Brief Reports

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Helicon-wave damping in a periodic structure

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Damping of helicon waves propagating in a sinusoidally modulated structure is treated on the basis of linear-response theory. Numerical application to the charge-density-wave state of potassium shows that damping has a deleterious effect on the high-frequency helicon modes predicted earlier.

I. INTRODUCTION

In a previous paper¹ the dispersion relations were derived for helicon waves propagating in a periodic structure with a charge density which is modulated along one dimension, but which is essentially free-electron-like along the remaining two. The derivation was carried out on the basis of linear-response theory by generalizing the standard formulation for a free-electron gas^{2,3} to the case of periodic structures. Numerical application was made to the so-called charge-density-wave (CDW) state of potassium,⁴ in which there is a sinusoidal modulation of charge density. The dispersion relations so calculated were in basic agreement with the earlier results of McGroddy et al.⁵ The dispersion curve showed a maximum and a sharp drop, and the helicon-wave propagation was restricted to a very small part of the Brillouin zone. In addition, a band of high-frequency helicons with frequencies very near the cyclotron frequency ω_c , but well below it, were found. These high-frequency helicon modes had their origin in the one-dimensional band structure induced by the CDW and in the resonant nature of the dielectric tensor. The exact nature of these modes was not clear, but it was thought that these modes would provide, if confirmed experimentally, additional evidence for the CDW state. It was further noted that more theoretical work regarding the damping of these modes was required before the existence of these modes could be firmly established. It is the purpose of this Brief Report to present the results of a theoretical study of the damping of helicon waves in a periodic structure, with numerical applications to the CDW state of potassium. The study is carried out within the framework of linear-response theory by including an imaginary part for the frequency in the response functions. Expressions are given for the real and imaginary parts of the complex frequency of the helicon modes. Numerical

application to the CDW state of potassium shows that damping has a deleterious effect on the high-frequency helicon modes.

II. LINEAR-RESPONSE THEORY FOR HELICON DAMPING IN A PERIODIC STRUCTURE

Consider a system with an electronic structure which is free-electron-like along the x and the y directions, but is periodic along the z direction. Applied along the z direction is a static magnetic field \mathbf{B}_0 , described by a vector potential \mathbf{A}_0 , whose components in the Landau gauge are $(0, B_0 X, 0)$. There is also an electromagnetic disturbance that varies as $\exp(i\mathbf{q}\cdot\mathbf{r}-i\omega t)$. The wave vector \mathbf{q} is also taken to be along the z direction. $\mathbf{A}_1(\mathbf{r},t)$ is taken to be the vector potential for the selfconsistent field produced by the disturbance. SI units are used throughout.

We assume that the medium is nonmagnetic. The electric and the magnetic fields associated with the wave are related through the Maxwell's equations. Using the notation of Ref. 1, it can be shown that the frequencies of the helicon waves are determined from

$$\epsilon_{\pm}(q,\omega)\omega_{\pm}^2 = c^2 q^2 . \qquad (2.1)$$

Here $\epsilon_{\pm}(q,\omega)$ are the wave-vector- and frequencydependent components of the dielectric tensor in the polarization representation and are given in terms of the corresponding Cartesian components by

$$\boldsymbol{\epsilon}_{\pm}(\boldsymbol{q},\boldsymbol{\omega}) = \boldsymbol{\epsilon}_{\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{q},\boldsymbol{\omega}) \pm i \boldsymbol{\epsilon}_{\boldsymbol{x}\boldsymbol{y}}(\boldsymbol{q},\boldsymbol{\omega}) , \qquad (2.2)$$

and c is the speed of light.

The dielectric tensor is related to the conductivity tensor $\underline{\sigma}(q,\omega)$ according to

$$\underline{\epsilon}(\mathbf{q},\omega) = \epsilon_1 \underline{\mathbb{1}} + \frac{i\underline{\sigma}}{\omega\epsilon_0} . \tag{2.3}$$

36 8147

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BRIEF REPORTS

Here ϵ_1 is the dielectric constant of the lattice and $\underline{1}$ is the unit tensor. As has been described in Ref. 1, an ex-

pression for the conductivity tensor on the basis of linear-response theory can be obtained as

$$\sigma_{\pm} = \frac{i\omega_{p}^{2}\epsilon_{0}}{\omega} \left[1 + (\hbar\omega_{c}/N) \sum_{\substack{n,k_{y},k_{z} \\ l,l'}} \Lambda(nk_{y}k_{z}ll') \sum_{K,K'} b_{l}'^{*}(k_{z}+q+K)b_{l}(k_{z}+K)b_{l}^{*}(k_{z}+K')b_{l'}(k_{z}+q+K') \right], \quad (2.4)$$

where

$$\Lambda(nk_{y}k_{z}ll') = (n+1)\frac{\left[f_{0}(E(n+1,k_{z}+q,k_{y},l')) - f_{0}(E(n,k_{z},k_{y},l))\right]}{E(n+1,k_{z}+q,k_{y},l') - E(n,k_{z},k_{y},l) - \hbar(\omega \pm \omega_{c})}$$
(2.5)

Here ω_p is the plasma frequency, ω_c the cyclotron frequency, and N the number of electrons. The other quantities entering Eqs. (2.4) and (2.5) refer to the energy eigenvalue

$$E(n,k_z,k_y,l) = (n+\frac{1}{2})\hbar\omega_c + \varepsilon_l(k_z)$$
(2.6)

associated with the eigenstate

$$|nk_{z}k_{y}l\rangle = e^{ik_{y}Y}U_{n}(x+l_{H}^{2}k_{y})\sum_{K}b_{l}(k_{z}+K)e^{i(k_{z}+K)z}$$
(2.7)

of the unperturbed Hamiltonian

$$H_0 = (\mathbf{P} - e \,\mathbf{A}_0)^2 / 2m + V(z) , \qquad (2.8)$$

where V(z) is the periodic potential along z.

The f_0 's refer to the Fermi factors, U_n are the harmonic oscillator wave functions, and $l_H = (\hbar/m\omega_c)^{1/2}$ is the magnetic length. The $b_l(k_z + K)$ are the expansion coefficients associated with a set of plane-wave basis functions as described in Ref. 1.

Damping effects can be considered by replacing the frequency ω in Eq. (2.5) by a complex quantity $\omega - i/\tau$, as a result of which the dielectric tensor becomes a complex quantity:

$$\boldsymbol{\epsilon}_{+}(\boldsymbol{q},\omega) = \boldsymbol{\epsilon}_{+}^{\prime}(\boldsymbol{q},\omega) + i\boldsymbol{\epsilon}_{+}^{\prime\prime}(\boldsymbol{q},\omega) . \qquad (2.9)$$

We choose to work with a real wave vector q and a complex frequency in the dispersion relation given by Eq. (2.1). Furthermore, we focus on the mode associated with the positive sign and henceforth drop the subscript and the arguments (q, ω) . The real part ω' and the imaginary part ω'' of the helicon-mode frequency are then given by

$$\omega^{\prime 2} - \omega^{\prime \prime 2} = c^2 q^2 \epsilon^{\prime} / (\epsilon^{\prime 2} + \epsilon^{\prime \prime 2}) , \qquad (2.10)$$

$$2\omega'\omega'' = -c^2 q^2 \epsilon'' / (\epsilon'^2 + \epsilon''^2) . \qquad (2.11)$$

III. RESULTS AND DISCUSSION

The variation of both the real and the imaginary parts of the helicon-mode frequency as a function of the wave vector have been calculated for the CDW model of potassium using Eqs. (2.10) and (2.11) and the same values of the model parameters as those in Ref. 1. The disper-

sion of ω' is shown in Fig. 1 for several values of the collision parameter τ . Figure 2 shows the variation of ω'' with the wave vector q for the same values of τ .

As can be seen, there is no significant change in the dispersion of the low-frequency helicon branch due to collision damping and, in fact, the dispersion curve, say for $\omega_c \tau = 10^5$, is practically identical to the one given in Ref. 1. The big difference, however, is that there are no high-frequency helicon modes when collision damping is included.

In Ref. 1, the dispersion relation was determined in the following way. First a value of q was chosen, and the dielectric tensor $\epsilon_+(q,\omega)$ was calculated as a function of the frequency ω , by carrying out the sum in Eq. (2.4) in the Brillouin zone. The particular value of ω for which the value of the product $\omega^2 \epsilon_+(q,\omega)$ equals the



FIG. 1. Real part of the helicon-mode frequency vs wave vector q.



FIG. 2. Imaginary part of the helicon-mode frequency vs wave vector q.

value of the product c^2q^2 (within the accuracy of eight significant digits) would then give the frequency of the helicon wave of wave vector q. This is illustrated⁶ graphically in Fig. 2 for the high-frequency modes, where $\omega^2 \epsilon_+(q, \omega)$ is plotted as a function of ω for a given value of q. The helicon-mode frequencies correspond to the intersections of this curve, with the straight line corresponding to c^2q^2 . The high-frequency modes really correspond to those regions when $\epsilon_+(q, \omega)$ is increasing sharply, as indicated by the dashed lines. However, when collision damping is included, $\omega^2 \epsilon_+(q, \omega)$ does not go to ∞ , but its variation is shown by the thick line in Fig. 3, which does not intersect the horizontal line corresponding to c^2q^2 . Thus there are no high-frequency helicon modes for any real value of q.

For smaller values of the collision damping term $\omega_c \tau$, there is little qualitative difference in the dispersion curve, but quantitatively, the frequency becomes somewhat smaller and the range of wave-vector values in the Brillouin zone where helicon propagation is possible is further reduced.

As far as the imaginary part of the frequency is concerned, one can discern two distinctly different patterns. For the part which corresponds to the region where the real part of the frequency increases with q, the damping is small, and ω'' increases slightly with q. In the other part, where the real part of the frequency decreases with q, the damping is larger by several orders of magnitude and ω'' decreases with increasing q.

It may be noted that one could have studied the spa-



FIG. 3. Graphical solution of the characteristic equation.

tial damping by considering the frequency to be real and the wave vector to be complex in Eq. (2.1). However, in view of the reasons mentioned earlier, it was not considered likely to find actual roots for the dispersion in the high-frequency region.

The dispersion relation in Eq. (2.1) has solutions which exist in a fourfold space spanned by the real and the imaginary parts of the frequency ω' and ω'' and the real and the imaginary parts of the wave vector q' and q''. When the choice of an entirely real wave vector is made, only a part of the fourfold space is considered and no roots are found for the dispersion in the highfrequency region. Similarly, the choice of an entirely real frequency but complex wave vector would result in sampling a different region of the fourfold space. Whether or not actual roots are found for the dispersion relation in the high-frequency region with either of the two restricted choices considered above, the dielectric tensor still has a resonant character in the region of the high-frequency modes. It appears likely, therefore, that there may be maxima in the absorption of energy at these high-frequency mode positions. These absorption maxima, if observed experimentally, could be considered as evidence of the existence of the high-frequency modes and hence of the CDW state in potassium. It is worth mentioning that the possible existence of these modes as a probe of the CDW state in potassium has acquired additional significance in view of the very recent negative results obtained in neutron-diffraction experiments⁷ and in synchrotron x-ray experiments.8

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- ¹B. N. Narahari Achar, Phys. Rev. B 35, 7334 (1987).
- ²J. J. Quinn and S. Rodriguez, Phys. Rev. **128**, 2487 (1962).
- ³M. P. Green, H. J. Lee, J. J. Quinn, and S. Rodriguez, Phys. Rev. 177, 1019 (1969).
- ⁴A. W. Overhauser, Phys. Rev. Lett. 13, 190 (1964).
- ⁵J. C. McGroddy, J. L. Stanford, and E. A. Stern, Phys. Rev. **141**, 437 (1966).
- ⁶P. R. Wallace, *Mathematical Analysis of Physical Problems* (Holt, Rinehart and Winston, New York, 1972), p. 332.
- ⁷L. Pintschovius, O. Blaschko, G. Krexner, M. dePodesta, and R. Currat, Phys. Rev. B **35**, 9330 (1987).
- ⁸H. You, J. D. Axe, D. Hohlwein, and J. B. Hastings, Phys. Rev. B **35**, 9333 (1987).