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Wave-vector-nonconserving optical transitions in a model dilute alloy

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We explore the theory of the imaginary part $\epsilon_2(\omega)$ of the dielectric constant for a simple model alloy, with emphasis on the possibility of studying critical points in the host band structure through wave-vector-nonconserving transitions induced by impurities. We find Van Hove singularities in the host band structure produce discontinuities in slope of $\partial\epsilon_2(\omega)/\partial\omega$ at photon energies equal to the absolute magnitude of the difference between the Fermi energy and those of the critical points. The paper presents a study of $\epsilon_2(\omega)$ and its frequency derivative for a single impurity placed in a host with nondegenerate conduction band of tight-binding form.

I. INTRODUCTION

For many years the study of optical absorption in solids has been a primary method of probing their electronic band structure. If one considers optical absorption in a perfectly pure crystal with rigid lattice, a photon can be absorbed by inducing a transition between an occupied electron state of wave vector $\vec{k}$ in band n and an empty state of wave vector $\vec{k}$ in a different band n'. The structure in $\epsilon_2(\omega)$, the imaginary part of the dielectric constant, produced by such transitions occurs at the Van Hove critical points of the joint density of states formed from the appropriate convolution of the density of states of the occupied levels with that of the empty levels. The locations of the Van Hove singularities in the joint density of states are controlled by the *relative* position of singular features in the host band structure. If E_1 and E_2 are the energies of two such features, the structure in $\epsilon_2(\omega)$ occurs when $\hbar\omega = E_1 - E_2$ for $E_1 > E_2$.

If a small concentration of impurities is introduced into the rigid lattice, the presence of the impurities produces transitions which do not conserve wave vector. The purpose of the present paper is to study theoretically the structure in $\epsilon_2(\omega)$ produced by such wave-vector-nonconserving transitions in a model sufficiently simple to allow explicit and detailed calculation, yet with Van Hove critical points in the host band structure representative of real metals in three dimensions.

Although it is well known that such wave-vector-nonconserving optical transitions occur in solids, theorists have devoted rather little attention to this area. Earlier studies[1] of optical absorption in dilute alloys focus primary attention on the use of this method to study virtual levels induced by the impurities. In these theories, the host electronic density of states is taken to be structureless. Velicky and Levin[2] have presented a theoretical study close in spirit to the present. Indeed, for reasons discussed below, we have re-examined the same basic model that forms the basis of their work. Finally, the present authors have studied the behavior of $\epsilon_2(\omega)$ in a model insulator in one dimension,[3] with a single impurity present. The impurity-induced indirect transitions (wave-vector-nonconserving transitions) produced step discontinuities in $\epsilon_2(\omega)$ at photon energies where structure is absent for the pure matrix. While this calculation shows dramatic structure in $\epsilon_2(\omega)$ can be produced by an impurity, it is of more general interest to explore $\epsilon_2(\omega)$ in a three-dimensional model, where the Van Hove singularities in the electronic density of states are less violent than those found in one dimension.

In the present study, we explore the behavior of the impurity induced contribution to $\epsilon_2(\omega)$ for a simple-cubic model solid with a nondegenerate partially filled conduction band. An impurity is introduced that perturbs the electrons by means of a localized potential.

As remarked above, Velicky and Levin studied impurity-induced absorption for the same model. They calculate $\epsilon_2(\omega)$ to find gentle structure at some (but not all) transitions between the Fermi level and energies characteristic of Van Hove singularities in the one-electron density of states of the host. Our study was motivated by the desire to understand more fully the nature of the singularity in $\epsilon_2(\omega)$ present at such energies. Velicky and Levin use the coherent-potential-approximation (CPA) to study by numerical methods optical absorption in a rather concentrated alloy (impurity concentration 10 at.%), where lifetime effects present in the CPA may blur out the singularities in $\epsilon_2(\omega)$. Thus, we wish to study optical absorption induced by a single isolated impurity to analyze the nature of the singularities in $\epsilon_2(\omega)$.

We find $\epsilon_2(\omega)$ to have continuous slop with continuous derivative $\partial\epsilon_2(\omega)/\partial\omega$ at these energies, while $\partial\epsilon_2(\omega)/\partial\omega$ has a discontinuity in slope there. The critical-point structure in $\epsilon_2(\omega)$ is thus quite hard to perceive even in our study of the one-impurity problem. As in the paper of Velicky and Levin, we find some but not all critical points can be seen as subtle features in $\epsilon_2(\omega)$. There seems to be no obvious reason why some critical points fail to show up, save for the fact that the features are sufficiently delicate that their presence may not be noted, in calculations at our level of precision. However, when we examine $\partial\epsilon_2/\partial\omega$ at the same level of computational precision, we find *all* of the critical points show up cleanly.

The remarks in the preceding paragraph suggest that the study of optical absorption in dilute alloys may be a powerful method of studying the *absolute* (not relative) position of critical points in the host band structure. Following Velicky and Levin, we find the photon energies at which the structure occurs equal the *magnitude* of the difference between the energy of the critical point and the Fermi energy. This means one can study either critical points above or those below the Fermi energy, to locate their absolute position with the Fermi energy as a fiducial mark. In essence, the impurity can serve as a point probe that can be used to elucidate features in the host band structure, provided the alloy is sufficiently dilute that the process of alloying does not perturb the host band structure. Our result that structures show clearly in $\partial\epsilon_2/\partial\omega$, but are difficult to see in ϵ_2 itself, suggests use of derivative spectroscopy to study $\partial\epsilon_2/\partial\omega$ (or better yet $\partial^2\epsilon_2/\partial\omega^2$, where step discontinuities will occur quite similar to those we found in ϵ_2 in our earlier study of the one dimensional example).

In a pure material, thermal vibrations (phonons) produce disorder, to produce wave-vector-non-conserving transitions qualitatively similar to the impurity-induced transitions studied here. These phonon-assisted indirect transitions should also produce (temperature-dependent) features in $\partial\epsilon_2(\omega)/\partial\omega$. We understand this phenomenon is under investigation by Allen and his co-workers.[4]

The present paper is a full account of material discussed by us in a brief and preliminary fashion at a recent conference.[5]

II. GENERAL REMARKS

In our preceding paper,[3] the general expression for $\epsilon_2(\omega)$ provided by the one electron theory of solids was expressed in terms of the Green's functions that describe electron propagation in the disordered material. These results are easily reduced to expressions suitable for the present study by suppressing band indices (we consider here a metal with a single nondegenerate conduction band) and making some minor rearrangements. The fundamental quantity that enters is a spectral density function $\rho(\vec{k},\vec{k}';\epsilon)$ defined by the statement

$$\rho(\vec{k},\vec{k}';\epsilon)=(1/i\pi)\,[G(\vec{k},\vec{k}';\epsilon+i\eta)\\ -G(\vec{k},\vec{k}';\epsilon-i\eta)]\,, \tag{1}$$

where

$$G(\vec{k},\vec{k}';z)=\langle\vec{k}|(H-z)^{-1}|\vec{k}'\rangle\,, \tag{2}$$

with H the Hamiltonian that describes the disordered material, and $|\vec{k}\rangle$, $|\vec{k}'\rangle$ are Bloch states of the pure host matrix. If Ω is the volume of the crystal and m is the free-electron mass, then for an optically isotropic material

$$\epsilon_2(\omega)=\frac{4\pi^2e^2}{\Omega m^2\omega^2}(1-e^{-\beta\omega})\\ \times\sum_{\vec{k}\vec{k}'}\int_{-\infty}^{+\infty}d\epsilon\, f(\epsilon)[1-f(\epsilon+\omega)]\\ \times \mathrm{Re}\,[\langle\vec{k}'|p_x|\vec{k}'\rangle\langle\vec{k}|p_x|\vec{k}\rangle\rho(\vec{k},\vec{k}';\epsilon)\\ \times\rho(\vec{k}',\vec{k};\epsilon+\omega)]\,. \tag{3}$$

Here $f(\epsilon)=\{\exp[\beta(\epsilon-\mu)]+1\}^{-1}$ is the Fermi-Dirac function, and p_x is the x component of the electron momentum. The momentum matrix elements in Eq. (3) may be related to the group velocity $v_x(\vec{k})=\hbar^{-1}\partial E(\vec{k})/\partial k_x$ by the result[6]

$$\langle\vec{k}|p_x|\vec{k}\rangle=m\,v_x(\vec{k})\,, \tag{4}$$

so we have, using units where $\hbar=1$,

$$\epsilon_2(\omega)=\frac{4\pi^2e^2}{\Omega\omega^2}(1-e^{-\beta\omega})\\ \times\int_{-\infty}^{+\infty}d\epsilon\, f(\epsilon)[1-f(\epsilon+\omega)]\varphi(\epsilon,\omega)\,, \tag{5}$$

where

$$\varphi(\epsilon,\omega)=\sum_{\vec{k}\vec{k}'}v_x(\vec{k})\,v_x(\vec{k}')\,\rho(\vec{k},\vec{k}';\epsilon)\\ \times\rho(\vec{k}',\vec{k};\epsilon+\omega)\,. \tag{6}$$

We consider a single impurity placed at the origin in a monatomic simple-cubic lattice. The conduction band of the host is described by the Hamiltonian

$$H_0=\sum_k E(\vec{k})\,c_{\vec{k}}^{\dagger}\,c_{\vec{k}}\,, \tag{7}$$

where

$$E(\vec{k})=-\tfrac{1}{3}\,W\,[\cos k_x a_0+\cos k_y a_0+\cos k_z a_0) \tag{8}$$

describes the conduction band of tight-binding form with first neighbors overlaps. The bottom of the conduction band is at $-W$, and the top is at $+W$, with $2W$ its width. The impurity produces a localized perturbation that we write

$$V=\frac{v}{N}\sum_{\vec{k}\vec{k}'} c^{\dagger}_{\vec{k}} c_{\vec{k}'} \,. \tag{9}$$

The Green's function $G(\vec{k},\vec{k}';z)$ has the well-known Slater-Koster form that formed the basis of our earlier analysis of the two-band insulator

$$G(\vec{k},\vec{k}';z)=G_0(\vec{k},z)\,\delta_{\vec{k}\vec{k}'}+\Delta G(\vec{k},\vec{k}';z)\,, \tag{10}$$

where $G_0(\vec{k},z)=[E(\vec{k})-z]^{-1}$ and

$$\Delta G(\vec{k},\vec{k}';z)=-\frac{v}{N}\,\frac{G_0(\vec{k},z)\,G_0(\vec{k}',z)}{1+v\,F(z)} \tag{11a}$$

and

$$F(z)=\frac{1}{N}\sum_{\vec{k}} G_0(\vec{k},z)\,. \tag{11b}$$

Here N is the number of unit cells in the crystal.

Following Eq. (10), the spectral density will be split into two parts

$$\rho(\vec{k},\vec{k}';\epsilon)=\delta_{\vec{k}\vec{k}'}\,\delta(E(\vec{k})-\epsilon)+\frac{1}{N}\,\Delta\rho(\vec{k},\vec{k}';\epsilon)\,. \tag{12}$$

The imaginary part of the dielectric constant then becomes

$$\epsilon_2(\omega)=\epsilon_{2a}(\omega)+\epsilon_{2b}(\omega)+\epsilon_{2c}(\omega)\,, \tag{13a}$$

with

$$\epsilon_{2a}(\omega)=\frac{4\pi^2e^2}{\Omega_0\omega^2}(1-e^{-\beta\omega})\frac{1}{N}\sum_{\vec{k}} v_x^2(\vec{k})f(E(\vec{k}))\,[1-f(E(\vec{k})+\omega)]\,\Delta\rho(\vec{k},\vec{k};E(\vec{k})+\omega)\,, \tag{13b}$$

$$\epsilon_{2b}(\omega)=\frac{4\pi^2e^2}{\Omega_0\omega^2}(1-e^{-\beta\omega})\frac{1}{N}\sum_{\vec{k}} v_x^2(\vec{k})f(E(\vec{k})-\omega)\,[1-f(E(\vec{k}))]\,\Delta\rho(\vec{k},\vec{k};E(\vec{k})-\omega)\,, \tag{13c}$$

and

$$\epsilon_{2c}(\omega)=\frac{4\pi^2e^2}{\Omega_0\omega^2}(1-e^{-\beta\omega})\int_{-\infty}^{+\infty} d\epsilon\, f(\epsilon)\,[1-f(\epsilon+\omega)]\,\frac{1}{N^2}\sum_{\vec{k}\vec{k}'} v_x(\vec{k})\,v_x(\vec{k}')\,\Delta\rho(\vec{k}',\vec{k};\epsilon+\omega)\,\Delta\rho(\vec{k},\vec{k}';\epsilon)\,. \tag{13d}$$

In our model, the impurity potential produces s wave scattering only, and as a consequence $\Delta\rho(\vec{k},\vec{k}';\epsilon)$ depends on $\vec{k}$ and $\vec{k}'$ in a separable manner and is independent of their relative directions. It follows that $\epsilon_{2c}(\omega)$ vanishes identically. This is a special feature of the model used here and, in general, all three terms will be nonvanishing. We note that the decoupling procedure used by Velicky and Levin fails to produce a contribution to $\epsilon_2(\omega)$ analogous to that in Eq. (13d). Thus, in general, their decoupling scheme fails to produce the proper expression for $\epsilon_2(\omega)$ in the one impurity limit. However, because s wave scattering only is present in the model explored by them (and by us), in this special case they recover the proper one impurity limit. As we remarked earlier,[3] in language appropriate to a treatment based on the Boltzmann equation, their decoupling scheme is equivalent to ignoring the "scattering in" terms which in general are the same order of magnitude as the "scattering out" terms.

After some straightforward algebra, $\epsilon_{2a}(\omega)$ and $\epsilon_{2b}(\omega)$ may be cast into the form (for $T=0$),

$$\epsilon_{2a}(\omega)=\frac{4\pi^2e^2}{\Omega\omega^4}\,v^2 \times\int_{\epsilon_F-\omega}^{\epsilon_F}\frac{v_x^2(\epsilon)\,\rho(\epsilon)\rho(\epsilon+\omega)\,d\epsilon}{[1+vF_R(\epsilon+\omega)]^2+\pi^2v^2\rho^2(\epsilon+\omega)} \tag{14a}$$

and

$$\epsilon_{2b}(\omega)=\frac{4\pi^2e^2}{\Omega\omega^4}\,v^2 \times\int_{\epsilon_F}^{\epsilon_F+\omega}\frac{v_x^2(\epsilon)\rho(\epsilon)\rho(\epsilon-\omega)\,d\epsilon}{[1+vF_R(\epsilon-\omega)]^2+\pi^2v^2\rho^2(\epsilon-\omega)}\,. \tag{14b}$$

In these expressions, ϵ_F is the Fermi energy, $\rho(\epsilon)$ the host density of states, $F_R(\epsilon)$ the real part of $F(\epsilon+i\eta)$ [Eq. (11.b)], and we introduce

$$v_x^2(\epsilon)=\frac{1}{N\rho(\epsilon)}\sum_{\vec{k}} v_x^2(\vec{k})\delta(\epsilon-\epsilon(\vec{k}))\,. \tag{15}$$

It is convenient to define a frequency-dependent relaxation time $\tau(\omega)$ for the electrons by comparing the forms in Eqs. (14) to the result of the Drude model of conductivity in the limit $\omega\tau(\omega)$

$\gg 1$. If n is the electron density, we have

$$\epsilon_2(\omega) = (4\pi n e^2/m\omega^3)[1/\tau(\omega)]\,, \tag{16}$$

so comparison with Eqs. (14) yields

$$1/\tau(\omega) = 1/\tau_a(\omega) + 1/\tau_b(\omega)\,, \tag{17}$$

where

$$\frac{1}{\tau_a(\omega)} = \frac{\pi m}{\Omega n}\frac{v^2}{\omega} \times \int_{\epsilon_F-\omega}^{\epsilon_F} \frac{v_x^2(\epsilon)\rho(\epsilon)\rho(\epsilon+\omega)d\epsilon}{[1+vF_R(\epsilon+\omega)]^2+\pi^2 v^2\rho^2(\epsilon+\omega)}\,, \tag{18a}$$

and

$$\frac{1}{\tau_b(\omega)} = \frac{\pi m}{\Omega n}\frac{v^2}{\omega} \times \int_{\epsilon_F}^{\epsilon_F+\omega} \frac{v_x^2(\epsilon)\rho(\epsilon)\rho(\epsilon-\omega)d\epsilon}{[1+vF_R(\epsilon-\omega)]^2+\pi^2 v^2\rho(\epsilon-\omega)}\,. \tag{18b}$$

The relaxation rate defined above may be expressed conveniently in terms of the energy dependent phase shift $\delta(\epsilon) = \tan^{-1}\{\pi v\rho(\epsilon)/[1+vF_R(\epsilon)]\}$ for scattering from the impurity. One has

$$\frac{1}{\tau_a(\omega)} = \frac{m}{\pi\Omega n\omega}\int_{\epsilon_F-\omega}^{\epsilon_F}\frac{v_x^2(\epsilon)\rho(\epsilon)}{\rho(\epsilon+\omega)} \times \sin^2[\delta(\epsilon+\omega)]d\epsilon\,, \tag{19a}$$

$$\frac{1}{\tau_b(\omega)} = \frac{m}{\pi\Omega n\omega}\int_{\epsilon_F}^{\epsilon_F+\omega}\frac{v_x^2(\epsilon)\rho(\epsilon)}{\rho(\epsilon-\omega)} \times \sin^2[\delta(\epsilon-\omega)]d\epsilon\,. \tag{19b}$$

From the form of Eq. (19a), it is evident that $1/\tau_a(\omega)$ has its origin in processes where the photon lifts an electron of energy ϵ to the final state $\epsilon+\omega$, where it scatters from the impurity. Equation (19b) describes an event where the hole scatters off the impurity to break down wave-vector conservation. As $\omega \to 0$, the relaxation time $\tau(\omega)$ defined above reduces to

$$\frac{1}{\tau(0)} = \frac{2}{3\pi\Omega}\frac{mv_F^2(\epsilon_F)}{n}\sin^2\delta(\epsilon_F)\,. \tag{20}$$

For a parabolic band, with $mv_F(\epsilon_F) = k_F$ and $n = k_F^3/6\pi^2$, [the explicit factor of 2 for spin has been omitted from Eqs. (19)], we have the standard result[7]

$$1/\tau(0) = (4\pi/\Omega m k_F)\sin^2[\delta(\epsilon_F)]\,. \tag{21}$$

In Sec. III, we explore the behavior of $\tau(\omega)$ quantitatively.

III. RESULTS AND DISCUSSION

From the general structure of the expressions in Eqs. (18a) and (18b), it is quite clear that $\tau(\omega)^{-1}$ will be influenced only modestly by the Van Hove singularities in the density of states $\rho(\epsilon)$. In our model, as in any three-dimensional model, the Van Hove singularities are discontinuities in slope of $\rho(\epsilon)$, at certain special energies. The products $\rho(\epsilon)\rho(\epsilon\pm\omega)$ are the controlling factors in Eqs. (18a) and (18b), but since they appear under the integral sign, the influence of the Van Hove singularities can at most be very subtle and hard to perceive.

A much more satisfactory procedure is to study not $\tau(\omega)^{-1}$, but rather its frequency derivative. From the experimental point of view, this suggests use of derivative spectroscopy in the study of the optical spectrum of alloys. Upon differentiating Eq. (18a) with respect to frequency, we find

$$\frac{\partial}{\partial\omega}\left(\frac{1}{\tau_a(\omega)}\right) = \frac{\pi m}{\Omega n}\frac{v^2}{\omega}\frac{v_x^2(\epsilon_F)\rho(\epsilon_F)\rho(\epsilon_F+\omega)}{[1+vF_R(\epsilon_F+\omega)]^2+\pi^2v^2\rho^2(\epsilon_F+\omega)} - \frac{1}{\omega}\frac{1}{\tau_a(\omega)} - \frac{\pi m}{\Omega n}\frac{v^2}{\omega}\int_{\epsilon_F-\omega}^{\epsilon_F}\frac{d\epsilon\,\rho(\epsilon+\omega)}{[1+vF_R(\epsilon+\omega)]^2+\pi^2v^2\rho^2(\epsilon+\omega)}\frac{\partial}{\partial\epsilon}[v_x^2(\epsilon)\rho(\epsilon)]\,. \tag{22}$$

A similar expression obtains for the frequency derivative of $\tau_b(\omega)^{-1}$.

The first term in Eq. (22) allows the Van Hove singularities in the density of states to be probed directly through the factor $\rho(\epsilon_F+\omega)$. Structure in the frequency derivative $\partial\epsilon_2(\omega)/\partial\omega$ (discontinuities in slope) whenever ω matches the difference between the Fermi energy and the energy of a critical point located *above* the Fermi level. The frequency derivative $\partial\tau_b(\omega)^{-1}/\partial\omega$ contains a similar term with $\rho(\epsilon_F-\omega)$ rather than $\rho(\epsilon_F+\omega)$, so one also obtains structure when ω matches the difference in energy between the Fermi energy and that of a critical point located *below* the Fermi level.

In Eq. (22), the structure in $\partial[\tau_a(\omega)]^{-1}/\partial\omega$ at a Van Hove critical point is controlled by the first term, with the remaining two terms only modestly

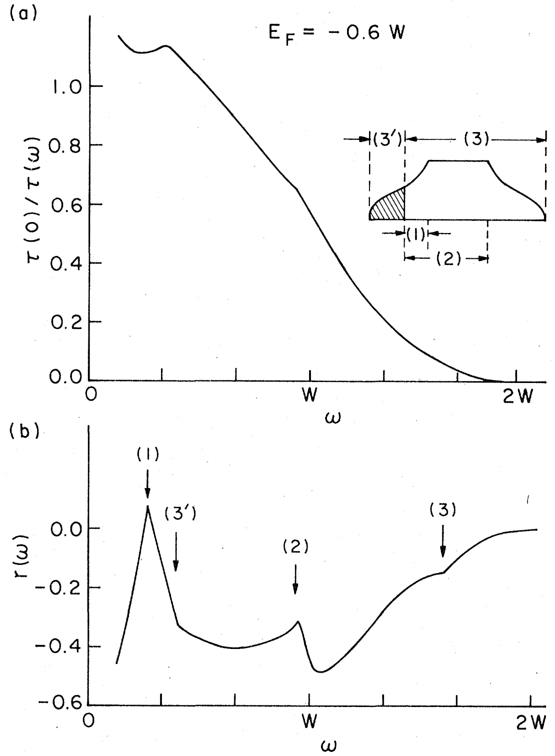

FIG. 1. Ratios (a) $\tau(0)/\tau(\omega)$ and (b) $r(\omega)$ for the potential $v = 0.02W$, and for the Fermi energy illustrated in the inset. The relevant transition energies are indicated by arrows in (b).

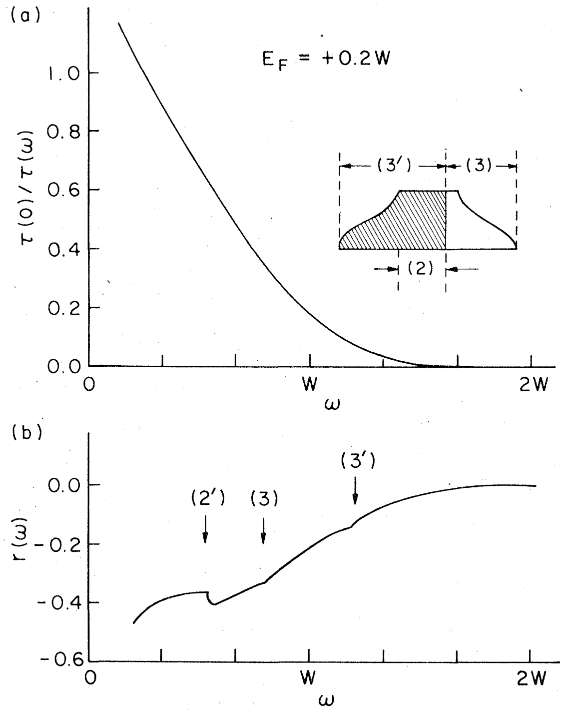

FIG. 2. Ratios (a) $\tau(0)/\tau(\omega)$ and (b) $r(\omega)$ for the potential $v = 0.02W$ and for the Fermi energy illustrated in the inset. The relevant transition energies are indicated by arrows in (b).

affected. We have already argued that $\tau_a(\omega)^{-1}$ itself shows no discontinuity in slope, and for our model we may show that the combination $v_x^2(\epsilon)\rho(\epsilon)$ is smoothly varying with continuous slope throughout the band, with no Van Hove singularities. Thus, like $[\tau_a(\omega)]^{-1}$ itself, the third term in Eq. (22) is smooth near the critical points.

We now turn to our numerical calculations, which serve to illustrate these points. For the energy band function in Eq. (8), the band width is $2W$ with the zero of energy at the midpoint of the band. The density of states is symmetrical about the midpoint of the band, with critical points located at the energies $\pm\frac{1}{3}W$. Of course, the band edges are also critical points, since the slope of $\rho(\epsilon)$ jumps from $+\infty$ (at the bottom) to zero, or $-\infty$ (at the top) to zero. We shall calculate the dimensionless ratio $\tau(0)/\tau(\omega)$ and also $r(\omega) = W\tau(0)\partial[\tau(\omega)]^{-1}/\partial\omega$. These two quantities may be calculated once the value of the two dimensionless parameters E_F/W and v/W are given.

In Figs. 1 and 2, we show the behavior of $\tau(0)/\tau(\omega)$ and of $r(\omega)$ for the weak scattering limit with $v = 0.02\,W$. We have chosen two positions of the Fermi level, as indicated on the insets. The strength for the potential is that used in the earlier work of Velicky and Levin. The calculated curves of $\tau(0)/\tau(\omega)$ are very similar to theirs, as they should be. We remark that we have used the Green's functions computed by Oitmaa[8] in all the numerical work reported here.

Close inspection of the behavior of $\tau(\omega)^{-1}$ shows gentle structure appears at some of the transition energies between the Fermi level and the critical points. Not all of the transitions can be perceived by the eye in $\tau(\omega)^{-1}$, and the ones that appear are gentle. This is the case also in the earlier work of Velicky and Levin.

The frequency derivative $r(\omega)$ does display clear discontinuities in slope at each critical point, as indicated in the Fig. 1 and 2. The structure should be even more prominent in the second derivative $\partial r(\omega)/\partial\omega$ of the relaxation rate, although we have not calculated the second derivative.

In our earlier study of the one dimensional model insulator, we noted that while the *position* of the impurity-induced structure is controlled (in the dilute limit) by the position of the critical points in the host band structure, the *shape* of the features is controlled by the details and strength of the impurity potential. We find similar results in the present study. We illustrate this in Figs.

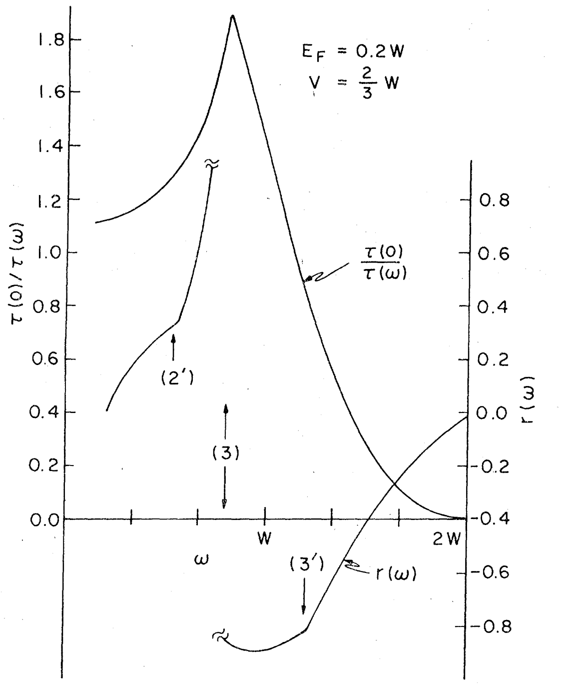

FIG. 3. Ratios $\tau(0)/\tau(\omega)$ and $r(\omega)$, for $v = \frac{2}{3} W3$ and $E_f = + 0.2W$. The values of $\tau(0)/\tau(\omega)$ and $r(\omega)$ are to be read from the right-hand scale.

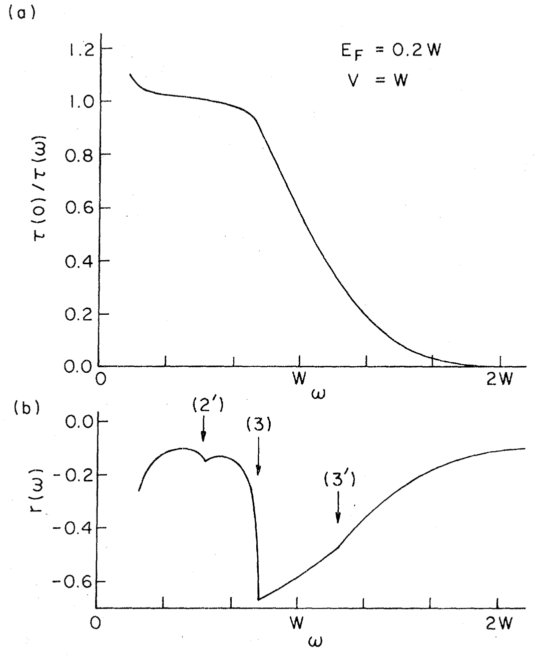

FIG. 4. Ratios (a) $\tau(0)/\tau(\omega)$ and (b) $r(\omega)$ for the potential $v = W$, and $E_f = + 0.2W$.

3 and 4, where both $\tau(0)/\tau(\omega)$ and $r(\omega)$ are displayed for the Fermi energy fixed as in Fig. 2, but for various values of the scattering potential v. Figure 3 is particularly dramatic, with a scattering resonance located near one of the critical energies.

It is evident from Figs. 1- 3 that no simple general statement can be made about the shape of the impurity induced structure in $\partial\epsilon_2(\omega)/\partial\omega$. Indeed, if calculations such as those presented here can be carried out for models of real metals, the shape of the critical-point structures in $\partial\epsilon_2(\omega)/\partial\omega$ may provide detailed information about the potential near the impurity. We are presently exploring the possibility of calculating $\partial\epsilon_2(\omega)/\partial\omega$ for a tight binding description of the d bands in Ni based alloys.

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[6] See, C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), p. 185.

[7] Compare with Eq. (4) in Chap. 18 of Ref 6, noting here only the s-wave phase shift is nonvanishing.

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