# Attenuation of phase excitations in charge-density wave systems

M. L. Boriack and A. W. Overhauser Purdue University, West Lafayette, Indiana 47907

(Received 13 February 1978)

The attenuation of collective excitations (phasons) corresponding to phase modulation of a charge-density wave (CDW) caused by electron-phason interaction is studied. Phason attenuation is a nonlocal effect and must be treated microscopically because the pertinent length scale is determined by the CDW wave vector  $\vec{Q}$ rather than the phason wave vector  $\vec{q}$ . In three-dimensional jellium, phasons with  $\vec{q}$  parallel to  $\vec{Q}$  are predominantly attenuated by scattering electrons (in  $\vec{k}$  space) near the CDW energy gaps, and the attenuation rate is independent of temperature. The phason attenuation rate is  $\gamma \equiv (1/E) dE/dt$ , for a phason with energy E. We find  $\gamma \sim q \cos^2 \theta$ , where  $\theta$  is the angle between  $\vec{q}$  and  $\vec{Q}$ . For  $\vec{q}$  parallel to  $\vec{Q}$ ,  $\gamma$ is approximately 0.3 times the phason frequency; i.e., phasons are underdamped. Phasons with  $\vec{q}$ perpendicular to  $\vec{Q}$  are not attenuated. If heterodyne gaps (caused by potentials of periodicity  $\vec{Q} \pm 2\pi \vec{G}$ ) cut the Fermi surface, the attenuation is increased by a factor of 3.

## I. INTRODUCTION

In three-dimensional metals exchange interactions and electron-electron correlations can give rise to a charge-density wave (CDW) instability<sup>1</sup> which breaks the translation symmetry of the crystal. In the presence of a CDW the spatial density of conduction electrons is of the form

$$\rho = \rho_0 \left[ \mathbf{1} + p \cos(\mathbf{Q} \cdot \mathbf{r} + \varphi) \right], \tag{1}$$

where p is the fractional amplitude of the electron-density modulation,  $\rho_0$  is the mean electron density,  $\vec{Q}$  is the CDW wave vector, and  $\varphi$  is the CDW phase. This new periodicity arises in addition to the normal periodicity of the crystal lattice; and since Q is nearly equal to the diameter  $2k_F$  of the Fermi surface, the CDW periodicity is, in general, incommensurate with that of the lattice. The resulting structure is multiply periodic, and the crystal no longer has a translation group since no two ions are equivalent.

A CDW instability can occur only if the electronic charge density is locally neutralized by an accompanying lattice distortion.<sup>1</sup> Each positive ion will be displaced from its equilibrium lattice site  $\vec{L}$  by

$$\vec{u}(\vec{L}) = \vec{A}\sin(\vec{Q}\cdot\vec{L}+\varphi).$$
<sup>(2)</sup>

Because  $\vec{\mathbf{Q}}$  is incommensurate with the lattice, the energy of the system must be independent of the spatial position of the CDW as determined by the phase  $\varphi$ . It then follows that there will be lowfrequency collective excitations corresponding to  $\varphi$  varying slowly in space and time. These elementary excitations are called phasons<sup>2</sup> and have important consequences for experiments which try to detect a CDW with Bragg diffraction of x rays, neutrons, or electrons or through Knightshift or hyperfine-field effects.<sup>3</sup>

Because phasons have important experimental consequences, it is of interest to determine their rate of attenuation. Our purpose in this paper is to study the attenuation of phasons caused by electron-phason interaction.

We demonstrate below that the length scale of the electron-phason interaction is determined by the CDW wave vector  $\vec{Q}$  and not the phason wave vector  $\vec{q}$ . Because the wavelength of the interaction is the order of a lattice spacing, the electron mean free path will always be long compared to the wavelength of the interaction. Thus, phason attenuation is a nonlocal effect and is correctly described by "Golden Rule" quantum mechanics.

It is certainly incorrect to use Ohm's law or a transport equation with relaxation to a local equilibrium distribution in calculating the phason attenuation rate. Herein lies a major difference between the attenuation of phasons and the attenuation of long-wavelength acoustical phonons, i.e., ultrasonic attenuation. This difference is made manifest in the following argument. Consider a longitudinal acoustical phonon with wavelength  $2\pi/q$  equal to, say, 1000 lattice constants and amplitude A. Let us take a length of 100 lattice constants to define a macroscopic chunk of sample. The ion displacements are  $u = A \sin \mathbf{q} \cdot \mathbf{r}$ . The mean displacement of an ion in a typical "chunk" will be  $\sim A$  since the displacements are all, in general, in phase. Equivalently, there is a macroscopic motion of the charge density. Now consider a phason with wavelength  $2\pi/q$  equal to 1000 lattice constants. As shown below the displacements of the ions are  $u \sim A \sin[(\vec{Q} \pm \vec{q}) \cdot \vec{r}]$ . That is, the periodicity of the ion displacements is determined by  $Q \gg q$  and is the order of one lattice cons-

17

4549

tant. Since  $2\pi/Q$  is much smaller than the length of the 100-lattice-constant chunk, the mean displacement of an ion in the chunk is ~0. Thus a long-wavelength phason (unlike a phonon) is not accompanied by a macroscopic motion of the charge density.

McMillan<sup>4</sup> has dealt briefly with the problem of phason attenuation within the context of timedependent Landau theory. The relation of his work to that in this paper is disucssed in the Appendix.

### **II. PHASONS AND ELECTRON-PHASON INTERACTION**

In this section we review some of the properties of phasons assuming negligible damping. A more detailed discussion can be found in a previous work by one of the authors.<sup>2</sup> We also derive the electron-phason interaction.

Consider a single incommensurate CDW as described by Eqs. (1) and (2). Since the energy of the CDW is independent of phase  $\varphi$ , it follows that there will be low-frequency collective excitations corresponding to  $\varphi$  varying slowly in space and time. We express  $\varphi(\mathbf{L}, t)$  as an expansion in running waves,

$$\varphi(\vec{\mathbf{L}},t) = \sum_{\vec{\mathbf{q}}} \varphi_{\vec{\mathbf{q}}} \sin(\vec{\mathbf{q}} \cdot \vec{\mathbf{L}} - \omega_{\vec{\mathbf{q}}} t).$$
(3)

This approach is analogous to treating lattice dynamics in the continuum approximation.

The phason wave vectors  $\{\mathbf{\hat{q}}\}\$  are assumed small compared to the Brillouin zone.  $\{\omega_{\mathbf{\hat{q}}}\}\$  and  $\{\varphi_{\mathbf{\hat{q}}}\}\$  are the frequencies and amplitudes of the normal modes, respectively.

For simplicity consider only a single phason mode to be excited. The atomic displacements relative to the crystal lattice sites are

$$\mathbf{\tilde{u}}(\mathbf{\vec{L}},t) = \mathbf{\vec{A}} \sin[\mathbf{\vec{Q}} \cdot \mathbf{\vec{L}} + \varphi_{\mathbf{\vec{q}}} \sin(\mathbf{\vec{q}} \cdot \mathbf{\vec{L}} - \omega t)].$$
(4)

For the present study we take the amplitude  $\vec{A}$  of the atomic displacements to be parallel to  $\vec{Q}$ .

For small  $\dot{\varphi}_{\mathbf{d}}$  we can express  $\mathbf{u}$  approximately as

$$\mathbf{\tilde{u}}(\vec{\mathbf{L}},t) \cong \vec{\mathbf{A}} \sin \vec{\mathbf{Q}} \cdot \vec{\mathbf{L}} + \frac{1}{2} \vec{\mathbf{A}} \varphi_{\mathbf{\tilde{q}}} \sin[(\vec{\mathbf{Q}} + \vec{\mathbf{q}}) \cdot \vec{\mathbf{L}} - \omega t] - \frac{1}{2} \vec{\mathbf{A}} \varphi_{\mathbf{\tilde{q}}} \sin[(\vec{\mathbf{Q}} - \vec{\mathbf{q}}) \cdot \vec{\mathbf{L}} + \omega t].$$
(5)

If  $\overline{\mathbf{q}}$  is perpendicular to  $\overline{\mathbf{Q}}$ , the local direction of the CDW wave vector is slightly rotated. If  $\overline{\mathbf{q}}$  is parallel to  $\overline{\mathbf{Q}}$ , the local magnitude of the CDW wave vector is periodically modulated. Equation (5) also shows the relation between phasons and the phonon modes of the undistorted lattice. The last two terms, which represent phason deviations from the equilibrium CDW state, constitute a coherent superposition of phonon modes with wave vectors  $\overline{\mathbf{Q}} + \overline{\mathbf{q}}$  and  $\overline{\mathbf{Q}} - \overline{\mathbf{q}}$ . The energy density of a phason can be written<sup>2</sup>

$$E_{\mathbf{\dot{q}}} = \frac{1}{4} n M A^2 \omega^2 \varphi_{\mathbf{\dot{q}}}^2 , \qquad (6)$$

where n is the number of ions per unit volume and M is the ion mass.

It is expected that  $\omega_{\vec{q}}$  vs  $\vec{q}$  will be highly anisotropic because a local rotation of  $\vec{Q}$  requires less energy than a change in its magnitude. Consequently the surfaces of constant phason energy will be very flat (pancake-shaped) ellipsoids. The anisotropy could be as high as 100 to 1, especially if the Fermi surface is nearly spherical as is the case for the isotropic metals of primary interest in this work. Denoting components of  $\vec{q}$  parallel (longitudinal) and perpendicular (transverse) to  $\vec{Q}$  as  $q_{\parallel}$  and  $q_{\perp}$ , we can write  $\omega_{\vec{q}}$  as

$$\omega_{e}^{2} = c_{\perp}^{2} q_{\perp}^{2} + c_{\parallel}^{2} q_{\parallel}^{2} , \qquad (7)$$

where  $c_{\perp}$  and  $c_{\parallel}$  are the corresponding components of phason velocity and  $c_{\parallel}/c_{\perp}$  may be as great as 100. The phason frequency spectrum is plotted schematically in Fig. 1. Note that the phason spectrum is a continuous function of the angle between  $\vec{q}$  and  $\vec{Q}$ . The terms "longitudinal" and "transverse" are used here merely for convenience in specifying the special cases of  $\vec{q}$  parallel and perpendicular to  $\vec{Q}$  and do not have the same meaning as when they are applied to phonons.

For the electron density to be modulated as in Eq. (1) requires that the total self-consistent potential in the one-electron Schrödinger equation be of the form<sup>1</sup>

$$V(\mathbf{\tilde{r}}) = G\cos(\mathbf{Q} \cdot \mathbf{\tilde{r}} + \varphi) .$$
(8)

Taking a single phason mode  $\overline{\mathbf{q}}$  to be excited, we have for small  $\varphi_{\overline{\mathbf{q}}}$ 

$$V(\mathbf{\hat{r}}) = G \cos[\mathbf{\vec{Q}} \cdot \mathbf{\hat{r}} + \varphi_{\mathbf{\hat{q}}} \sin(\mathbf{\hat{q}} \cdot \mathbf{\hat{r}} - \omega t)]$$
  

$$\cong G \cos \mathbf{\vec{Q}} \cdot \mathbf{\hat{r}} + \frac{1}{2} \varphi_{\mathbf{\hat{q}}} G \cos[(\mathbf{\vec{Q}} + \mathbf{\hat{q}}) \cdot \mathbf{\hat{r}} - \omega t]$$
  

$$-\frac{1}{2} \varphi_{\mathbf{\hat{q}}} G \cos[(\mathbf{\vec{Q}} - \mathbf{\hat{q}}) \cdot \mathbf{\hat{r}} + \omega t].$$
(9)

The term  $G\cos \vec{Q}\cdot \vec{r}$  is the CDW potential in the absence of phasons. The second and third terms



FIG. 1. Schematic illustration of the vibrational modes in a metal having a CDW structure. The frequency of the phason branch goes to zero at  $\vec{Q}$ , the location of the CDW satellite reflection in  $\vec{k}$  space. Such a diagram has only an approximate meaning since an incommensurate CDW structure does not have a Brillouin zone.

4550

give the electron-phason interaction,

$$V_{e\varphi} = \frac{1}{2} \varphi_{\mathbf{q}} G \cos\left[ (\mathbf{Q} + \mathbf{\bar{q}}) \cdot \mathbf{\bar{r}} - \omega t \right] -\frac{1}{2} \varphi_{\mathbf{q}} G \cos\left[ (\mathbf{\bar{Q}} - \mathbf{\bar{q}}) \cdot \mathbf{r} + \omega t \right].$$
(10)

Note that the wavelengths of the periodic potentials are determined by the CDW wave vector  $\vec{Q}$ which is much larger than the phason wave vector  $\vec{q}$ . Thus, phason attenuation is a nonlocal effect as discussed in Sec. I.

### **III. SCATTERING OF "BELLY" ELECTRONS**

The one-electron Schrödinger equation which incorporates the CDW potential is

$$\mathcal{K} = p^2 / 2m + G \cos \mathbf{Q} \cdot \mathbf{\vec{r}}, \qquad (11)$$

where  $\varphi$  has been chosen equal to zero without loss of generality. This potential deforms the electron wave functions by mixing the plane wave state  $\vec{k}$  with  $\vec{k} \pm \vec{Q}$  and leads to the modulated electron density of Eq. (1). The electron energy spectrum is also altered. As shown in Fig. 2, the CDW potential leads to energy gaps of magnitude G at  $\vec{k}$  $=\pm\frac{1}{2}\vec{Q}$ . Figure 2 also shows the lemon-shaped Fermi surface which results for the case of critical contact, i.e., when the Fermi surface touches the energy gaps at a point.

We shall show that there are two regions in  $\bar{k}$  space where electrons are scattered by phasons: electrons near the "belly" of the lemon and "conical point" electrons near the energy gap. For simplicity we begin by considering the "belly" electrons.

Far away from the energy gaps, the electron states which diagonalize the Hamiltonian (11) are easily found using first-order perturbation theory. A state  $\Psi_{r}$  below the energy gap is

$$\Psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}} + \left[G/2(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{Q}})\right]e^{i(\vec{k}-\vec{Q})\cdot\vec{r}} + \left[G/2(\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{Q}})\right]e^{i(\vec{k}+\vec{Q})\cdot\vec{r}}, \qquad (12)$$



FIG. 2. One-electron energy spectrum and Fermi surface of a metal with a CDW of wave vector  $\vec{Q}$ . Energy gap caused by the CDW periodic potential is G. Distortion of the Fermi surface at the conical point P is exaggerated. Electron wave functions most severely deformed are those between the conical point P and the plane w. Electrons which contribute to phason attenuation are those labeled B near the belly and C near the conical point.

where  $\epsilon_{k} \equiv \hbar^{2}k^{2}/2m$ . It is sufficiently accurate to take the energy of  $\Psi_{k}^{*}$  to be the free-electron energy  $\epsilon_{k}^{*}$ . We will be considering only the zero-temperature limit so that only states below the gap are needed for the Fermi surface of Fig. 2. We assume  $\hbar\omega_{\tilde{q}} \ll G$ , i.e., phasons do not cause interband transitions.

Phasons are attenuated by scattering electrons from states  $\Psi_{\vec{k}}$  below the Fermi surface to states  $\Psi_{\vec{k}'}$  above the Fermi surface. We now can write down the golden rule transition rate. Confining the region of interest temporarily to "belly" states, we find the transition rate using Eq. (10) for the electron-phason interaction,

$$w_{\vec{k} \to \vec{k} + \vec{q}} = (2\pi/\hbar) (\frac{1}{4} \varphi_{\vec{q}} G)^2 |\mathfrak{M}|^2 \delta(\epsilon_{\vec{k} - \vec{q}} - \epsilon_{\vec{k}} - \hbar \omega_{\vec{q}}) \\ \times f_{\vec{k}} (1 - f_{\vec{k} + \vec{q}}), \qquad (13)$$

where

$$\left|\mathfrak{M}\right|^{2} = \left(\frac{1}{2} G\right)^{2} \left[1/(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{Q}}) - 1/(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}-\vec{Q}+\vec{q}}) - 1/(\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{Q}+\vec{q}}) + 1/(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}+\vec{Q}+\vec{q}})\right]^{2}.$$
 (14)

The Fermi-occupation probabilities  $f_{\vec{k}}$  and  $f_{\vec{k}+\vec{q}}$  weight the transition rate by the probability that the initial state is filled and the final state is empty.

The phason loses energy to the electrons at the

rate

$$\frac{dE_{\mathbf{q}}}{dt} = -\hbar\omega_{\mathbf{q}} \sum_{\mathbf{k}} w_{\mathbf{k}\to\mathbf{k}+\mathbf{q}} .$$
(15)

Conservation of energy required by the  $\delta$  function makes  $\epsilon_{\mathbf{k}+\mathbf{q}}^* = \epsilon_{\mathbf{k}}^* + \hbar \omega$ . In the  $q \to 0$  limit it follows that the scattered electrons are those with velocity  $\mathbf{v}$  such that the component of  $\mathbf{v}$  along  $\mathbf{q}$  is equal to the phason velocity. This condition is the same as that for ultrasonic attenuation. For longitudinal phasons the energy conserving transitions satisfy  $\cos\theta_{\mathbf{k},\mathbf{q}}^* = c_{\parallel}/v_F \sim 10^{-3}$ . The scattered electrons lie on a ring at the belly of the lemon as indicated in Fig. 2. For these electrons  $f_{\mathbf{k}}^*(1-f_{\mathbf{k}+\mathbf{q}}^*)$  $\rightarrow \frac{1}{2}\hbar\omega_{\mathbf{q}}^*\delta(\epsilon_{\mathbf{k}}^* - E_F)$  in the zero-temperature limit.  $E_F$  is the Fermi energy.

Furthermore,

$$|\mathfrak{M}|^{2} \cong (4mGq_{\parallel}/\hbar^{2}Q^{3})^{2}$$
(16)

plus higher-order terms in  $q_{\parallel}/Q$ . Since the matrix element for the transition depends on  $q_{\parallel}$ , transverse phasons, for which  $\vec{q} \cdot \vec{Q} = 0$ , are not attenuated. The matrix element for electron-phason scattering depends on the difference of plane-wave coefficients for CDW electrons separated by  $\vec{q}$  in  $\vec{k}$ space. Since these coefficients are functions only of the component of  $\vec{k}$  parallel to  $\vec{Q}$ , the difference must be zero for  $\vec{q}$  perpendicular to  $\vec{Q}$ .

Changing the sum over  $\vec{k}$  in (15) to an integral and performing the integration gives

(17)

The energy attenuation coefficient is  $\gamma_{\dot{\mathbf{q}}} \equiv -(1/E_{\dot{\mathbf{q}}})^2$ × $dE_{\dot{\mathbf{r}}}/dt$ . Combining Eqs. (6) and (17) obtains

$$\gamma_{\mathbf{d}} = (6\pi\hbar Q^2 / MA^2) (mG/\hbar^2 Q^2)^4 q \cos^2\theta_{\mathbf{Q},\mathbf{d}}, \quad (18)$$

where  $\theta_{\vec{Q},\vec{q}}$  is the angle between  $\vec{Q}$  and  $\vec{q}$ , and we have used the relation  $n = k_F^3/3\pi^2$ . Note that  $\gamma_{\vec{q}}$  is independent of temperature.

Our primary interest in this work is the alkali metals and, in particular, potassium. The CDW hypothesis has been successful in explaining quantitatively several of the anomalous properties of potassium including the anomalous optical absorption,<sup>5</sup> splitting of the conduction-electron spin-resonance g factor,<sup>6</sup> and the anisotropic residual resistivity.<sup>7</sup> Moreover, the question of phasons is of interest in potassium since the phason Debye-Waller factor would likely greatly reduce the intensity of CDW diffraction satellite peaks.<sup>2,3</sup> The intensity would not be lost but would be transferred into a pancake-shaped phason cloud about the satellite position. Special techniques that integrate over this diffuse phason pancake may be required to detect the effects of the CDW in a diffraction experiment.

We, therefore, evaluate  $\gamma_{\mathbf{q}}$  for the proposed CDW in potassium. Taking  $G/E_F = 0.3$ ,  $A \cong 0.1$  Å,  $Q \cong 2k_F$ , and longitudinal phasons, for which  $\theta_{\mathbf{q},\mathbf{q}}^{\bullet} = 0$ , we obtain

$$\gamma_{q}^{\bullet} \cong (20 \text{ cm/sec})q. \tag{19}$$

A useful quantity is the phason quality factor  $\mathfrak{Q} \equiv \omega_{\mathbf{q}}^{-}/\gamma_{\mathbf{q}}^{-}$  which gives the number of phason cycles during the mean lifetime  $1/\gamma_{\mathbf{q}}^{-}$  of the phason. While there is no experimental knowledge of the phason spectrum, a reasonable estimate is that the longitudinal phason velocity is comparable to the longitudinal phonon velocity, i.e.,  $c_{\parallel} \sim 3 \times 10^5$  cm/sec. Note that since both  $\gamma_{\mathbf{q}}^{-}$  and  $\omega_{\mathbf{q}}^{-}$  depend linearly on q,  $\mathfrak{Q}$  is independent of q. For longitudinal phasons  $\mathfrak{Q} \sim 1.5 \times 10^4$  so that considering only the "belly" electrons leads to negligible damping. Note from (7) and (18) that  $\mathfrak{Q}$  is monotonically increasing as  $\theta_{\mathbf{Q},\mathbf{q}}^{-}$  increases from 0 to  $\frac{1}{2}\pi$ . For transverse phasons  $\gamma_{\mathbf{q}} \equiv 0$ .

### IV. SCATTERING OF "CONICAL POINT" ELECTRONS

In the discussion following Eq. (15) we found that the electrons scattered by a phason in the limit q - 0 are those with velocity  $\vec{v}$  such that the component of  $\vec{v}$  along  $\vec{q}$  is equal to the phason velocity. In addition to the electrons near the belly, discussed in Sec. III, there exist electrons in  $\vec{k}$  space near the energy gaps which satisfy this criteria for energy conserving transitions. This can be seen from Fig. 2. Owing to Bragg reflection by the periodic CDW potential, electrons at  $\bar{k} = \pm \frac{1}{2}Q$  have zero velocity in the  $\bar{Q}$  direction. For the Fermi surface in Fig. 2, the other velocity components are also zero for the states at  $\pm \frac{1}{2}Q$ . It follows that electrons near the conical points also contribute to phason attenuation. For each phason only electrons near one of the conical points contribute since the other electrons move in the wrong direction.

The most severely deformed wave functions and energies are for states in the conical point regions. Sufficiently accurate CDW electron wave functions can be found near the energy gap at  $\frac{1}{2} \vec{Q}$  by considering only the plane wave states  $\vec{k}$  and  $\vec{k} - \vec{Q}$ . These plane wave states are degenerate at  $\vec{k} = \frac{1}{2} \vec{Q}$ in the absence of the CDW potential. Diagonalizing the Hamiltonian (11) exactly on this basis leads to the wave functions and energies of states above and below the gap. For the present work only states below the gap need to be considered. It is convenient to move the origin in  $\vec{k}$  space to  $\frac{1}{2} \vec{Q}$ . For the remainder of this section  $\vec{k}$  will be measured from this new origin. A state  $\Psi_{\vec{k}}^*$  below the energy gap is

$$\Psi_{\vec{k}} = e^{i\vec{Q}\cdot\vec{r}/2}(\cos\xi \, e^{i\vec{k}\cdot\vec{r}} - \sin\xi \, e^{i(\vec{k}-\vec{Q})\cdot\vec{r}})\,, \qquad (20)$$

and has energy

$$E_{\vec{k}} = \hbar^{2} (k^{2} + \frac{1}{4} Q^{2}) / 2m - \frac{1}{2} \left[ (\hbar^{2} \vec{k} \cdot \vec{Q} / m)^{2} + G^{2} \right]^{1/2}.$$
(21)

The coefficients  $\cos \xi$  and  $\sin \xi$  are defined by

$$\sin 2\xi = G[(\hbar^2 \mathbf{k} \cdot \mathbf{Q}/m)^2 + G^2]^{-1/2}.$$
(22)

The golden rule transition rate for a phason to scatter an electron from state  $\Psi_{\mathbf{k}}^*$  below the Fermi surface to a state  $\Psi_{\mathbf{k}+\mathbf{q}}^*$  above is given by (13) with  $\boldsymbol{\epsilon}_{\mathbf{k}}$  replaced by  $E_{\mathbf{k}}$  and

$$\mathfrak{M}|^{2} = (\cos\xi\sin\xi' - \sin\xi\cos\xi')^{2}.$$
(23)

Note that  $\mathfrak{M}$  depends on cross terms, i.e., the coefficient of  $e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}$  is multiplied by the coefficient of  $e^{i(\vec{\mathbf{k}}'-\mathbf{Q})\cdot\vec{\mathbf{r}}}$ , etc.

Energy conservation requires  $E_{\vec{k}+\vec{q}} = E_{\vec{k}} + \hbar \omega$ . For longitudinal phasons the scattered electrons are found using (21) to be those which satisfy

$$k_{g} = -[mc_{\parallel}(\hbar Q^{2}/2mG) - 1)] - \frac{1}{2}q.$$
(24)

In the limit  $q \rightarrow 0$  this reduces to the requirement that the component of electron velocity along  $\bar{q}$  is equal to the phason velocity. Near the energy gaps the electrons behave as if they had effective mass  $m(\hbar^2Q^2/2mG-1)^{-1}$ . If  $\frac{1}{2}q$  is greater than the first term on the right-hand side in (24), the electron will be scattered from a state  $\Psi_{\bar{k}}$  on one side of the conical point to  $\Psi_{\bar{k}+\bar{q}}$  on the other side. For the Fermi surface in Fig. 2, the electron is scattered from the conical point on the right to that on

4552

the left. We shall discuss this point in more detail below.

It is straightforward to evaluate (23) and to perform the integration over  $\bar{k}$  space in (15). The rate at which the phason loses energy to the electrons is

$$dE_{\vec{d}}/dt = \left(\varphi_{\vec{d}}^2 Q^2 \hbar \omega^2 q / 128\pi\right) \cos^2 \theta_{\vec{Q},\vec{d}}.$$
 (25)

Note that (24) is independent of the CDW energy gap. M depends on the difference in the coefficients of the wave functions describing states separated by  $\vec{q}$  in  $\vec{k}$  space. Near the energy gaps the electron effective mass is smaller than the freeelectron mass by a factor of order  $G/E_{F}$ . Thus a small change by  $\vec{q}$  in  $\vec{k}$  space results in a large change in  $\mathfrak{M}$ . Expression (24) is valid for q/Q $< 2mG/\hbar^2 Q^2$ . With  $G/E_F \cong 0.3$  as proposed for potassium  $q \leq 10^7$  cm<sup>-1</sup>. Since  $dE_{\mathfrak{q}}/dt$  depends on  $\cos^2\theta_{\vec{Q},\vec{q}}$ , transverse phasons are not attenuated by scattering conical point electrons.

The temperature-independent energy attenuation coefficient for longitudinal phasons in potassium is

$$\gamma_{\mathfrak{d}} \cong (1.1 \times 10^5 \text{ cm/sec})q. \tag{26}$$

Taking  $c_{\parallel} \sim 3 \times 10^5$  cm/sec gives a phason quality factor  $\mathcal{Q} \sim 2.7$ . Since both  $\omega_{\vec{a}}$  and  $\gamma_{\vec{a}}$  depend linearly on q, 2 is independent of q. Thus longitudinal phasons are underdamped but, nevertheless, rather strongly attenuated. The  $\mathcal{Q}$  obtained here depends on the specific values chosen for A and  $c_{\mu}$ .

This strong scattering by phasons of conicalpoint electrons should have important experimental consequences. The strong attenuation of longitudinal phasons should effect their contribution to the low-temperature specific heat. Due to phason scattering electrons near a conical point will have a short lifetime. The high rate of scattering of electrons from one conical point to the other may have important consequences for magnetotransport. The short lifetime of conical point electrons is also important to the de Haasvan Alphen effect. For an applied magnetic field parallel to  $\vec{Q}$ , the important cyclotron orbits for the de Haas-van Alphen effect are those at the belly of the 'lemon where phason scattering is negligible. As the magnetic field is tilted away from  $\vec{\mathbf{Q}}$ , the important cyclotron orbits will intersect the conical points. An electron on this orbit will be "killed" before it can complete the orbit, and the de Haas-van Alphen signal should disappear. This loss of signal as the orientation of the crystal changes has been observed in certain samples of potassium<sup>8</sup> and is difficult to explain on the basis of free-electron theory.

With a CDW present, the potential in a metal will have terms with periodicity  $\vec{Q}$  and  $2\pi \vec{G}$ , where

⊨ |2#Ğ-Q | -Heterodyne Gap

FIG. 3. If "heterodyne" gaps caused by potentials with periodicity  $2\pi \vec{G} \pm \vec{Q}$ cut the Fermi surface as shown, there are two additional sets of electrons,  $H_1$  and  $H_2$ , which contribute to attenuation for a longitudinal phason with velocity to the right.

 $\mathbf{\tilde{G}}$  is a reciprocal lattice vector. In addition there will be "heterodyne" terms with periodicity  $\vec{\mathbf{Q}}$  $\pm 2\pi \vec{G}$ .<sup>9</sup> If  $\vec{Q} \pm 2\pi \vec{G}$  is less than the diameter of the Fermi surface, there will be additional "heterodyne" gaps in the electron energy spectrum and the Fermi surface will be multiply connected as in Fig. 3. There will now be two additional places where longitudinal phasons will be strongly attenuated since Eq. (25) is valid as long as q is small enough as that the scattered electrons are within the strongly deformed regions of the energy spectrum. The quality factor for longitudinal phasons will be  $2 \sim 1$ . In the presence of heterodyne gaps as in Fig. 3, longitudinal phasons will be (approximately) critically damped, but transverse phasons will remain undamped.

We have shown above that phasons with  $\overline{q}$  perpendicular to Q are not attenuated in jellium. A question which arises is: do the ionic potentials in a real metal lead to finite attenuation of transverse phasons? We have investigated this problem by including the effects of ionic potentials following the method of pseudopotentials. We have found that the first-order matrix element for golden rule transitions is still zero for transverse phasons. However, there is a small but finite attenuation in the next order, i.e., the transition rate depends on the fourth power of the pseudopotential. Thus transverse phasons remain very much underdamped.

#### V. CONCLUSIONS

We have derived the electron-phason interaction and have shown that the wavelength of the interaction is determined by the CDW wave vector  $\vec{Q}$ and not the wave vector  $\vec{q}$  of the phason. Phason attenuation is, therefore, a nonlocal phenomenon and is correctly treated quantum mechanically. Because long-wavelength phasons are not accompanied by macroscopic motion of the charge density, the attenuation of phasons cannot be treated by Ohm's law. Phasons are predominantly attenuated by scattering electrons near the CDW energy gaps. The attenuation rate is independent of temperature. However, transverse phasons are



Q

not attenuated. The scattering of conical point electrons leads to phasons which are underdamped; but for longitudinal phasons the damping is strong, and the attenuation rate is ~0.3 times the phason frequency for the proposed phasons in potassium. If heterodyne gaps cut the Fermi surface, electrons near these gaps also contribute strongly to phason attenuation (and longitudinal phasons may be nearly critically damped).

### APPENDIX

McMillan<sup>4</sup> has dealt briefly with the problem of phason attenuation within the context of time-dependent Landau theory. McMillan described the shortwavelength components of charge density by an order parameter  $\Psi(\tilde{\mathbf{r}})$ . He treated the long-wavelength components of the conduction-electron charge density as an incompressible fluid with velocity field  $\tilde{\mathbf{v}}(\tilde{\mathbf{r}})$ . He then wrote an "Ohm's law" expression for the power dissipation and found equations of motion for  $\Psi$  and  $\tilde{\mathbf{v}}$  which resulted in overdamped phasons.

From the discussion in Sec. I of this work, it is clear that McMillan's "Ohm's law" approach is not valid. Phasons are not accompanied by a macroscopic motion of the charge density. The

- <sup>1</sup>A. W. Overhauser, Phys. Rev. <u>167</u>, 691 (1968).
- <sup>2</sup>A. W. Overhauser, Phys. Rev. <u>B</u> 3, 3173 (1971).
- <sup>3</sup>A. W. Overhauser, Hyperfine Interactions
- 4, 786 (1978).
- <sup>4</sup>W. L. McMillan, Phys. Rev. B <u>12</u>, 1197 (1975).
- <sup>5</sup>A. W. Overhauser and N. R. Butler, Phys. Rev. B <u>14</u>, 3371 (1976).

length scale important to phason attenuation is determined by the CDW wave vector  $\vec{Q}$  and not the phason wave vector  $\vec{q}$ . It is incorrect to apply Ohm's law on a 1-Å scale.

McMillan finds that the lifetime of the phason decreases with increasing conductivity. In other words, the rate of attenuation increases as the conductivity increases. This result is analogous to the (incorrect) result obtained in the theory of ultrasonic attenuation when nonlocal effects are disregarded. The mechanism for phason attenuation, as we have shown, is scattering of electrons near the CDW energy gaps and is nonlocal. It should also be noted that McMillan's result for the attenuation rate is temperature dependent since it is proportional to the (temperature-dependent) conductivity. This is in direct contrast to our temperature-independent result.

McMillan finds that the phason lifetime  $\tau \sim 1/q^2$ (in contrast to the correct result,  $\sim 1/q$ ). An important question, then, is why his phasons are not oscillatory (underdamped) in the  $q \rightarrow 0$  limit where  $\tau \rightarrow \infty$ . The reason is that McMillan's equations do not allow for oscillatory solutions. The kinetic energy term containing  $(\partial \Psi/\partial t)^2$  which would lead to a second-order differential equation for the order parameter was omitted.

- <sup>6</sup>A. W. Overhauser and A. M. deGraaf, Phys. Rev. <u>168</u>, 763 (1968).
- <sup>7</sup>M. F. Bishop and A. W. Overhauser, Phys. Rev. Lett. <u>39</u>, 632 (1977).
- <sup>8</sup>D. Shoenberg and P. J. Stiles, Proc. R. Soc. A <u>281</u>, 62 (1964).
- <sup>9</sup>A. W. Overhauser, Phys. Rev. B 9, 2441 (1974).