is CV's estimate. Larger values of g_0 (~ 1) might be relevant for commensurate systems (polyacetylene) or elastically softer CDW materials.

IV. FLEXURE AND RAYLEIGH WAVES IN PLATE GEOMETRY

The work reported in this section extends the work of Sec. III in order to treat flexure waves in thin samples of TaS_3 used by BR to investigate the dependence of the elastic modulus on an applied electric field.

The mathematical treatment of flexure, Rayleigh-, and longitudinal-wave propagation in thin samples is similar in nature. However, it has not been possible to extend the analysis of Sec. III to these problems beyond second order in the coupling coefficient $g_0=V_0/Mc_L^2$. In view of the fact that c/c_L in the bulk one-dimensional case actually can go to zero if g_0 is large enough, one might expect similar behavior in three-dimensional finite geometries.

There is, however, a distinct difference between longitudinal and flexure waves which motivates this derivation; for flexural waves the frequency is *quadratic* in wave number q. For simplicity, we have treated the geometry in a thin infinite plate, rather than the rod geometry experimentally used by BR; since flexural waves in both cases have $w \sim q^2$, this should not qualitatively alter the results. Modification of our results to consider rodlike geometries will be discussed later.

An excellent discussion of these problems when CDW waves are absent is given by Landau and Lifshitz[15] (LL) (cf. Sec. 25).

A. Elastic equations for plate geometry

Equation (1′) of Sec. III is easily generalized to treat vibrations in a plate geometry. One has

$$\ddot{\mathbf{u}}=c_T^2\nabla^2\mathbf{u}+(c_L^2-c_T^2)\nabla(\nabla\cdot\mathbf{u}) + \mathbf{e}_z(QV_0/M)\sin[Q(z+vt+u_z)] \quad (41)$$

where the sliding CDW is restricted to the z direction, $\mathbf{e}_z$ being a unit vector in the z direction. In Eq. (41), c_T is the transverse sound velocity (assuming isotropy in the x-y plane) and c_L is the longitudinal velocity. In an isotropic material, they can be expressed in terms of Young's modulus E and Poisson's ratio σ. From LL, one has

$$c_T=\{E/[2(1+\sigma)\rho]\}^{1/2}$$

and (42)

$$c_L=\{E(1-\sigma)/[(1+\sigma)(1-2\sigma)\rho]\}^{1/2} ,$$

where ρ is the sample density. Lear *et al.*[16] estimate an average value of $\sigma \sim 0.3$ for $NbSe_3$, presumably similar to TaS_3, so $c_T \cong c_L/2$. The displacement vector $\mathbf{u}=(u_x,u_y,u_z)$ will be restricted to motion in the x-z plane so that $u_y=0$ hereafter.

1. Boundary conditions for thin-plate geometry

Our plate occupies the space $-a<x<a$, $-\infty<y,z<\infty$. The boundary conditions for our *free* plate are the stress-free conditions given by (cf. LL, Ref. 15, Chap. III)

$$\frac{\partial u_x}{\partial x}+\zeta\frac{\partial u_z}{\partial z}=\frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}=0 \quad (43)$$

at the bounding surface $x=\pm a$. The parameter ζ is given by

$$\zeta=1-2b \quad (44)$$

with

$$b=(c_T/c_L)^2 . \quad (45)$$

The parameter b occurs in many different places in the remainder of this paper.

2. Dynamic equilibrium displacement $\mathbf{u}_0$

In the weak-coupling case, the dynamic equilibrium displacement vector $\mathbf{u}_0=(u_x,0,u_z)$. It is convenient to use

$$\theta=Q(z+vt) , \quad (8')$$

$$Qu_x=Y_x\cos(\theta),\quad Qu_y=Y_y\sin(\theta) , \quad (46)$$

and

TABLE I. Sound velocity as a function of (q,v,g_0) for one-dimensional continuum CV model.

				c/c_L		
q/Q	v/c_L	$g_0=0.1$	$g_0=0.5$	$g_0=1$	$g_0=3$	$g_0=5$
0	0	0.9901	0.8040	0.5152	0.0942	0.0250
0.1	0	0.9897	0.7985	0.5085	0.0927	0.0246
0.2	0	0.9883	0.7804	0.4879	0.0882	0.0234
0	0.01	0.9899	0.8004	0.5077	0.0840	0.0143
0.1	0.01	0.9895	0.7947	0.5008	0.0825	0.0139
0.2	0.01	0.9880	0.7760	0.4798	0.0780	0.0126
0	0.02	0.9897	0.7966	0.4999	0.0733	0.001 95
0.1	0.02	0.9893	0.7907	0.4929	0.0718	0.001 50
0.2	0.02	0.9877	0.7714	0.4715	0.0672	0.000 16

$$D=\frac{d}{dx}\ , \tag{47}$$

so that

$$\begin{vmatrix} D^2-bK_{\rm T}^2 & Q(1-b)D \\ -Q(1-b)D & bD^2-K_{\rm L}^2 \end{vmatrix} \begin{vmatrix} Y_x \\ Y_z \end{vmatrix} = \begin{vmatrix} 0 \\ Q^2 g_0 \end{vmatrix}\ , \tag{48}$$

where g_0 is defined by Eq. (25). The parameters

$$K_{\rm L,T}=Q[1-(v/c_{\rm L,T})^2]^{1/2} \tag{49}$$

are characteristic wave vectors for transverse- and longitudinal-wave propagation associated with the homogeneous part of Eq. (48). The boundary conditions, Eq. (43), become

$$DY_x+\zeta DQY_z=DY_z-QY_x=0 \ \text{ at } x=a\ . \tag{50}$$

The following abbreviations will be used:

$$d_{\rm L,T}=\cosh(K_{\rm L,T}a),\ \ t_{\rm L,T}=\tanh(K_{\rm L,T}a)\ . \tag{51}$$

The general solution of Eq. (48) which satisfies Eq. (50) is

$$Y_x=K_{\rm L}\sinh(K_{\rm L}x)A_{\rm L}/d_{\rm L}-Q\sinh(K_{\rm T}x)A_{\rm T}/d_T\ , \tag{52}$$

$$Y_z=g_1-Q\cosh(K_{\rm L}x)A_{\rm L}/d_{\rm L}+K_{\rm T}\cosh(K_{\rm T}x)A_{\rm T}/d_{\rm T}\ , \tag{53}$$

where $g_1=g_0/[1-(v/c_{\rm L})^2]$ as defined by Eq. (11). The coefficients $A_{\rm L,T}$ are given by

$$A_{\rm T}=2QK_{\rm L}t_{\rm L}A_{\rm L}/[(Q^2+K_{\rm T}^2)t_{\rm T}]\ , \tag{54}$$

$$A_{\rm L}=-Qg_1(Q^2+K_{\rm T}^2)(c_{\rm L}/c_{\rm T})^2/D_0\ , \tag{55}$$

with

$$D_0=[K_{\rm T}^2+Q^2]^2-4Q^2K_{\rm T}K_{\rm L}(t_{\rm L}/t_{\rm T})\ . \tag{56}$$

When x is close to either surface $x=-a$ or $+a$, the dynamic equilibrium displacement amplitudes vary rapidly as one goes toward the center of the plate because $Qa=2k_Fa\gg 1$, even for samples a few micrometers thick as is the case in the BR samples.

3. *Dynamic equilibrium displacement when $v=0$*

When $v\ll c_{\rm L}$, which is usually the case, one can get a good idea about the behavior of u_0 from Y_x and Y_z at $v=0$ given by

$$Y_x=(g_0\zeta/2)\exp[-Q(a-x)] \times[(1-b)Q(x-a)-1]/[b(1-b)]\ , \tag{57}$$

$$Y_z=g_0\{1-(\zeta/2)\exp[-Q(a-x)] \times[(1-b)Q(x-a)+b]/[b(1-b)]\}\ . \tag{58}$$

The magnitude of the dynamic equilibrium surface displacement u_x is $|Y_x|/Q$ and at $x=a$ it is $g_0(\zeta/2)/[b(1-b)Q]$. Coppersmith and Varma estimate $g_0\cong 0.1$, and if $b=0.25$ the dynamic equilibrium displacement near the surface could amount to 0.16 Å. This u_x displacement varies rapidly near the surface and approaches zero as one goes toward the sample center, in a distance of the order of $1/k_F\cong 10$ Å. This may affect the results of surface-sensitive experiments such as electron diffraction.

B. Equations for the vibrational spectrum

The vibrational amplitude $\mathbf{u}_1$ for plate geometry is obtained from Eq. (41) when $\mathbf{u}$ is expanded about the dynamic equilibrium amplitude $\mathbf{u}_0$. One finds that

$$\ddot{\mathbf{u}}_1/c_{\rm L}^2=\nabla^2\mathbf{u}_1+(1-b)\nabla(\nabla\cdot\mathbf{u}_1)+\mathbf{e}_z f\ . \tag{59}$$

where

$$f=Q^2(g_0/2)[2\cos(\theta)-g_0Y_z(x)]u_{1z}\ , \tag{60}$$

$\theta=Q(z+vt)$, and $\sin^2(\theta)=[1-\cos(2\theta)]/2$ has been replaced by $\frac{1}{2}$. The analysis of Sec. III shows that the $\cos(2\theta)$ term leads to higher-order corrections, namely g_0^4 terms.

To obtain the vibrational spectrum from Eq. (59), one can expand $\mathbf{u}_1$ in double Fourier integral

$$\mathbf{u}_1=\int dq\int dw\exp[i(qz-wt)]\begin{bmatrix} h_x(x;q,w) \\ 0 \\ -ih_z(x;q,w)\end{bmatrix}\ . \tag{61}$$

The functions h_x and h_z are real with the inclusion of the imaginary coefficient in Eq. (61) and satisfy

$$\begin{bmatrix} D^2-bp_T^2 & (1-b)qD \\ -(1-b)qD & bD^2-p_L^2\end{bmatrix}\begin{bmatrix} h_x \\ h_z\end{bmatrix}=\begin{bmatrix} 0 \\ -F\end{bmatrix}\ , \tag{62}$$

where

$$F=Q^2(g_0/2)[-g_0Y_z(x)h_z(x;q,w) +h_z(x;q-Q,w+w_v) +h_z(x;q+Q,w-w_v)] \tag{63}$$

and

$$p_{\rm L,T}(q,w)=[q^2-(w/c_{\rm L,T})^2]^{1/2} \tag{64}$$

are the characteristic wave vectors associated with the homogeneous part of Eq. (62).

The boundary conditions for Eq. (62) are

$$Dh_x(x;q,w)+\zeta qh_z(x;q,w) =Dh_z(x;q,w)-qh_x(x;q,w)=0 \tag{65}$$

at the boundaries $x=-a$ and $+a$.

One can show, by direct substitution, that a particular solution of Eq. (62) is

$$h_{xp}=(c_{\rm L}/w)^2qD[Y(x,p_{\rm T})-Y(x,p_{\rm L})]\ , \tag{66a}$$

$$h_{zp}=(c_{\rm L}/w)^2[-p_{\rm T}^2Y(x,p_{\rm T})+q^2Y(x,p_{\rm L})]\ , \tag{66b}$$

with $D=d/dx$, and

$$Y''(x,p)-p^2Y(x,p)=-F(x;q,w)\ . \tag{67}$$

The left-hand side of Eq. (67) is simply the scalar wave equation for transverse or longitudinal waves when $p=p_{\rm T}$ or $p_{\rm L}$. Since $p_{\rm T}=p_{\rm L}=q$ when $w=0$, h_{xp} and h_{zp} are finite as $w \to 0$. Equation (67) is satisfied by the particular solution

$$Y(x,p) = \int_{-a}^{a} dx'\, U_1(x_>,p) U_2(x_<,p) F(x';q,w) , \quad (68)$$

where

$$U_1(x,p) = \sinh[p(a-x)]/[\sinh(pa)] \quad (69)$$

and

$$U_2(x,p) = \sinh[p(a+x)]/[2p\cosh(pa)] \quad (70)$$

are *regular* functions of p. In Eq. (68) the symbols $x_>$ and $x_<$ have their customary meaning, namely $x_>$ means $x > x'$, etc.

The choice of U_1 and U_2 is dictated by symmetry requirements. If $F(-x) = \pm F(x)$, $Y(-x) = \pm Y(x)$ and $Y'(-x) = \mp Y'(x)$. This means that Eq. (68) can be used for both transverse, $h_z(-x) = -h_z(x)$, and longitudinal, $h_z(-x) = h_z(x)$, excitations.

C. Flexure modes

The vibrational spectrum for flexure modes can be determined from Eqs. (65), (66), and (68) requiring $h_x(x) = h_x(-x)$ and $h_z(x) = -h_z(-x)$. This last condition requires that $F(x) = -F(-x)$ also. Hence, the general solution of Eq. (62) for flexures modes in a plate is

$$h_x = h_{xp} + qA_L\cosh(p_L x)/\cosh(p_L a) - qA_T\cosh(p_T x)/\cosh(p_T a) , \quad (71)$$

$$h_z = h_{zp} - q^2 A_L \sinh(p_L x)/\cosh(p_L a) + p_T^2 A_T \sinh(p_T x)/\cosh(p_T a) . \quad (72)$$

Since $h_z(x) = -h_z(-x)$, $F(x) = -F(-x)$ and the boundary conditions at $x = -a$ will *automatically* be satisfied if they are satisfied at $x = a$. This is consistent with the appearance of only two constants A_T and A_L in Eqs. (71) and (72). h_{xp} and h_{zp} are defined by Eq. (68) and can now be calculated using the symmetry properties of Eq. (68) for the half-space $0 < x < a$. For convenience, this solution will be labeled Y_F are shown below:

$$Y_F(x,p) = \int_0^a dx'\, g(x,x';p) F(x') , \quad (73)$$

where

$$g(x,x';p) = \sinh[p(a-x)]\sinh(px')/[p\sinh(pa)] \quad (74)$$

for $x > x'$. For $x < x'$, interchange x and x' in Eq. (74).

For brevity, only $h_z(x;q,w)$ will be given in this paper. It completely fixes the vibrational spectrum since $F(x)$ depends on h_z and not h_x. Using Eqs. (73), (65), and the boundary conditions at $x = a$, the coefficients A_L and A_T are fixed. One finds, after much algebra, that

$$h_z(x;q,w) = \int_0^a dx'\, G_{zz}(x,x';q,w) F(x';q,w) , \quad (75)$$

where

$$G_{zz} = G_{zz}^{(1)} + G_{zz}^{(2)} . \quad (76)$$

The Green's function

$$G_{zz}^{(1)}(x,x';q,w) = L_F(q,w) Y_F(x;q,w) Y_F(x';q,w) \quad (77)$$

with

$$Y_F(x;q,w) = (c_L/w)^2[-2q^2 U_F(x;p_L) + (p_T^2 + q^2) U_F(x;p_T)] \quad (78)$$

and

$$L_F(q,w) = (w/c_L)^2 p_T \tanh(p_T a)/D_F \quad (79)$$

with

$$D_F(q,w) = 4p_T^2 q^2 (T_T/T_L) - (p_T^2 + q^2)^2 \quad (80)$$

and

$$T_{T,L} = \tanh(p_{T,L} a)/(p_{T,L} a) . \quad (81)$$

The function U_F in Eq. (68) is given by

$$U_F(x;p) = \sinh(px)/\sinh(pa) . \quad (82)$$

Finally,

$$G_{zz}^{(2)}(x,x';q,w) = (c_L/w)^2[q^2 g(x,x';p_L) - p_T^2 g(x,x';p_T)] , \quad (83)$$

where $g(x,x';p)$ is defined by Eq. (74).

The Green's function $G_{zz}(x,x';q,w)$ is made up of terms, each of which is an *analytic* function of q and w. In particular, the functions which contain p, p_T, or p_L have power-series expansions that are *even* functions of p, p_T, or P_L so no branch cut appears in any of the functions. For small values of q and w, $L_F(q,w)$ has a pole at the flexure-mode resonance frequency $w_F(q)$ given by the zero in D_F for small values of q and w.

As mentioned previously, h_x and h_z obey the boundary conditions for arbitrary $F(x;q,w)$. Hence, one can use the integral equation for $h_z(x;q,w)$ to construct solutions for $h_z(x;q+Q, w-w_v)$, which involve $h_z(x';q+2Q, w-2w_v)$ and $h_z(x';q,w)$. The terms involving $(q-Q, w+w_v)$ give new terms involving (q,w) and $(q-2Q, w+2w_v)$. If one repeats these processes, an integral equation is obtained for $h_z(x;q,w)$ which depends upon a new iterated Green's function called $K_F(x,x';q,w)$ which is correct to g_0^2. Our new integral equation becomes

$$h_z(x;q,w) = \int_0^a dx'\, K_F(x,x';q,w) h_z(x';q,w) , \quad (84)$$

where

$$K_F = K_F^{(1)} + K_F^{(2)} , \quad (85)$$

with

$$K_F^{(m)} = -Q^2(g_0^2/2) G_{zz}^{(m)}(x,x';q,w) Y_z(x') + (Q^2 g_0/2)^2 \sum_{q',w'} \int_0^a dx''\, G_{zz}^{(m)}(x,x'';q,w) G_{zz}(x'',x';q',w') , \quad (86)$$

where the summation contains two terms:

$$(q',w')=(q+Q,\, w-w_v) \text{ and } (q-Q,\, w+w_v) \;. \tag{87}$$

The pole in G_{zz}, coming from $D_F(q,w)$, for small (q,w), dominates the behavior of the flexure kernel $K_F(x,x';q,w)$. Since $G_{zz}^{(1)}$ is separable, one can write Eq. (85) as

$$h_z(x)=L_F Y_L(x) A_F + \int_0^a dx' K_F^{(2)}(x,x';q,w) h_z(x') \;, \tag{88}$$

where the constant A_F is fixed by

$$A_F=\int_0^a dx' \left[-Q^2(g_0^2/2) Y_z(x') Y_F(x';q,w) + (Q^2 g_0/2)^2 \sum_{q',w'} \int_0^a dx'' \, Y_F(x'';q,w) G_{zz}(x'',x';q',w') \right] h_z(x';q,w) \;. \tag{89}$$

The method used to obtain the vibrational spectrum from Eqs. (88) and (89) is analogous to that used in Sec. III for the one-dimensional problem. There, one set $A_n=(g_0/2)A_0 G_n B_n$ for $n\neq 0$ and obtained an equation for A_0. Setting the coefficient of A_0 equal to zero fixed $w(q)$. Here, one can set

$$h_z(x;q,w)=L_F(q,w) A_F b_z(x;q,w) \;, \tag{90}$$

and then

$$b_z(x;q,w)=Y_F(x;q,w)+\int_0^a dx' K_F^{(2)}(x,x';q,w) b_z(x';q,w) \;. \tag{91}$$

Equation (91) can now be solved as a completely determined function of x, q, and w for small (q,w) to get the flexure modes. [Of course, $L_F(q,w)$ possesses higher-order poles corresponding to higher-frequency vibrations, but we are not interested in these in this paper.] When h_z from Eq. (90) is substituted into Eq. (89), one obtains an equation for the vibrational spectrum since the coefficient of A_F must *vanish*. The result correct to g_0^2 terms, is obtained by dropping the last term in Eq. (91), i.e., take $b_z=Y_F$ so that

$$1=L_F(q,w)(Qg_0/2)^2 \int_0^a dx \left[-2Y_z(x) Y_F(x;q,w) + Q^2 \sum_{q',w'} \int_0^a dx' \, Y_F(x';q,w) G_{zz}(x,x';q',w') \right] Y_F(x;q,w) \;. \tag{92}$$

The integrals in this equation can all be evaluated analytically. However, for small q and w it is necessary to make power-series expansions of rather involved functions. In particular, for small (q,w),

$$L_F(q,w)=-(c_T p_T)^2 ab / \{ w^2-[w_F(q)]^2 \} \;, \tag{93}$$

where

$$w_F(q)=2qc_T(qa)[(1-b)/3]^{1/2} \tag{94}$$

is the well-known flexure-mode frequency [cf. LL, Ref. 15, Sec. 25] for an infinite plate of thickness $2a$.

For samples whose length l is a few millimeters, only modes whose wave vectors q are greater than $2\pi/l$ can be excited. This is the case with the TaS_3 experiments of BR and Brill.[4] In this situation, one obtains from Eq. (92)

$$w=qc \;, \tag{95}$$

where

$$(c/c_T)^2=(qa)^2[4(1-b)/3-(g_0^2/6b)(3+8vc/c_L^2)] \;, \tag{96}$$

provided $Qa \gg 1$.

In the weak-coupling limit, $g_0 \ll 1$, the change in the flexure-mode frequency due to the CDW in the presence of an electric field can be expressed, using Eqs. (94)–(96), as

$$\Delta w_F/w_F=-g_0^2(qa)(v/c_T)/[3(1-b)]^{1/2} \;. \tag{97}$$

The presence of the qa factor in Eq. (97) comes from the term vc/c_L^2 in Eq. (96), which *dramatically* reduces $\Delta w_F/w_F$ as a function of the CDW drift velocity v. Equation (32) shows that $(\Delta c/c_L)_{\text{bulk}}$ is *orders of magnitude larger* than that for flexure waves.

D. Rayleigh-mode frequencies

The procedures discussed in the preceding subsection can be extended to examine Rayleigh modes near the surface of a thick plate. In the absence of CDW coupling, one can read LL (cf. Sec. 24). The functions L_F, Y_F, and G_{zz} must be changed, of course, with the poles of the appropriate L function fixing $w(q)$. For brevity, the details will be omitted and some of the results reported. One finds

$$\Delta w_R/w_R \cong -0.2 g_0^2 (v/c_T) \tag{98}$$

for the case $(c_T/c_L)^2 \ll 1$.

V. DISCUSSION

The Coppersmith-Varma model[5] has been generalized to treat the influence of a sliding CDW at long wavelengths for *arbitrary lattice distortions* leaving the CDW *undistorted.*

A derivation of the CV model was given in Sec. II based on the FL model and applied to the one-dimensional problem in Sec. III for an arbitrary coupling $g_0=V_0/Mc_L^2$. It was noted that the sound velocity c in this one-dimensional CV model can become arbitrarily small if g_0 is large enough. The results are summarized in Table I.

In Sec. IV the vibrational spectrum for plate geometry was investigated for flexure modes in considerable detail for a sample of thickness $2a$. An equation determining the flexure-mode frequency was derived and analyzed for the case $Qa \gg 1$, $qa \ll 1$ in the weak-coupling limit $g_0 \ll 1$.

As Coppersmith and Varma note in their paper, it appears that the CV model in the weak-coupling limit leads to $\Delta w/w$ changes described by

$$\Delta w/w = d g_0^2 (vc/c_L^2) , \tag{99}$$

where d is a constant of the order of unity.

For a thin rod, the unperturbed frequencies are given by

$$w_F' = 2q^2 a (E/12\rho)^{1/2} , \tag{100}$$

which in comparing Eqs. (94), (42), and (45) corresponds to

$$b = \tfrac{1}{2}, \quad c_T = c_L/2^{1/2}, \quad \text{and } \sigma = 0$$

(as expected), so that Eq. (97) becomes

$$\Delta w'/w' = -g^2 (qa) 3^{1/2} v/c . \tag{97$'$}$$

BR noted 1% changes in the flexural resonant frequency of TaS_3 samples of length $l \sim 3$ mm for electric fields above threshold. CV estimate $g_0 \cong 0.1$. Taking $q \sim 10$ cm^{-1} and $v/c_L \sim 10^{-5}$, the CV result would give, for bulk acoustic phonons, $\Delta w/w \sim 10^{-7}$. The results for flexural waves in the CV model is even smaller, as shown by Eq. (97′), by $qa \sim 10^{-3}$ with $a \cong 1$ μm.

One must conclude that the *weak-coupling* CV model cannot explain the BR flexure-mode data. This observation does not rule out a modified CV approach being appropriate. As noted in our derivation of the CV model in Sec. II, one should definitely use a more realistic phase function $\Phi(\mathbf{r},t)$, especially for small v near threshold. Moreover, if g_0 is not small one *cannot* use perturbation theory to solve for either u_0, the dynamic equilibrium displacement vector, or u_1, needed to derive the flexure-mode spectrum for small q and w.

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