Helicon-wave propagation in a periodic structure

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Dispersion relations have been obtained on the basis of linear-response theory for helicon waves propagating in a periodic structure with a modulation of charge density along one dimension, but with an essentially free-electron-like behavior in the other two. Numerical applications are made to the so-called "charge-density-wave" state of potassium, in which there is a sinusoidal modulation of charge density, and the results are in basic agreement with those obtained by Overhauser and collaborators in some earlier studies. In addition, a band of high-frequency helicon modes well below the cyclotron frequency occurs as a result of the one-dimensional band structure induced by the periodic modulation.

I. INTRODUCTION

It is well known that under the influence of a strong magnetic field, a conducting medium can support the propagation of electromagnetic waves,[1,2] which are transverse, circularly polarized, and propagate along the axis of the applied magnetic field. Aigrain[3] termed such waves "helicon waves." Helicon waves are generally slow, relatively loss free, and span a convenient frequency range for experimental work. Consequently, they are found to have many applications in solid-state physics, including dynamic Hall-effect[4] and Fermi-surface measurements.[5] There exists a vast literature on helicon waves embodying several review articles and monographs.[6–11] Although helicon waves (corresponding to the propagating solutions pertaining to a homogeneous medium) have been studied in many systems such as metals, semiconductors, superconductors, and ferromagnets, helicon propagation in periodic structures has not received as much attention. It is to be expected that the periodic modulation would give rise to "band-structure" type of effects in the dispersion relations, i.e., there would be "forbidden" regions. The periodic structure envisaged here is characterized by a charge density which is strongly modulated along one dimension but is essentially free-electron-like in the other two. Such a periodic structure is typified by a semiconductor superlattice or by a free-electron system which has undergone a charge-density-wave (CDW) modulation.

Baynham and Boardman[9,12] have studied the propagation of helicon waves in a Kronig-Penney type of periodic structure in the local limit. They find that in the absence of scattering, the dispersion equation breaks up into bands of allowed and forbidden propagation regions. When scattering is taken into account, there occurs a blurring of the band edge and, in addition, there arises a second propagating solution. In the strong scattering limit, the two propagating circularly polarized solutions collapse into a single plane polarized wave. Because of the resulting mathematical simplifications, Baynham and Boardman chose to limit their studies to the Kronig-Penney type of sandwich structure only. A more serious limitation of the Baynham and Boardman approach is the local approximation used in their study. Helicon waves were shown to be possible in a superlattice consisting of a periodic array of two-dimensional layers of free-electron gas by Das Sarma and Quinn.[13] The dispersion relations for helicons propagating in such a system were obtained by Tselis *et al.*[14(a)] on the basis of linear-response theory and Maxwell's equations. Although the approach used by Tselis *et al.* is more general than that of Baynham and Boardman, numerical applications were made[14(b)] in the quasiclassical approximation, and the effect of the periodicity on the dispersion relations was not brought out clearly. The studies mentioned above basically dealt with the Kronig-Penney model either in its finite width version,[9–12] or in the δ-function version.[13,14(a),14(b)]

In a much earlier study on helicon wave propagation, Overhauser and Rodriguez[15] had considered the propagation of helicon waves in the so-called charge-density-wave (CDW) model for potassium.[16] According to Overhauser,[16] the ground state in the CDW model is characterized by a sinusoidal modulation of the charge density, and a lemon-shaped Fermi surface. Overhauser and Rodriguez[15] studied the position of "Kjeldaas edge," i.e., the onset of absorption of energy by the electrons from the helicon waves, when the condition for Doppler-shifted cyclotron resonance first occurs for the CDW model and concluded that the helicon wave dispersion near the Kjeldaas edge was sensitive to the electronic band structure. The dispersion relations for this model were calculated by McGroddy *et al.*[17] and were found to be double valued, and the range of the associated wave vector was limited to a very small region of the Brillouin zone due to the presence of the Kjeldaas edge.

It appears, therefore, that there is need to reexamine the theory for propagation of helicon waves in a periodic structure to bring out clearly when "band-structure" type of effects occur. It is the purpose of this paper to study helicon wave propagation in a periodic structure on the basis of linear-response theory. In Sec. II, the dispersion relation for helicons propagating parallel to the applied magnetic field is obtained by generalizing to periodic structures the standard linear-response theory used for a free electron gas.[18–20] Numerical applications are made to the Overhauser CDW model for potassium by specializing to sinusoidal modulation. Application to semiconductor superlattices will be considered in a future publication.

II. LINEAR-RESPONSE THEORY FOR HELICONS 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 $(0,B_0X,0)$. 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 self-consistent field produced by the disturbance. SI units are used throughout.

In the absence of the magnetic field, the system is described by the Hamiltonian, in the usual notation,

$$\mathscr{H}=p^2/2m+V(z)\ , \tag{2.1}$$

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

The stationary states belonging to the wave vector $\mathbf{k}$ are given by

$$|k_xk_yk_z,l\rangle=e^{i\mathbf{k}\cdot\mathbf{r}}\zeta_l(k_z,z)\ , \tag{2.2}$$

where $\zeta_l(k_z,z)$ satisfies the equation

$$\frac{d^2\zeta_l}{dz^2}+2ik_z\frac{d\zeta_l}{dz}+[\varepsilon_l(k_z)-V(z)]\zeta_l=0\ . \tag{2.3}$$

Here l is the band index and $\varepsilon_l(k_z)$ is the energy of the one-dimensional band. The eigenvalue of the state in Eq. (2.2) is given by

$$E_l(k_xk_yk_z)=(\hbar^2/2m)(k_x^2+k_y^2)+\varepsilon_l(k_z)\ . \tag{2.4}$$

When the uniform magnetic field is applied along the z direction, the system is characterized by the Hamiltonian

$$\mathscr{H}_0=(\mathbf{p}-e\,\mathbf{A}_0)^2/2m+V(z) \tag{2.5}$$

with the eigenstates

$$|k_yk_znl\rangle=e^{i(k_yy+k_zz)}U_n(x+l_H^2k_y)\zeta_l(k_z,z)\ . \tag{2.6}$$

Here $U_n(x)$ are the harmonic-oscillator wave functions, $l_H=(\hbar/mw_C)^{1/2}$ is the magnetic length, and $\omega_C=eB_0/m$ is the cyclotron frequency. Spin-dependent effects have been neglected. Using a collective index ν to denote the eigenstate as $|\nu\rangle$, the eigenvalue is given by

$$E(\nu)=E(k_ynk_zl)=(n+\tfrac{1}{2})\hbar\omega_C+\varepsilon_l(k_z)\ . \tag{2.7}$$

The eigenfunctions $\zeta_l(k_z,z)$ satisfying Eq. (2.3) can be expanded in terms of plane-wave basis functions according to[21]

$$\zeta_l(k_z,z)=\sum_K b_l(k_z+K)e^{iKz}\ , \tag{2.8}$$

where K's are the one-dimensional reciprocal-lattice vectors and $b_l(k_z+K)$ are the expansion coefficients satisfying the usual orthogonality and closure conditions[21]

$$\sum_K b_n^*(k_z+K)b_l(k_z+K)=\delta_{nl}\ , \tag{2.9}$$

$$\sum_l b_l^*(k_z+K)b_l(k_z+K')=\delta_{KK'}\ . \tag{2.10}$$

The eigenstates in Eq. (2.6) can then be written as

$$|\nu\rangle=e^{ik_yy}U_n(x+l_H^2k_y)\sum_K b_l(k_z+K)e^{i(k_z+K)z}\ . \tag{2.11}$$

With the perturbing electromagnetic field, the Hamiltonian is

$$\mathscr{H}=(\mathbf{p}-e\,\mathbf{A}_0-e\,\mathbf{A}_1)^2/2m+V(z)\ . \tag{2.12}$$

To first order in $\mathbf{A}_1$, this can be written as

$$\mathscr{H}=\mathscr{H}_0+\mathscr{H}_1\ . \tag{2.13}$$

With $\mathscr{H}_0$ given by Eq. (2.5) and

$$\mathscr{H}_1=-e[\mathbf{v}\cdot\mathbf{A}_1+\mathbf{A}_1\cdot\mathbf{v}]/2\ , \tag{2.14}$$

where $\mathbf{v}$ is the velocity operator

$$\mathbf{v}=(\mathbf{p}-e\,\mathbf{A}_0)/m\ . \tag{2.15}$$

Using linear-response theory, an expression for the conductivity tensor can be obtained as[20]

$$\tilde{\sigma}(\mathbf{q},\omega)=i\omega_p^2\epsilon_0[\tilde{1}+\tilde{I}(\mathbf{q},\omega)]/\omega\ . \tag{2.16}$$

Here w_p is the plasma frequency, $\tilde{1}$ is the unit tensor, and the tensor $\tilde{I}(\mathbf{q},\omega)$ is given by

$$\tilde{I}(\mathbf{q},\omega)=\frac{2m}{N}\sum_{\nu,\nu'}\Lambda_{\nu\nu'}\langle\nu'|\mathbf{v}(\mathbf{q})|\nu\rangle\langle\nu|\mathbf{v}(\mathbf{q})|\nu'\rangle\ , \tag{2.17}$$

where

$$\Lambda_{\nu\nu'}=\{f_0(E(\nu'))-f_0[E(\nu)]\}/\{E(\nu')-E(\nu)-\hbar(\omega-\omega_C)\}\ . \tag{2.18}$$

The f_0's are the Fermi factors and the operators $\mathbf{v}(\mathbf{q})$ are given by

$$\mathbf{v}(\mathbf{q})=(e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{v}+\mathbf{v}e^{i\mathbf{q}\cdot\mathbf{r}})/2\ . \tag{2.19}$$

In writing down the expression for the conductivity tensor in Eq. (2.16), relaxation effects have not been considered, but they can be included in a straightforward manner.[20] The expression in Eq. (2.16) will be used in the next section to obtain the dispersion relations for helicon waves.

A. The dispersion relations

We assume that the medium is nonmagnetic. The electric and the magnetic fields associated with the wave are related through Maxwell's equations

$$\mathrm{curl}\mathbf{e}=-\frac{\partial\mathbf{B}}{\partial t}\ , \tag{2.20}$$

$$\mathrm{curl}\mathbf{B}=\mu_0\left[\mathbf{J}+\epsilon_1\epsilon_0\frac{\partial\mathbf{e}}{\partial t}\right]\ , \tag{2.21}$$

where $\mathbf{J}$ is the current density and ϵ_1 is the dielectric constant of the lattice. The fields are assumed to vary as $\exp(i\mathbf{q}\cdot\mathbf{r}-i\omega t)$. Expressing the current density $\mathbf{J}$ in terms of $\tilde{\sigma}$ Eq. (2.20) and (2.21) become

$$\mathbf{q}\times\mathbf{e}=\omega\mathbf{B}\ , \tag{2.22}$$

$$\mathbf{q}\times\mathbf{B}=-\omega/C^2(i\tilde{\sigma}/\omega\epsilon_0+\epsilon_1\tilde{1})\mathbf{e}\ . \tag{2.23}$$

One can introduce an effective dielectric tensor

$$\tilde{\epsilon}(\mathbf{q},\omega)=\epsilon_1\tilde{1}+\frac{i\tilde{\sigma}}{\omega\epsilon_0} \tag{2.24}$$

and eliminate the **B** field in Eqs. (2.22) and (2.23) and obtain a set of homogeneous equations for the components of **e**. The determinant of the coefficients in these equations is the required secular equation giving the frequency of oscillation ω for the helicon waves of wave vector **q**. For waves propagating along the magnetic field, the dispersion relation is most conveniently expressed in the polarization representation in which the field components are given by

$$e_\pm=e_x\pm ie_y \tag{2.25}$$

and e_z. In this representation the dielectric tensor is diagonal with the components

$$\epsilon_\pm(q,\omega)=\epsilon_{xx}(q,\omega)\pm i\epsilon_{xy}(q,\omega) \tag{2.26}$$

and $\epsilon_{zz}(q,\omega)$. The equations for the field components $e_\pm$ are

$$(C^2q^2-\omega^2\epsilon_\pm)e_\pm=0\ . \tag{2.27}$$

Therefore the frequencies of the helicon waves are determined from

$$\epsilon_\pm(q,\omega)\omega_\pm^2=C^2q^2\ . \tag{2.28}$$

The relevant matrix elements appearing in Eq. (2.17) needed for the calculation of $\epsilon_\pm(q,\omega)$ are given by

$$\langle\nu'\,|\,v_x(q)\,|\,\nu\rangle=i(\hbar\omega_C/2m)\{(n+1)^{1/2}\delta_{n',n+1}-n^{1/2}\delta_{n',n-1}\}\sum_K\delta_{k_y'k_y}\delta_{k_z',k_z+q+K}b_{l'}^*(k_z+q+K)b_l(k_z+K)\ , \tag{2.29}$$

$$\langle\nu'\,|\,v_y(q)\,|\,\nu\rangle=(\hbar\omega_C/2m)^{1/2}\{(n+1)^{1/2}\delta_{n',n+1}+n^{1/2}\delta_{n',n-1}\}\sum_K\delta_{k_y'k_y}\delta_{k_z',(k_z+q+K)}b_{l'}^*(k_z+q+K)b_l(k_z+k)\ , \tag{2.30}$$

and the components of the conductivity tensor required in Eq. (2.28) for the dielectric tensor components $\epsilon_\pm$ are given by

$$\sigma_\pm=\frac{i\omega_p^2\epsilon_0}{\omega}\left\{1+\hbar\omega_C/N\sum_{\substack{n,k_y k_z\\ ll'}}\Lambda(nk_yk_zll')\sum_{KK'}b_{l'}^*(k_z+q+K)b_l(k_z+K)b_l^*(k_z+K')b_{l'}(k_z+q+K')\right\}\ , \tag{2.31}$$

where

$$\Lambda(nk_yk_zll')=(n+1)\frac{\{f_0[E(n+1,k_z+q,k_y,l')]-f_0[E(n,k_z,k_y,l)]\}}{E(n+1,k_z+q,k_y,l')-E(n,k_z,k_y,l)-\hbar(\omega-\omega_C)}\ . \tag{2.32}$$

We will concentrate on the mode corresponding to the plus sign in the numerical applications in the next section.

III. NUMERICAL APPLICATION

The dispersion relation given by Eq. (2.28) has been evaluated numerically for the Overhauser CDW model of potassium at absolute zero. The values of the parameters taken from Ref. 15 are the following: $\varepsilon_F=2.14$ eV, the energy gap at the zone boundary $Q/2=0.62$ eV and the CDW wave vector $Q=1.33\times2\pi/a$ where a is the lattice constant for potassium. The static magnetic field B_0 was assumed to be 2 T and corresponded to a cyclotron frequency $\omega_C=3.516\times10^{11}\ \mathrm{s}^{-1}$.

The band structure was calculated by using a basis set of five plane waves. This was found to be adequate since the potential causing the sinusoidal modulation in the CDW model involves only a single Fourier coefficient. The dielectric tensor $\epsilon_+(q,\omega)$ was evaluated by summing over points in the Brillouin zone. No significant differences were found when the number of waves in the basis set was increased to fifteen.

The dispersion relation was determined in the following way: First, a value of the wave vector q was chosen, and the dielectric tensor $\epsilon_+(q,\omega)$ was calculated as a function of the frequency ω. The particular value of ω, for which the product $\omega^2\epsilon_+(q,\omega)$ is equal to 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. The dispersion so calculated is shown in Fig. 1.

It can be seen that the range of q, for which helicon wave propagation is possible, is restricted to a very small part of the Brillouin zone. In fact, we had to use the long-wavelength expansion of the dielectric tensor component $\epsilon_+(q,\omega)$, retaining terms up to q^2, in obtaining the dispersion for $q/Q\le1.0\times10^{-5}$. The dispersion curve exhibits a maximum and then a sharp drop and agrees quite well with that given in Ref. 17, although the frequencies given in the present work are somewhat higher.

We find additional high-frequency modes ranging from $\omega=3.1\times10^{11}\ \mathrm{s}^{-1}$ at $q/Q\cong1.0\times10^{-5}$ to $\omega=2.4\times10^{11}\ \mathrm{s}^{-1}$ at $q/Q\cong1.0\times10^{-3}\ \mathrm{s}^{-1}$. These modes are discrete, and form, at each value of the wave vector q in this range, a band of 1–5 closely spaced modes lying well below the cyclotron frequency, ω_C. While the exact nature of these modes is still not clear, a clue as to their origin can be given. These modes satisfy Eq. (2.28), of course, and arise when the components of the dielectric

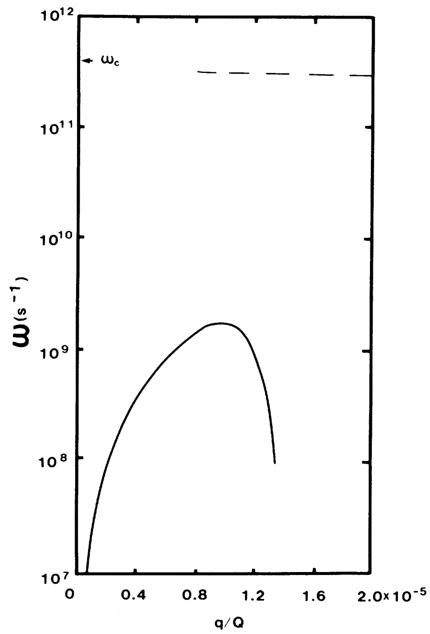

FIG. 1. Helicon wave dispersion in the CDW state of potassium.

tensor increases sharply. This means that the physical origin of these modes, as indicated by Eq. (2.32), lies in the resonant nature of the dielectric tensor and the one-dimensional band structure induced by the CDW which is responsible for it. It would appear, therefore, that an experimental confirmation of these modes would provide additional evidence for the CDW state. More theoretical work regarding the damping of these modes is required before the nature of these modes becomes clear.

IV. CONCLUSIONS

In this paper, helicon wave propagation in a periodic structure has been studied on the basis of linear-response theory and numerical applications have been made to the Overhauser model of potassium. The dispersion curve obtained is in basic agreement with the earlier results. Helicon wave propagation is severely restricted to a small part of the Brillouin zone—mainly, it appears, due to nonlocal effects. Additional high-frequency modes appear as a result of the resonance nature of the dielectric tensor.

"Band-structure" type of effects are not apparent in the system, unless one interprets the high-frequency helicon modes as part of the "band structure." One would have to consider other periodic structures to look for band-structure type of effects. Semiconductor superlattices may be the most likely candidates. It is planned to study these systems in the future.

Additional theoretical work regarding the damping of the high-frequency modes is also required.

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