Total Dielectric Function Approach to Electron and Phonon Response in Solids

David R. Penn
Electron and Optical Physics Division, Physics Laboratory
National Institute of Standards and Technology
Technology Administration, Department of Commerce
Gaithersburg, MD 20899

and

Steven P. Lewis
Department of Physics, University of California
Berkeley, CA 94720
and
Materials Sciences Division
Lawrence Berkeley Laboratory
Berkeley, CA 94720
and
Department of Physics, State University of New York
Stony Brook, New York 11794-3800*

and

Marvin L. Cohen
Department of Physics, University of California
Berkeley, CA 94720
and
Materials Sciences Division
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Abstract

The interaction between two test charges, the response of a solid to an external field, and the normal modes of the solid can be determined from a total dielectric function that includes both electronic and lattice polarizabilities as well as local field effects. In this paper we examine the relationship between superconductivity and the stability of a solid and derive new sum rules for the electronic part of the dielectric function. It is also shown that there must be negative eigenvalues of the total static dielectric function implying the possibility of an attractive interaction between test charges. An attractive interaction is required for superconductivity.

1 Introduction

The dielectric function is of fundamental importance in understanding many properties of solids. It describes the response of the solid to an external field, the elementary excitations of the solid, and the screening in the solid. The *total* dielectric function includes not only the screening by the electrons but also the polarizability of the lattice [1]. The presence of a lattice serves to modify the electron wave functions and consequently the electronic screening, leading to local field effects. In addition, over-screening by the lattice results in an attractive total pairing interaction which may lead to superconductivity. In the absence of local field effects, the electron-phonon coupling only involves the longitudinal phonons [2]. The presence of local field effects allows coupling between the transverse phonon modes and the electrons through Umklapp processes and enhances the strength of the attractive electron-electron interaction.

In this paper we study $\epsilon^{-1}_{\rm TOT}$, the inverse total dielectric function that describes the electronic and lattice screening including local field effects. In addition we consider the interaction of two test charges, $V_{\rm INT} = \epsilon^{-1}_{\rm TOT}\, v$, where v is the bare Coulomb interaction. The interaction between the two test charges is simpler than that between two electrons because of exchange and correlation interactions with other electrons. A direct derivation of $\epsilon^{-1}_{\rm TOT}$ in the random phase approximation (RPA) has been given by Allen, Cohen and Penn [1]. Their results are in agreement with earlier work by Maksimov [3], who took a different approach by deriving the total interaction, $V_{\rm INT}$, and defining $\epsilon^{-1}_{\rm TOT}$ by $\epsilon^{-1}_{\rm TOT} = V_{\rm INT}/v$.

Although the concept of the total dielectric function has not been a subject of active study, there are a number of useful applications of this approach. Besides determining the total interaction between two test charges, the inverse dielectric function describes the response of the system to an external field. Also, $\epsilon^{-1}_{\rm TOT}$ has poles at energies corresponding to collective elementary excitations. The poles determine the plasmon and phonon modes [1] of the solid as well as any other collective modes that might exist. Another important reason for studying $\epsilon^{-1}_{\rm TOT}$ is that stability considerations place restrictions on this function [1], [4].

Finally, a further reason for working with $\epsilon^{-1}_{\rm TOT}$ is that this approach treats the electrons and ions on an equal footing. Hence, the final results do not depend on an arbitrary division between the electronic and ionic systems. For example, this approach is appropriate whether the

ions are treated as pseudopotentials or as bare nuclei and is independent of the division of the Hamiltonian with regard to electron, phonon, and electron-phonon contributions. In this paper we restrict ourselves primarily to results at zero frequency, i.e., the static dielectric function.

In section 2 we discuss the background and formulation of the theory pertaining to the total dielectric function, $\epsilon_{\rm TOT}$. This function is defined in section 2.A, and related stability conditions are given. The electronic part of the susceptibility is discussed in section 2.B and the lattice part in section 2.C. In section 2.D, $\epsilon^{-1}_{\rm TOT}$ is given as well as the electron-phonon coupling and the dynamical matrix. These quantities result in a natural way when $\epsilon_{\rm TOT}$ is inverted to obtain $\epsilon^{-1}_{\rm TOT}$. In section 2.E, sum rules involving the electronic part of the dielectric function, $\epsilon^{-1}_{\rm el}$, are given. These sum rules are a consequence of the existence of a lattice. The best known one is the acoustic sum rule which is expressed in terms of $\epsilon^{-1}_{\rm el}$. We derive a second sum rule, the translational sum rule, which has been stated incorrectly in previous literature [1], [5]. Making use of these two sum rules, we derive sum rules involving $\epsilon_{\rm el}$ rather than $\epsilon^{-1}_{\rm el}$. The relationship between $\epsilon^{-1}_{\rm TOT}$ and BCS theory is discussed in section 2.F. In section 2.G, we argue that for $\omega = 0$, $\epsilon^{-1}_{\rm TOT}$ has one negative eigenvalue for each spatial dimension of the system. A negative eigenvalue implies the possibility of an attractive screened Coulomb interaction, $\epsilon^{-1}_{\rm TOT}\ v$. We also show that the frequency-dependent $\epsilon_{\rm TOT}$ has zeros at the phonon frequencies; in other words there is an eigenvalue of $\epsilon_{\rm TOT}$ which is zero for $\omega = \omega_Q$ where ω_Q is a phonon frequency. Section 2.H shows how the stability conditions for the individual electronic and lattice parts of the system are related to that for the total system. In section 3 analytic results are given for the value of $\epsilon_{\rm el}$ in one dimension for the case $Q \rightarrow 0$ where Q is the reduced wave vector. A one-dimensional model for $\epsilon_{\rm el}$ is introduced in section 4, and numerical results are obtained for $\epsilon^{-1}_{\rm TOT}$ as well as for the phonon frequencies. The sum rules are used to limit the parameters of the models. Conclusions of the paper are presented in section 5.

2 Theory and Formulation

The purpose of this section is first to review relevant previous results and then to present new theory.

A. Definition of Inverse Dielectric Function and Stability Conditions

The inverse dielectric function $\epsilon^{-1}_{\rm TOT}$ is defined by the change in potential at a point $\vec{r}$ and time t due to an infinitesimal perturbing potential $\delta V_{\rm EXT}(\vec{r}', t')$

$$\delta V_{\rm TOT}(r,t) \;=\; \int_{-\infty}^{t} dt' \int d^3r' \; \epsilon^{-1}_{\rm TOT}(r,r',t-t') \; \delta V_{\rm EXT}(r',t') \quad . \tag{1}$$

The dielectric function $\epsilon_{\rm TOT}$ is related to $\epsilon^{-1}_{\rm TOT}$ by

$$\int_{-\infty}^{\infty} dt'' \int d^3r'' \; \epsilon_{\rm TOT}(r,r'',t-t'') \; \epsilon^{-1}_{\rm TOT}(r'',r',t''-t') \;=\; \delta(r-r') \; \delta(t-t') \quad . \tag{2}$$

A change in the external potential results in a change in the charge density of the system, $\delta \rho_{\rm TOT}(\vec{r}, t)$, related to the susceptibility, χ, by

$$\delta \rho_{\rm TOT}(r,t) \;=\; \int_{-\infty}^{t} dt' \int d^3r' \; \chi(r,r',t-t') \; \delta V_{\rm EXT}(r',t') \tag{3}$$

where $\delta \rho_{\rm TOT}$ includes the change in both the electronic charge density and the nuclear charge density. Equation (3) serves to define the susceptibility χ. The change in charge density $\delta \rho_{\rm TOT}$ is given by the change in the expectation value of the operator

$$\hat{\rho}_{\rm TOT}(r) \;=\; Z \sum_{l} \delta(r - R_l) \;-\; \sum_{i} \delta(r - R_i) \tag{4}$$

where Ze is the charge of the nuclei which are assumed identical for simplicity, $\vec{R}_l$ is the nuclear coordinate at the lattice site l. Charge densities are in units of inverse volume, and potentials have units of energy, not work per unit charge.

Schematically, Eq. (1) is $\delta V_{\rm TOT} = \epsilon^{-1}_{\rm TOT} \; \delta V_{\rm EXT}$, and Eq. (3) is $\delta \rho_{\rm TOT} = \chi \; \delta V_{\rm EXT}$. Because $\delta V_{\rm TOT} = \; \delta V_{\rm EXT} + v \, \delta \rho_{\rm TOT}$ where v is the Coulomb interaction, it follows that $\epsilon^{-1}_{\rm TOT} = 1 \; + \; v \, \chi$, i.e.,

$$\epsilon^{-1}_{\rm TOT}(r,r',t-t') \;=\; \delta(r-r') \, \delta(t-t') \; + \; \int d^3r'' \; \frac{e^2}{|r-r''|} \; \chi(r'',r',t-t') \quad . \tag{5}$$

It is useful to deal with the Fourier transform of the time. Thus if $\delta V_{\rm EXT}(\vec{r}',t') \propto e^{-i\omega t'}$, then $\epsilon^{-1}_{\rm TOT} = \epsilon^{-1}_{\rm TOT}(\vec{r},\vec{r}',\omega)$ and $\chi = \chi(\vec{r},\vec{r}',\omega)$. Similarly, $\epsilon_{\rm TOT}$ and $\epsilon^{-1}_{\rm TOT}$ satisfy

$$\int d^3r''\, \epsilon_{\rm TOT}(r,r'',\omega)\, \epsilon^{-1}_{\rm TOT}(r'',r',\omega) = \delta(r-r') \quad . \tag{6}$$

In the case of a homogeneous electron gas, $\epsilon^{-1} = \epsilon^{-1}(\vec{r}-\vec{r}',t'-t)$ which can be Fourier transformed to obtain $\epsilon^{-1} = \epsilon^{-1}(\vec{q},\omega)$.

It is clear from Eq. (1) that ϵ^{-1} is a causal response function for any value of q, while it has been shown [6] that ϵ is causal only at $q = 0$. The Kramer-Kronig relations, which hold for causal response functions, are

$$Re\, \epsilon^{-1}(\vec{q},\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{d\omega'\,\omega'}{\omega'^2-\omega^2}\, Im\, \epsilon^{-1}(q,\omega') \quad , \tag{7a}$$

$$Re\, \epsilon(0,\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{d\omega'\,\omega'}{\omega'^2-\omega^2}\, Im\, \epsilon(0,\omega') \quad , \tag{7b}$$

and since a stable system in its ground state can only absorb energy, $Im\,\epsilon(q,\omega) > 0$ and $Im\,\epsilon^{-1}(q,\omega) \equiv Im\,\frac{1}{\epsilon(q,\omega)} < 0$. Setting $\omega = 0$ in Eq. (7) yields the conditions [7]-[9]

$$\frac{1}{\epsilon(\vec{q},0)} < 1 \quad , \tag{8a}$$

$$\epsilon(0,0) > 1 \quad . \tag{8b}$$

These conditions can be generalized to the case of a solid with a periodic lattice as discussed by Car, Tosatti, Baroni, and Leelaprute [4]. In the case of a periodic lattice $\epsilon^{-1}_{\rm TOT}(\vec{r},\vec{r}',\omega) = \epsilon^{-1}_{\rm TOT}(\vec{r}+R^0_L,\vec{r}'+R^0_L,\omega)$, so that $\epsilon^{-1}_{\rm TOT} = \epsilon^{-1}_{\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega)$, where $\vec{Q}$ is a reduced wave vector, and $\vec{G},\vec{G}'$ are reciprocal lattice vectors. Equation (1) becomes

$$\delta V_{\rm TOT}(\vec{Q}+\vec{G},\omega) = \sum_{G'} \epsilon^{-1}_{\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega)\, \delta V_{\rm EXT}(\vec{Q}+\vec{G}',\omega) \quad , \tag{9}$$

where $\delta V_{\rm TOT}(Q+G,\omega)$ is the Fourier transform of $\delta V_{\rm TOT}(r,t)$.

It has been shown by Car *et al.* [4] and verified in reference 1 that the generalization of Eq. (8a) to the case of a periodic lattice is

$$\epsilon^{-1}_{\mu}(\vec{Q}) < 1 \quad , \tag{10}$$

where $\epsilon^{-1}_{\mu}(\vec{Q})$ is any eigenvalue of the matrix $\epsilon^{-1}_{\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega=0)$. In the present case, Eq. (10) includes the lattice as well as the electronic polarizability whereas Car *et al.*, [4] were

interested only in the electronic response. Nevertheless, their proof holds for the more general case.

A violation of the condition in Eq. (10) implies an instability of the combined electronic and lattice systems. The relationship between this type of instability and an instability in either the electronic or lattice part of the system is discussed in section 2.H. Equations (8a) and (10) allow for negative values of $\epsilon^{-1}(q)$ and $\epsilon_\mu^{-1}(Q)$ with the consequence that $V_{\rm INT}$ can be attractive and the system stable, as required for superconductivity. It is expected [1] that near a phase transition there will be some eigenvalue of $\epsilon_{\rm TOT}^{-1}$ that is large and negative.

It can also be shown [1] that the diagonal part of $\epsilon_{\rm TOT}^{-1}$ satisfies

$$\epsilon_{\rm TOT}^{-1}(\vec{Q}+\vec{G},\vec{Q}+\vec{G},\omega=0) \;<\; 1 \quad , \tag{11}$$

which means that the macroscopic dielectric function, $\epsilon_M(Q,Q)$, satisfies [10], [11]; $1/\epsilon_M(Q,Q) \equiv \epsilon_{\rm TOT}^{-1}(\vec{Q},\vec{Q},\omega=0) < 1$. Equation (11) is a weaker condition than Eq. (10); if Eq. (10) is satisfied then so is Eq. (11). Similarly, the generalization of (8b) takes the form

$$\frac{1}{\epsilon_{\rm TOT}^{-1}(Q+0,Q+0,\omega=0)} \;>\; 1 \quad . \tag{12}$$

Equations (10) and (12) must be satisfied to ensure the stability of the solid. We have written the subscript "TOT" on $\epsilon_{\rm TOT}^{-1}$ to emphasize that it is the response of the total system (electrons plus lattice), rather that just the electronic part $\epsilon_{\rm el}^{-1}$, that obeys (10) and (12). It is shown in Appendix A that the eigenvalues of $\epsilon_{\rm el}^{-1}$ satisfy $\left(\epsilon_{\rm el}^{-1}\right)_\mu < 1+\Gamma_\mu$ where $\Gamma_\mu > 0$.

B. Electronic Part of the Susceptibility

The electronic portion of the susceptibility, $\chi_{\rm el}$, and the inverse dielectric function $\epsilon_{\rm el}^{-1}$ have been derived [10]-[12] in the random phase or mean field approximation for the case of a periodic lattice. The relationship between the exact expressions for ϵ and χ is given by Eq. (5) in the form $\epsilon^{-1} \;=\; 1 + v\,\chi$ where v is the Coulomb interaction. The change in the charge density, $\delta\rho$, induced by the external field $\delta V_{\rm EXT}$ is given by Eq. (3) as $\delta\rho \;=\; \chi\,\delta V_{\rm EXT}$. In the mean field approximation it is assumed that $\delta\rho \simeq \chi_0^{\rm el}(\delta V_{\rm EXT} + v\,\delta\rho)$ where $\chi_0^{\rm el}$ is the susceptibility for a system of electrons which do not interact with each other. Thus $\chi = \left(1 - v\,\chi_0^{\rm el}\right)^{-1} \cdot \chi_0^{\rm el}$, and ϵ

takes the form $\epsilon_{\rm MF,el} = 1 - v\,\chi_0^{\rm el}$ where $\epsilon_{\rm MF,el}$ is the mean field dielectric function. In this case

$$\chi_0^{\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega) = \sum_{kl'l} \frac{(f_{k+Q,l'} - f_{k,l})\ M_{k+Q,l,l'}(G,G')}{\epsilon_{k+Q,l'} - \epsilon_{k,l} - \hbar\omega + i\alpha} \quad , \tag{13a}$$

$$M_{\vec{k}+\vec{Q},l,l'}(\vec{G},\vec{G}') = \left\langle \vec{k}+\vec{Q}\ l' \left| e^{i(\vec{Q}+\vec{G})\cdot\vec{r}} \right| \vec{k}\, l \right\rangle \left\langle \vec{k}\, l \left| e^{-i(\vec{Q}+\vec{G}')\cdot r} \right| \vec{k}+\vec{Q}\, l' \right\rangle \quad , \tag{13b}$$

where $f_{k,l}$ is the Fermi factor for the state $|kl\rangle$, $\epsilon_{k,l}$ is the corresponding energy, and l is a band index.

It will be convenient to work with the symmetric form of ϵ^{-1}; $\epsilon_S^{-1} = 1 + v^{1/2}\,\chi\, v^{-1/2}$ where $v^{1/2}(Q) = \sqrt{4\pi\, e^2/\Omega}/Q$, and Ω is the crystal volume:

$$\epsilon_S^{-1}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega) = \delta_{GG'} + \frac{4\pi\, e^2}{\Omega} \frac{1}{|\vec{Q}+\vec{G}|}\, \chi(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega)\, \frac{1}{|\vec{Q}+\vec{G}'|} \quad . \tag{14}$$

For the electronic case (no lattice polarizability) the symmetric form of the dielectric function in the mean field approximation is

$$\epsilon_{S,\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega) = \delta_{GG'} - \left(\frac{4\pi\, e^2}{\Omega}\right) \frac{1}{|\vec{Q}+\vec{G}|}\, \chi_0^{\rm el}\,(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega)\, \frac{1}{|\vec{Q}+\vec{G}'|} \quad , \tag{15}$$

where $\chi_0^{\rm el}$ is given by Eq. (13a) and (13b).

In the random phase approximation at $\omega = 0$ the eigenvalues of $\epsilon_{S,\rm el}$ are positive [4] and a static, attractive electron-electron interaction, $\epsilon^{-1}\, v$, is not possible with only electronic screening.

It should be noted that the $G = 0$ and $G' = 0$ components of $\epsilon_{S,\rm el}(\vec{Q},+\vec{G},\vec{Q}+\vec{G}';\omega)$ are not continuous at the origin. In particular, $\epsilon_{S,\rm el}(\vec{Q}\equiv 0,\vec{G};\omega) = \delta_{0,G}$, which is not the limit of $\epsilon_{S,\rm el}(\vec{Q},\vec{Q}+\vec{G};\omega)$ as $\vec{Q}\to 0$. This follows from Eq. (15); for a system of dimension L, the Coulomb factor is not really infinite at $\vec{Q}+\vec{G}\equiv 0$, but rather is of order L. However, the matrix element in Eq. (13b) is zero for $\vec{Q}+\vec{G}\equiv 0$ because the wave functions are orthogonal. Thus, even in the limit of very large L, the last term in Eq. (15) is zero for $\vec{Q}+\vec{G}\equiv 0$ or $\vec{Q}+\vec{G}'\equiv 0$, whereas it does not necessarily vanish as $\vec{Q}+\vec{G}\to 0$ or $\vec{Q}+\vec{G}'\to 0$. This fact will be used in deriving the translational sum rule in section 2.E.

C. Lattice Part of the Susceptibility

The lattice contribution to the susceptibility has been derived in reference 1 using mean field theory for the case of one atom per unit cell. In this approximation a displaced ion feels

the average field due to all ions and electrons in their equilibrium states. The result is that the displaced ion acts like an independent Einstein oscillator with frequency Ω_0, and the lattice susceptibility is given by

$$\chi_0^L(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega) \;=\; N\,Z^2\,\frac{(\vec{Q}+\vec{G})\;\cdot\;(\vec{Q}+\vec{G}')}{M(\omega^2\;-\;\Omega_0^2)} \quad , \tag{16a}$$

where N is the number of atoms, Ze is the ionic charge, and

$$M\Omega_0^2 \;=\; \frac{-4\pi\,e^2\,Z^2}{3\Omega}\sum_G \rho_{\rm TOT}(\vec{G}) \quad , \tag{16b}$$

where $\rho_{\rm TOT}(\vec{G})$ is the Fourier transform of the equilibrium total charge density. Equation (16b), derived in Ref. [1], is valid for the case of a three dimensional lattice with cubic symmetry. For the one dimensional case (discussed in section 3) the right-hand side of Eq. (16b) is multiplied by 3. The reader is referred to Section IV of reference 1 for a complete derivation and discussion of Eqs. (16).

It will be useful to write the expression for χ_0^L in another form [1];

$$\chi_0^L(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega) \;=\; NZ^2\sum_{\alpha,\beta}(\vec{Q}+\vec{G})_\alpha\;D^\circ_{\alpha,\beta}(\omega)\;(\vec{Q}+\vec{G})_\beta \quad , \tag{17a}$$

where D° is the displacement-displacement correlation function,

$$[D^\circ\,(\omega)]^{-1}_{\alpha\beta} \;=\; M\,\omega^2\,\delta_{\alpha\beta} - K^\circ_{\alpha\beta} \quad , \tag{17b}$$

and

$$K^\circ_{\alpha\beta} \;=\; -\;\frac{4\pi\,e^2\,Z^2}{\Omega}\sum_{G\neq 0}\hat{G}_\alpha\,\hat{G}_\beta\left(1\;-\;\frac{\rho(\vec{G})}{\rho(0)}\right) \quad , \tag{17c}$$

where α,β denote x, y, or z, and $\rho(\vec{G})$ is the electronic charge density form factor.

D. Calculation of $\epsilon^{-1}_{\rm TOT}$

The total dielectric function in the mean field approximation is given by

$$\epsilon_{S,\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega) \;=\; \delta_{GG'} \;-\; \frac{4\pi\,e^2}{\Omega}\,\frac{1}{|Q+G|}\,\chi_0^{\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega)\,\frac{1}{|Q+G'|} \quad , \tag{18}$$

where $\chi_0^{\rm TOT} \;=\; \chi_0^{\rm el} + \chi_0^L$, and $\chi_0^{\rm el}$ and χ_0^L are given by Eqs. (13) and (16), respectively. It is $\epsilon^{-1}_{\rm TOT}$, and not $\epsilon_{\rm TOT}$, that is the causal response function and the physical quantity of interest. Equation (18) can be inverted [1] to obtain $\epsilon^{-1}_{\rm TOT}$ or equivalently $V_{\rm INT} \;=\; \epsilon^{-1}_{\rm TOT}\;v \;=\; v^{1/2}\,\epsilon^{-1}_{S,\rm TOT}\,v^{1/2}$,

$$V_{\rm INT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega) = v^{1/2}(Q+G)\,\epsilon^{-1}_{S,\rm TOT}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega)\,v^{1/2}(Q+G')$$

$$= \frac{4\pi e^2}{\Omega}\,\frac{1}{|\vec{Q}+\vec{G}|}\,\frac{1}{|\vec{Q}+\vec{G}'|}\,\Big\{\epsilon^{-1}_{S,\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega)$$

$$+ Z^2\,\frac{4\pi e^2}{\Omega}\sum_{\alpha\beta}\varphi^s_\alpha(\vec{Q}+\vec{G},\omega)\,D_{\alpha\beta}(\vec{Q},\omega)\,\varphi^s_\beta(\vec{Q}+\vec{G}',\omega)\Big\} \quad , \quad (19)$$

where $\epsilon^{-1}_{S,\rm TOT}$ denotes the total dielectric function and is given by the quantity in curly brackets. The quantity $\epsilon^{-1}_{S,\rm el}$ is the inverse of the electronic dielectric matrix $\epsilon_{S,\rm el}$ given by Eq. (15). The term in (19) involving $\epsilon^{-1}_{S,\rm el}$ describes the screening due to the electrons in the solid while the term proportional to Z^2 is the screening due to the lattice polarization. This latter term can be attractive, and if it is large the total interaction can be negative, i.e., have a negative eigenvalue. The electron-phonon coupling strength is

$$\varphi^s_\alpha(\vec{Q}+\vec{G},\omega) = \sum_{G''}\epsilon^{-1}_{S,\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}'';\omega)\,(\widehat{Q+G''})_\alpha \quad , \quad (20)$$

where $(\widehat{Q+G})$ denotes a unit vector. The phonon propagator D is given by

$$D^{-1}_{\alpha\beta}(\vec{Q},\omega) = M\,\omega^2\,\delta_{\alpha\beta} - K_{\alpha\beta}(\vec{Q},\omega) \quad . \quad (21)$$

where α,β denote cartesian components.

The phonon frequencies are the eigenvalues of the dynamical matrix, $K_{\alpha\beta}(\vec{Q},\omega)$,

$$M\,\omega^2\,\vec{\eta}_Q = K(\vec{Q},\omega)\,\vec{\eta}_Q \quad . \quad (22)$$

where ω and $\vec{\eta}_Q$ are eigenvalues and eigenvectors, respectively, of K. The dynamical matrix K is [13], [14]

$$K_{\alpha\beta}(\vec{Q},\omega) = \frac{4\pi e^2 Z^2}{\Omega}\Bigg[\sum_{GG'}(\widehat{Q+G})_\alpha\,\epsilon^{-1}_{S,\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}';\omega)\,(\widehat{Q+G'})_\beta$$

$$- \sum_{GG'\neq 0}\widehat{G_\alpha}\,S^{-1}_{S,\rm el}(\vec{G},\vec{G}',0)\,\hat{G}'_\beta\Bigg] \quad , \quad (23)$$

where $S^{-1}_{S,\rm el}$ is the inverse of $S_{S,\rm el}$ which is the same matrix as $\epsilon_{S,\rm el}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega)$ except that the row $\epsilon(\vec{Q},\vec{Q}+\vec{G},\omega)$ and the column $\epsilon(\vec{Q}+\vec{G},\vec{Q};\omega)$ are deleted. The matrix $S_{S,\rm el}$ is closely

related to the matrix involving $\epsilon_{S,\mathrm{el}}$ for $Q \equiv 0$ described in the last paragraph of section 2.B. The matrix $D(\vec{Q},\omega)$ appearing in Eq. (19) can be put in the form

$$D = \sum_j \eta_{Qj} \left[M\omega^2 - M\omega_{Qj}^2\right]^{-1} \eta_{Qj}^\dagger \quad , \tag{24}$$

where η_{Qj} is an eigenvector of $K(\vec{Q},\omega)$, and ω_{Qj}^2 is the corresponding eigenvalue as determined from Eq. (22). For $\omega = 0$, the dynamical matrix K is Hermitian, and ω_{Qj}^2 is positive. Negative values of ω_{Qj}^2 correspond to an unstable lattice. From Eq. (24) it is clear that if a phonon mode approaches zero, V_{INT} can become large and negative, and an attractive interaction results even though the system is stable.

E. Sum Rules

There are two important sum rules for $\epsilon_{\rm el}^{-1}$ evaluated at $\omega = 0$. The first is the acoustic sum rule which follows from the condition that the lattice acoustic modes go to zero frequency as Q approaches zero. The second sum rule which we will refer to as the translational sum rule is a consequence of the periodicity of the lattice. The acoustic sum rule has been derived by Pick *et al.* [13]; it can be shown that Eq. (23) can be put in the form (Appendix B)

$$\begin{aligned} K_{\alpha\beta}(\vec{Q},\omega) \;=\; & \frac{4\pi\, e^2\, Z^2}{\Omega} \left\{ \sum_G \epsilon_{S,\rm el}^{-1}(\vec{Q},\vec{Q}+\vec{G};\omega)\, \widehat{(Q+G)}_\alpha \, \frac{1}{\epsilon_{S,\rm el}^{-1}(\vec{Q},\vec{Q};\omega)} \right. \\ & \times \sum_{G'} \epsilon_{S,\rm el}^{-1}(\vec{Q},\vec{Q}+\vec{G}';\omega)^*\, \widehat{(Q+G')}_\beta \\ & + \sum_{GG'\neq 0} \Big[\widehat{(Q+G)}_\alpha\, S_{S,\rm el}^{-1}(\vec{Q},\vec{G},\vec{Q}+\vec{G}';\omega)\, \widehat{(Q+G')}_\beta \\ & \left. - \hat{G}_\alpha\, S_{S,\rm el}^{-1}(\vec{G},\vec{G}';\omega)\, \hat{G}'_\beta \Big] \right\} \quad , \end{aligned} \tag{25}$$

where S^{-1} is defined after Eq. (23). This expression for K leads directly to the acoustic sum rule which ensures that the acoustic phonon modes satisfy $\omega(Q) \to 0$ as $Q \to 0$. The term in Eq. (25) in the square brackets approaches zero as $Q \to 0$ because S^{-1} is analytic. Consequently, $K \to 0$ if

$$\lim_{Q\to 0} \sum_G \epsilon_{S,\rm el}^{-1}(\vec{Q},\vec{Q}+\vec{G})\, \widehat{(Q+G)}_\alpha \;=\; 0 \quad , \tag{26}$$

where $\epsilon^{-1}(\vec{Q},\vec{Q}+\vec{G}) \equiv \epsilon^{-1}(\vec{Q},\vec{Q}+\vec{G};\omega=0)$. This sum rule is satisfied automatically in metals because of the dependence of ϵ on Q, but is non-trivial for insulators as will be discussed in more detail below.

The translational sum rule was first derived by Keating [5] and rederived in ref. 1. It is stated incorrectly in both references where it had been assumed that $\epsilon^{-1}(Q,Q;0)$ is continuous as $Q \to 0$ contrary to our discussion at the end of section 2B. This sum rule is obtained by rigidly displacing the entire lattice and recognizing that the displaced ions produce a rigid displacement of the electronic charge density. It is derived in Appendix C.

The resulting sum rule is

$$\sum_{G'\neq 0} S_{S,\rm el}^{-1}(\vec{G},\vec{G}')\, \widehat{G}'_\alpha \;=\; \left(1 - \frac{\rho(\vec{G})}{\rho(0)}\right) \hat{G}_\alpha \quad ; \quad G \neq 0 \quad , \tag{27}$$

where $\rho(\vec{G})$ is the electronic form factor. Equation (27) will be referred to as the translational sum rule. One consequence of the translational sum rule is that off-diagonal matrix elements of $\epsilon_{S,\mathrm{el}}$ cannot be neglected for either metals or insulators. In the case of the acoustic sum rule this conclusion only follows for insulators, because metals automatically satisfy this sum rule. For the exact $\epsilon^{-1}_{S,\mathrm{el}}$ both sum rules are satisfied automatically while for models of $\epsilon^{-1}_{S,\mathrm{el}}$ the sum rules can be used to fix the adjustable parameters. It follows directly from Eq. (27) that $K^{\circ}_{\alpha\beta}$ of Eq. (17c) is given by

$$K^{\circ}_{\alpha\beta} \;=\; -\,\frac{4\pi\, e^2\, Z^2}{\Omega} \sum_{G,G'\neq 0} \hat{G}_\alpha \; S^{-1}_{S,\mathrm{el}}(\vec{G},\vec{G}')\, \vec{G}'_\beta \tag{28}$$

which is the second term on the right-hand side of Eq. (23) for $K_{\alpha\beta}$.

The two sum rules can be expressed in terms of $\epsilon_{S,\mathrm{el}}$ rather than $\epsilon^{-1}_{S,\mathrm{el}}$ and take the following form which is derived in Appendix D,

$$\sum_{G'\neq 0} \epsilon_{S,\mathrm{el}}(\vec{G},\vec{G}') \left(1-\frac{\rho(\vec{G}')}{\rho(0)}\right) \widehat{G'}_\alpha \;=\; \hat{G}_\alpha \qquad (G\neq 0) \quad , \tag{29a}$$

$$Q\to 0 \;:\; \sum_{G'\neq 0} \epsilon_{S,\mathrm{el}}(\vec{Q}+\vec{G}') \left(1-\frac{\rho(\vec{G}')}{\rho(0)}\right) \widehat{(Q+G')}_\alpha \;=\; \hat{Q}_\alpha \quad . \tag{29b}$$

Equation (29) holds only for insulators as is made clear in Appendix D. This form of the sum rules is useful when dealing with models that define $\epsilon_{S,\mathrm{el}}$ instead of $\epsilon^{-1}_{S,\mathrm{el}}$, as is usually the case.

F. Relationship Between V_{INT} and Superconductivity

As discussed in section 1 the total interaction between two electrons is not strictly $\epsilon^{-1}_{\mathrm{TOT}}\, v$. This latter expression describes the interaction between two test charges. Nevertheless, the effects of vertex corrections and nonlinear effects may be small or take the form of multiplicative corrections and we assume $V_{\mathrm{INT}} \;=\; \epsilon^{-1}_{\mathrm{TOT}}\, v$. The matrix element for scattering a Cooper pair from a state k to k' on the Fermi surface is [1]

$$V_{kk'} \;=\; \langle k'\uparrow, -k'\downarrow |V_{\mathrm{INT}}|\; k\uparrow, -k\downarrow\rangle \;=\; \langle g_{kk'}|\epsilon^{-1}_{\mathrm{TOT}} v|g_{kk'}\rangle \quad , \tag{30}$$

where

$$g_{kk'}(r) \;=\; \psi_{k'}(r)\, \psi^*_k(r) \quad , \tag{31}$$

and $V_{kk'}$ is related to the BCS interaction V_{BCS} by [15]

$$-\,N_\uparrow(0)\, V_{BCS} \;=\; N_\uparrow(0)\langle V_{kk'}\rangle_{FS} \;=\; \mu-\lambda \quad , \tag{32}$$

where $\langle\cdots\rangle_{FS}$ denotes a Fermi surface average, and $N_\uparrow(0)$ is the density of states at the Fermi energy for a given spin. The screened Coulomb interaction $\epsilon_{\rm el}^{-1}\ v$ is given by the first term in Eq. (19) and corresponds to μ, a repulsive interaction, while the attractive electron phonon part of $\epsilon_{\rm TOT}^{-1}\ v$ is given by the second term in Eq. (19) and produces λ. Taking account of various types of renormalization and retardation effects leads to more refined expressions [15] for λ and μ; i.e., $\lambda \to \lambda^* \sim \lambda/1+\lambda$ and $\mu \to \mu^* = \mu/[1+\mu\ln(E_F/\hbar\omega_D)]$, where E_F is the Fermi energy, and $\hbar\omega_D$ is the Debye energy.

In order to evaluate $V_{kk'}$ in Eq. (30) the quantity $g_{kk'}(r)$ is expanded in a Fourier series. The terms in the expansion corresponding to $G \neq 0$ lead to local field effects, and it is these effects that we focus on.

G. Sign of the Eigenvalues of $\epsilon_{S,\rm TOT}$

It was noted in section 2.A that the eigenvalues of $\epsilon_{S,\rm TOT}^{-1}(Q+G,Q+G';\omega=0)$ satisfy $\epsilon_{S,{\rm TOT},\mu}^{-1}(Q) < 1$. This condition allows for the possibility of negative eigenvalues, and consequently two test charges may experience an attractive interaction. If the test charges have charge density ρ given by Eq. (31) then the average total interaction between them is

$$\langle V_{\rm INT}\rangle = \langle\rho|\ v^{1/2}\ \epsilon_{S,\rm TOT}^{-1}\ v^{1/2}\ |\rho\rangle = \sum_{Q,\mu} \left|\langle\rho|\ v^{1/2}\ |Q,\mu\rangle\right|^2\ \epsilon_{S,{\rm TOT},\mu}^{-1}(Q) \tag{33}$$

where $|Q,\mu\rangle$ is an eigenvector of $\epsilon_{S,\rm TOT}^{-1}$ corresponding to the eigenvalue $\epsilon_{S,{\rm TOT},\mu}^{-1}(Q)$. Clearly $V_{\rm INT}$ can be attractive only if at least one of the eigenvalues of $\epsilon_{S,\rm TOT}^{-1}$ is negative.

It is proved in Appendix E that in one and three dimensions, at least one eigenvalue of $\epsilon_{S,\rm TOT}^{-1}(Q+G,G+G')$ is negative. This result is obtained by proving that

$$\det\left(\epsilon_{S,\rm TOT}^{-1}\right) = (-1)^d\ \frac{\det(-K^0)}{\det(K)}\ \det\left(\epsilon_{S,\rm el}^{-1}\right) \tag{34}$$

where $\det(A)$ means the determinant of A, d is the dimension of the space, K is the dynamical matrix defined in Eq. (23), and K^0 is given by Eq. (17b) evaluated at $\omega = 0$. In the mean field approximation, $\det\left(\epsilon_{S,\rm el}^{-1}\right) > 0$. The quantity $\det(K) > 0$ is a condition for the stability of the lattice, i.e., all the eigenvalues of K must be positive, and $\det(-K^0) > 0$. One can write

$$\det\left(\epsilon_{S,\rm TOT}^{-1}\right) = \prod_\mu\ \epsilon_{S,{\rm TOT},\mu}^{-1}(Q)\quad , \tag{35}$$

i.e., the determinant of a matrix is the product of its eigenvalues. It follows that if the right-hand side of Eq. (34) is negative then at least one of the eigenvalues of $\epsilon^{-1}_{S,\mathrm{TOT}}$ is negative. This holds for one or three dimensions. More precisely in one and three dimensions there are an odd number of negative eigenvalues while in two dimensions there are none or an even number.

In section 4 we find that for a particular one-dimensional model of ϵ_{el} a numerical study gives the result that there is a negative eigenvalue of ϵ_{TOT} that vanishes at $Q = 0$. This behavior is explained as follows. It is shown in Appendix F that

$$\sum_{G' \neq 0} \epsilon_{S,\mathrm{TOT}}(\vec{G},\vec{G}') \left(1 - \frac{\rho(\vec{G}')}{\rho(0)}\right) \hat{G}'_\alpha = 0 \tag{36}$$

which is an eigenvalue equation with eigenvalue 0 and eigenvector $\xi_\alpha = (1 - \rho(\vec{G}')/\rho(0))\hat{G}_\alpha$. This is one eigenvector, ξ_α, for each dimension. Equation (36) is consistent with the hypothesis that there is one negative eigenvalue in each dimension that vanishes at $Q = 0$.

The reason for the existence of negative eigenvalues of $\epsilon^{-1}_{\mathrm{TOT}}$ can be understood by examining the case $\omega \neq 0$. It is shown in appendix G that

$$\sum_{G'} \epsilon_{S,\mathrm{TOT}}(\vec{Q}+\vec{G},\vec{Q},+\vec{G}',\omega_{Qj})\, \varphi^s_{\alpha_j}(\vec{Q}+\vec{G}',\omega_{Qj}) = 0 \tag{37}$$

where φ^s_α is given by Eq. (20), ω_{Qj} is a phonon frequency, and α_j denotes the direction of the phonon polarization vector. In other words, $\epsilon_{S,\mathrm{TOT}}$ has an eigenvalue $\lambda_\alpha(Q,\omega)$ that vanishes when $\omega = \omega_{Qj}$, a phonon frequency. This corresponds to $\epsilon_{S,\mathrm{TOT}}$ "having a zero" at the phonon mode frequency and is analogous to a homogeneous system which has plasmon mode of frequency ω_{pl} given by $\epsilon_{\mathrm{el}}(Q,\omega_{pl}) = 0$. Below the curve defined by $\lambda_\alpha(Q,\omega) = 0$ in ω, Q space, we assume that $\lambda_\alpha(Q,\omega) < 0$, and consequently, $\lambda_\alpha(Q,\omega = 0) < 0$; i.e., there is one negative eigenvalue of $\epsilon_{S,\mathrm{TOT}}$ for each spatial dimension in the case $\omega = 0$.

H. Stability of the System

The condition for the stability of a purely electronic system is $\epsilon^{-1}_\mu(Q) < 1$, where $\epsilon^{-1}_\mu(Q)$ is an eigenvalue of $\epsilon^{-1}_{S,\mathrm{el}}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',\omega = 0)$. The condition that the lattice be stable is that the phonon frequencies be real, $\omega^2_{Qj} > 0$, where ω_{Qj} is defined in Eq. (24). From Eq. (19)

$$\epsilon^{-1}_{S,\mathrm{TOT}}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',0) \;=\; \epsilon^{-1}_{S,\mathrm{el}}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}',0)$$

$$- \frac{4\pi\, e^2\, Z^2}{\Omega} \sum_{\alpha\beta} \varphi^s_\alpha(\vec{Q}+\vec{G},0)\; K^{-1}_{\alpha\beta}(Q)\; \varphi^s_\beta(\vec{Q}+\vec{G}',0) \quad . \quad (38)$$

Making use of Eqs. (21), (24), and (38) yields

$$\epsilon^{-1}_{S,\mathrm{TOT},\nu}(Q) \;=\; \sum_{\mu} |\langle\nu|\mu\rangle|^2\, \epsilon^{-1}_{\mu}(Q) \;-\; \frac{4\pi\, e^2\, Z^2}{\Omega M} \sum_{j} \frac{1}{\omega^2_{Qj}} \left| \sum_{\alpha} \langle\nu|\,\varphi_\alpha\rangle\; (\hat{\alpha}\cdot\vec{\eta}_{Qj}) \right|^2 \quad , \quad (39)$$

where $|\nu\rangle$ and $|\mu\rangle$ are eigenfunctions of $\epsilon^{-1}_{S,\mathrm{TOT}}$ and $\epsilon^{-1}_{S,\mathrm{el}}$, respectively. The condition $\epsilon^{-1}_{S,\mathrm{TOT},\nu}(Q) < 1$ required for stability of the coupled electron-lattice system, can be shown directly from Eq. (39) to hold if $\epsilon^{-1}_{\eta}(Q) < 1$ and $\omega^2_{Qj} > 0$, i.e., the electronic and lattice portions of the system are separately stable. It also follows from Eq. (39) that $\epsilon^{-1}_{S,\mathrm{TOT},\nu}(Q) < 1$ is possible even if $\epsilon^{-1}_{\eta}(Q) > 1$ as long as $\omega^2_{Qj} > 0$, i.e., even if the electronic portion of the system would be unstable in the absence of a lattice. Similarly, if $\epsilon^{-1}_{S,\mathrm{TOT},\nu}(Q) < 1$ is also possible for some Q even if $\omega^2_{Qj} < 0$. However, if K is a continuous function of Q there will be some value of Q for which ω^2_{Qj} is negative but small in magnitude and $\epsilon^{-1}_{S,\mathrm{TOT},\nu} < 1$ is not possible, as is clear from Eq. (39). Thus, since stability requires $\epsilon^{-1}_{S,\mathrm{TOT},\nu}(Q) < 1$ for all Q, an instability of the lattice implies the system must be unstable.

In summary, the total system is necessarily stable if the electron and lattice systems are individually stable. Furthermore, the total system can be stable if the electronic portion is individually unstable and the lattice system is stable. However, the total system *cannot* be stable if the lattice system is unstable regardless of the stability of the electronic system.

3 Analytic Results for One Dimension and $Q \rightarrow 0$

In section 3 we carry out calculations on a one-dimensional solid in the limit $\omega = 0$. It is assumed that the one-dimensional solid has a one atom basis and that the set of reciprocal lattice vectors $\{0, G_0, -G_0\}$ where $G_0 = 2\pi/a$ are the only ones of importance. In this section we investigate analytic properties as $Q \rightarrow 0$ for the mean-field dielectric function (Eq. (13)). In the following section we present numerical results for a specific one-dimensional model of $\epsilon_{S,\mathrm{el}}$ for general Q. The dependence of $\epsilon_{S,\mathrm{el}}(\vec{Q}+\vec{G}, \vec{Q}+\vec{G}')$ for $Q \rightarrow 0$ can be determined from the mean-field equation, Eq. (13), and one obtains

$$Q \rightarrow 0: \quad \epsilon_{S,\mathrm{el}}(Q,Q) = \frac{\alpha^I}{|\vec{Q}|^2} + \alpha^{II} \tag{40a}$$

$$\epsilon_{S,\mathrm{el}}(Q,Q+G) = \frac{\beta^I(G)}{|\vec{Q}|} + \beta^{II}(G) \tag{40b}$$

$$\epsilon_{S,\mathrm{el}}(Q+G,Q+G') = \gamma^I(G,G') + \gamma^{II}(G,G') \quad , \tag{40c}$$

where α, β, and γ are determined from the $Q \rightarrow 0$ limit of Eq. (13) and where I denotes intraband terms, $l = l'$, and II denotes interband terms, $l \neq l'$ in Eq. (13). $\beta^I(G)$ and $\beta^{II}(G)$ are, respectively, even and odd functions of G, $\gamma^I(G,G')$ is an even function of G or G', and $\gamma^{II}(G,G')$ is an even function of G and G', i.e., $\gamma^{II}(G,G') = \gamma^{II}(-G,-G')$.

(a) For the case of an insulator there are no intraband terms, and in the limit $Q \rightarrow 0$ the symmetric dielectric matrix takes the form

$$\epsilon_{S,\mathrm{el}}(Q+G,Q+G')_{Q\rightarrow 0} = \begin{pmatrix} \alpha & \beta & -\beta \\ \beta & \gamma_a & \gamma_c \\ -\beta & \gamma_c & \gamma_a \end{pmatrix} \quad , \tag{41}$$

where we have omitted the superscript II for convenience. The inverse is given by

$$\epsilon^{-1}_{S,\mathrm{el}}(Q+G,Q+G')_{Q\rightarrow 0} = \frac{1}{\Delta} \begin{pmatrix} \gamma_a^2 - \gamma_c^2 & -\beta(\gamma_a+\gamma_c) & \beta(\gamma_a+\gamma_c) \\ -\beta(\gamma_a+\gamma_c) & \alpha\gamma_a - \beta^2 & -\beta^2 - \alpha\gamma_c \\ \beta(\gamma_a+\gamma_c) & -\beta^2 - \alpha\gamma_c & \alpha\gamma_a - \beta^2 \end{pmatrix} \tag{42a}$$

$$\Delta \;=\; \alpha\left(\gamma_a^2 \;-\; \gamma_c^2\right) \;-\; 2\beta^2\,(\gamma_a \;+\; \gamma_c) \quad . \tag{42b}$$

Making use of Eq. (23) the dynamical matrix takes the form

$$K(Q)_{\,Q\to 0} \;=\; \left(\frac{4\pi\, e^2}{\Omega}\right)\, Z^2\, \frac{(\gamma_a - \gamma_c - 2\beta)^2}{(\gamma_a - \gamma_c)\,[\alpha(\gamma_a - \gamma_c) - 2\beta^2]} \quad . \tag{43}$$

If the acoustic phonon mode has zero energy at $Q = 0$ then

$$\gamma_a - \gamma_c - 2\beta \;=\; 0 \quad . \tag{44}$$

The acoustic sum rule, Eq. (26), gives

$$0 \;=\; \frac{\gamma_a - \gamma_c - 2\beta}{\alpha(\gamma_a - \gamma_c) - 2\beta^2} \quad , \tag{45}$$

which is the same requirement. If β, γ_a, and γ_c are calculated from first principles the acoustic sum rule would be satisfied, however, we here view γ_a, γ_c, and β, as parameters. Similarly, the translational sum rule, Eq. (27), yields

$$1 \;-\; \frac{\rho(G)}{\rho(0)} \;=\; \frac{1}{(\gamma_a - \gamma_c)} \quad . \tag{46}$$

(b) In the case of a simple metal with no interband terms, $\epsilon_{S,\mathrm{el}}$ becomes, for $Q \to 0$,

$$\epsilon_{S,\mathrm{el}} \;=\; \begin{pmatrix} \frac{\alpha}{|Q|^2} & \frac{\beta}{|Q|} & \frac{\beta}{|Q|} \\ \frac{\beta}{|Q|} & \gamma_a & \gamma_c \\ \frac{\beta}{|Q|} & \gamma_c & \gamma_a \end{pmatrix} \quad . \tag{47}$$

Simple metals are commonly treated as having no off-diagonal terms for the dielectric function. However, Eq. (47) shows that this is not strictly correct.

The result for $K(Q)$ from Eq. (8a) is

$$K(Q)_{\,Q\to 0} \;=\; \frac{(\gamma_a - \gamma_c)\,|Q|^2}{\alpha(\gamma_a - \gamma_c) - 2\beta^2} \quad , \tag{48}$$

so that a metal automatically satisfies the condition that the acoustic mode have zero frequency at $Q = 0$.

The translational sum rule takes the form given by Eq. (46) and is not satisfied automatically even for a metal. It therefore would place restrictions on the parameters of the model.

(c) In the general case of a metal where both intraband and interband terms contribute to $\epsilon_{S,\mathrm{el}}$

$$\epsilon_{S,\mathrm{el}} = \begin{pmatrix} \frac{\alpha'}{|Q|^2} & \frac{\beta'}{|Q|} & \frac{\beta''}{|Q|} \\ \frac{\beta'}{|Q|} & \gamma_a' & \gamma_c' \\ \frac{\beta''}{|Q|^2} & \gamma_c' & \gamma_a' \end{pmatrix} , \tag{49}$$

where

$$\alpha' = \alpha^{\mathrm{I}} + \alpha^{\mathrm{II}}|Q|^2 \quad , \quad \beta' = \beta^{\mathrm{I}} + \beta^{\mathrm{II}}|Q| \quad , \quad \beta'' = \beta^{\mathrm{I}} - \beta^{\mathrm{II}}|Q|$$

$$\gamma_a' = \gamma_a^{\mathrm{I}} + \gamma_a^{\mathrm{II}} \quad , \quad \gamma_c' = \gamma_c^{\mathrm{I}} + \gamma_c^{\mathrm{II}} \quad , \tag{50}$$

and where I, II refer to intraband and interband, respectively.

The result for $K(Q \to 0)$ is

$$K(Q)_{Q\to 0} = \frac{\Gamma_1}{\Gamma_2 \delta} (\Gamma_2 - 2\beta^{\mathrm{II}})^2 \, |Q|^2 \quad . \tag{51a}$$

where

$$\Gamma_1 = \gamma_a' + \gamma_c' \quad , \quad \Gamma_2 = \gamma_a' - \gamma_c' \quad , \quad \delta = \alpha' \Gamma_1 \Gamma_2 \; - \; 2\beta'\beta'' \Gamma_2 - (\beta' - \beta'')^2 \, \frac{(\Gamma_1 + \Gamma_2)}{2} \quad . \tag{51b}$$

The acoustic sum rule takes the form

$$0 = \frac{\Gamma_1}{\delta} \left[\Gamma_2 - 2\beta^{\mathrm{II}}\right] \, |Q|^2 \quad , \tag{52}$$

which is automatically satisfied as $Q \to 0$. The translational sum rule is

$$1 - \frac{\rho(G)}{\rho(0)} = \frac{1}{\gamma_a' - \gamma_c'} \quad , \tag{53}$$

which has the same form as Eq. (46) for the insulator and the metal.

4 Johnson Model

A well known model dielectric function for an insulator proposed by Johnson [16] is used to illuminate some of the preceding concepts. The model takes the following form

$$\epsilon^{J}_{S,\mathrm{el}}(\vec{Q}+\vec{G},\vec{Q}+\vec{G}') \;=\; \delta_{GG'} \;+\; \frac{\alpha\,\rho(\vec{G}-\vec{G}')\,\widehat{(\vec{Q}+\vec{G})}\cdot\widehat{(\vec{Q}+\vec{G}')}}{\left[1+\kappa\left(\vec{Q}+\tfrac{1}{2}\{\vec{G}+\vec{G}'\}\right)^{2}\right]^{2}} \quad , \tag{54}$$

where α, κ, and $\rho(\vec{G})$ may be regarded as parameters with the meaning that $\epsilon_{S,\mathrm{el}}(0,0) \;=\; 1+\alpha$, κ measures the extent in real space of the response to an electric field, and $\rho(\vec{G})$ is the electronic form factor normalized to $\rho(0) = 1$. We again restrict ourselves to one dimension and the set of reciprocal lattice vectors $\{0, G_0, -G_0\}$, where $G_0 = 2\pi/a$ and a is the lattice constant.

Use of $\epsilon_{S,\mathrm{el}}$ in Eq. (54) for calculating the dynamical matrix $K(Q)$ given by Eq. (23) yields

$$K(Q) \;\propto\; A + \mathcal{O}\left(Q^2\right) \tag{55}$$

as $Q \rightarrow 0$, where A is a linear combination of various $Q = 0$ matrix elements of $\epsilon_{S,\mathrm{el}}$. Furthermore, use of Eq. (54) in conjunction with the acoustic sum rule, Eq. (26), gives $A = 0$. Consequently, the phonon frequency, $\omega(Q) \;\propto\; \sqrt{K(Q)} \;\propto\; Q$ as $Q \rightarrow 0$, as expected for acoustic phonons.

For a model dielectric function like the Johnson model in Eq. (54), the electronic form factors, $\rho(G)$, are not given *a priori*, but rather are adjustable parameters. It is required, of course, that these form factors be less than or equal to $\rho(0)$ in order to guarantee that the real-space charge density, $-e\rho(r)$, is everywhere negative. Since the form factor appears in Eq. (54) as $\rho(\vec{G}-\vec{G}')$, it is necessary to consider five form factors, $\rho(0)$, $\rho(\pm G_0)$, and $\rho(\pm 2G_0)$, in our truncated reciprocal space. The normalization $\rho(0) = 1$ fixes one of the form factors, and two others are fixed by inversion symmetry: $\rho(-G_0) = \rho(G_0)$ and $\rho(-2G_0) = \rho(2G_0)$.

The two remaining form factors, $\rho(G_0)$ and $\rho(2G_0)$ are also not free to vary. In order to have a physically reasonable model for a dielectric function, it is necessary that the acoustic and translational sum rules be obeyed, and these sum rules place constraints on the electronic form factors.

Because the Johnson model defines $\epsilon_{S,\mathrm{el}}$ and not $\epsilon^{-1}_{S,\mathrm{el}}$, it is convenient to apply the sum rules in the forms given by Eqs. (29) as opposed to Eqs. (26) and (27). This convenience becomes a necessity if more reciprocal lattice vectors are added to the basis. It is simplest to use Eq. (29b)

first, with the result that $\rho(G_0)$ is a solution to the quadratic equation

$$\rho(G_0)\,(1-\rho(G_0)) = \frac{(1+\frac{1}{4}\kappa G_0^2)}{2\alpha} \quad . \tag{56}$$

We now apply Eq. (29a) which gives the same result for both $G = G_0$ and $G = -G_0$, namely,

$$1 + \frac{\alpha}{(1+\kappa G_0^2)} - \frac{2\alpha}{(1+\frac{1}{4}\kappa G_0^2)}\,\rho(G_0) + \alpha\rho(2G_0) = 0 \quad . \tag{57}$$

This equation is easily solved for $\rho(2G_0)$.

Taken together, Eqs. (56) and (57) specify the two form factors in terms of two dimensionless parameters: α and κG_0^2. These two parameters are not freely varying either, but rather are constrained by the stability requirement addressed in section 2. In particular, acceptable values of α and κG_0^2 must give eigenvalues of $\epsilon^{-1}_{S,\mathrm{TOT}}(Q+G, Q+G')$ that satisfy

$$\epsilon^{-1}_{S,\mathrm{TOT},\mu}(Q) < 1 \tag{58}$$

for all μ and Q. This constraint plus the requirement that $|\rho(G)| \leq \rho(0)$ (see above) define a region of acceptable parameters in the two-dimensional parameter space which is shown in Fig. 1.

All dots in this figure mark acceptable parameters, however they are classified into three types. Blackened squares correspond to parameters that give eigenvalues of $\epsilon^{-1}_{S,\mathrm{el}}$ which are between 0 and 1 for all Q. This condition is not rigidly required by the theory, and as Fig. 1 shows, it places a severe constraint on the acceptable region of parameter space. However, it is worth pointing out that the RPA dielectric function does satisfy this condition. Therefore, a model which violates it is exhibiting non- RPA-like behavior. It is possible to modify the Johnson model slightly so that this condition on the eigenvalues of $\epsilon^{-1}_{S,\mathrm{el}}$ is automatically obeyed, as will be discussed later.

Crosses in Fig. 1 correspond to parameters which give at least one negative eigenvalue of $\epsilon^{-1}_{S,\mathrm{el}}$, but still none that are greater than one. This category clearly represents the largest portion of acceptable parameters in this model. Finally, unblackened squares denote parameters for which an eigenvalue of $\epsilon^{-1}_{S,\mathrm{el}}$ exceeds one for at least some range of Q. It was shown in section 2.H that this situation is actually allowed for a stable system, however this model suggests (not surprisingly) that it is rare. Section 2.H also showed that it is *not* possible to have a stable system if the lattice is unstable (*i.e.*, the dynamical matrix is not positive). This is borne out by the Johnson model in that the dynamical matrix is positive for all Q for all acceptable parameters.

It is interesting to see how physical quantities differ in the different regions of acceptable parameters. Figure 2 shows phonon frequency vs. wave vector for two choices of parameters.

The units are chosen such that $\omega = K^2$, where K is the dynamical matrix (or number, since this is a one-dimensional model) defined in Eq. (23). In Fig. 2(a) and 2(b), the parameters are $\alpha = 9$, $\kappa G_0^2 = 3.16$ and $\alpha = 4$, $\kappa G_0^2 = 0.22$, respectively. These parameters correspond to crosses and blackened squares, respectively, in Fig. 1. Both phonon dispersion curves vanish linearly as $Q \rightarrow 0$ as a result of the acoustic sum rule. Figure 2(a) exhibits a higher speed of sound than Fig. 2(b), which is primarily due to the higher value of α in the former. The dispersion curve in Fig. 2(b) remains linear throughout the Brillouin zone. This unphysical behavior is caused by the small value of κG_0^2, which makes the terms quadratic or higher-order in Q much smaller than the linear term over a large range of Q. Since all the parameters that give only positive eigenvalues of $\epsilon_{S,\mathrm{el}}^{-1}$ (*i.e.*, blackened squares in Fig. 1) have small values of κG_0^2, they will all produce unphysical phonon dispersion curves. We can conclude that this model is necessarily non-RPA-like, since the only physically reasonable choices of parameters produce electronic dielectric functions with a negative eigenvalue.

Bragg scattering of waves in crystals results in a flattening of dispersion curves at the boundary of the Brillouin żone (BZ). Therefore, the fact that this behavior is not seen in Fig. 2 is cause for concern. It can be shown, however, that phonon dispersion curves calculated using Eq. (23) do approach the BZ edge with zero derivative assuming all (infinitely many) reciprocal lattice vectors are used in the calculation. This result is obtained by showing (a) that $K_{\alpha\beta}(\vec{Q}) = K_{\alpha\beta}(-\vec{Q})$, and (b) that $K_{\alpha\beta}(\vec{Q} + \vec{G}) = K_{\alpha\beta}(\vec{Q})$, if all reciprocal lattice vectors are included. Thus, the unphysical behavior of Fig. 2 near the BZ edge can be attributed to truncating the reciprocal space basis.

Figures 3(a) and 3(b) display the Q dependence of the eigenvalues of $\epsilon_{S,\mathrm{el}}$ and $\epsilon_{S,\mathrm{TOT}}$ for the same two sets of parameters as in Fig. 2. By construction one of the eigenvalues of $\epsilon_{S,\mathrm{el}}$ in Fig. 3(a) is negative, whereas none are negative in Fig. 3(b). Figure 3 illustrates the result discussed in section 2.G, namely, that $\epsilon_{S,\mathrm{TOT}}$ has a negative eigenvalue which vanishes as $Q \rightarrow 0$. In Fig. 3(a) there is also a second negative eigenvalue of $\epsilon_{S,\mathrm{TOT}}$, but this one does not vanish and is unrelated to the result of section 2.G. It is more closely related to the behavior of the negative eigenvalue of $\epsilon_{S,\mathrm{el}}$, but this relationship has not been investigated. The curves in Fig. 3(b) show fairly uninteresting dispersion (mainly of quadratic order) which, again, is due to the small value of κG_0^2.

It is natural to ask whether adding more reciprocal lattice vectors to the basis would make

the model more flexible; i.e., allowing a larger parameter space for which $\epsilon^{-1}_{S,\mathrm{TOT}} < 1$. We have done calculations for the one-dimensional Johnson model including five G's, $\{0, \pm G_0, \pm 2G_0\}$, and seven G's, $\{0, \pm G_0, \pm 2G_0, \pm 3G_0\}$, and have found, conversely, that the model becomes *less* flexible as the basis increases. That is, the region in parameter space which both satisfies the sum rules and gives a stable system becomes increasingly small. One explanation is that the number of constraints increases more rapidly than the number of adjustable parameters as G's, are added. Each time a pair of G-vectors is added to the basis, two new form factors are added as parameters. For example, in going from $\{0, \pm G_0\}$ to $\{0, \pm G_0, \pm 2G_0\}$, the form factors $\rho(3G_0)$ and $\rho(4G_0)$ become parameters. However, *three* new constraints are added. One is from the sum rule in Eq. (29) for $G = 2G_0$ (the $G = -2G_0$ equation is the same), which fixes the value of one of the new form factors. The other two constraints come from the fact that there are two additional eigenvalues of $\epsilon^{-1}_{S,\mathrm{TOT}}$ which must be less than unity for system stability. This difficulty again illustrates the significant role of the sum rules.

As stated above, it is possible to modify the Johnson model slightly so that the eigenvalues of $\epsilon^{-1}_{S,\mathrm{el}}$ are guaranteed to be positive. This is useful if one wishes to avoid un-RPA-like behavior. If a dielectric function has the form

$$\epsilon_{S,\mathrm{el}}(Q+G, Q+G') = \delta_{G,G'} + f^*(Q+G) \cdot \rho(G-G') \cdot f(Q+G') \quad , \tag{59}$$

where f is any function, then it is easy to show that $\langle \nu | \epsilon_{S,\mathrm{el}} | \nu \rangle > 0$ for any vector $|\nu\rangle$. In particular, if $|\nu\rangle$ is an eigenvector of $\epsilon^{-1}_{S,\mathrm{el}}$, then this shows that all eigenvalues are positive. We call an electronic dielectric function of this form separable. The RPA dielectric function (Eq. (15)), for example, is separable. By choosing f to be

$$f(Q+G) = \frac{\sqrt{\alpha}}{1+\kappa(Q+G)^2} \cdot \widehat{(Q+G)} \quad , \tag{60}$$

the resulting separable dielectric function is very similar to the Johnson dielectric function, and, in fact, is identical to it along the diagonal. Physical quantities calculated using this electronic dielectric function behave similarly to those using the Johnson model.

5 Conclusions

We have studied the total dielectric function, which includes the lattice response as well as the electronic response of the solid. The focus has been on the possibility of an attractive interaction between two test charges as is required for superconductivity. A necessary condition for an attractive interaction is that the total static dielectric function have at least one negative eigenvalue. We have shown that there are an odd number of negative eigenvalues for one and three spatial dimensions and zero or an even number for two dimensions. We have also shown that it is highly plausible that there is one negative eigenvalue for each dimension of the system.

It is also required that the system be stable. The condition for this is that the eigenvalues, $\epsilon^{-1}_{S,\mathrm{TOT},\mu}$, of the total inverse dielectric function, must satisfy $\epsilon^{-1}_{S,\mathrm{TOT},\mu} < 1$. We have shown that the solid will be stable if the electronic and lattice portions of the system are individually stable; i.e., $\epsilon^{-1}_{S,el,\eta} < 1$, where $\epsilon^{-1}_{S,el,\eta}$ are the eigenvalues of the inverse electronic dielectric function, and the phonon frequencies are real. It is also *possible* to have a stable system if the electronic portion, regarded as an isolated system, is unstable provided the lattice portion is stable. However, if the lattice is unstable then the entire solid must also be unstable.

We have also derived a sum rule, the translational sum rule, that is analogous to the acoustic sum rule; it also places restrictions on components of the inverse electronic dielectric function. Unlike the acoustic sum rule, the translational sum rule is important for the case of a metal as well as an insulator. In addition we have recast the acoustic and translational sum rules in terms of components of the electronic dielectric function rather than its inverse. This is convenient because most theories give expressions for the dielectric function, not its inverse.

Finally, we have presented numerical results for a one-dimensional model dielectric function. The phonon spectrum and the eigenvalues of the total dielectric function are then calculated in order to make the formalism more concrete as well as to demonstrate the importance of the sum rules in restricting the parameters of models.

Acknowledgments

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Appendix A

The result $(\epsilon_{\rm el}^{-1})_\mu < 1 + \Gamma_\mu$ where $\Gamma_\mu > 0$ and $(\epsilon_{\rm el}^{-1})_\mu$ is an eigenvalue of $\epsilon_{\rm el}^{-1}$ is proved below. From Eq. (19),

$$\epsilon^{-1}_{S,\rm TOT} \;=\; \epsilon^{-1}_{S,\rm el} \;+\; \sum_{\alpha\beta} \langle \varphi^s_\alpha |\; D_{\alpha\beta} \;| \varphi^s_\beta \rangle \tag{A.1}$$

and D is given by Eq. (21). Let $\epsilon^{-1}_{S,el,\mu}$ and $\epsilon^{-1}_{S,\rm TOT,\nu}$ be eigenvalues of $\epsilon^{-1}_{S,\rm el}$ and $\epsilon^{-1}_{S,\rm TOT}$, respectively. Equation (A.1) may be written as

$$\sum_\nu |\langle \mu | \nu \rangle|^2 \, \epsilon^{-1}_{S,\rm TOT,\nu} \;=\; \epsilon^{-1}_{S,el,\mu} \;-\sum_j \frac{1}{\omega^2_{Qj}} \left| \sum_\alpha \langle \mu |\, \varphi^s_\alpha \rangle \; \hat{\alpha} \cdot \vec{\eta}_{Qj} \right|^2 \tag{A.2}$$

where $\omega = 0$ in Eq. (21), $|\nu\rangle$ and $|\mu\rangle$ are eigenfunctions of $\epsilon^{-1}_{S,\rm TOT}$ and $\epsilon^{-1}_{S,\rm el}$, respectively, $|\vec{\eta}_{Qj}\rangle$ is an eigenvector of $K_{\alpha\beta}$ and ω^2_j is the corresponding eigenvalue. Using $\epsilon^{-1}_{S,\rm TOT,\nu} < 1$ for all ν leads to

$$\epsilon^{-1}_{S,el,\mu} \;<\; 1 + \sum_j \frac{1}{\omega^2_{Qj}} \left| \sum_\alpha \langle \mu |\, \varphi^s_\alpha \rangle \; \hat{\alpha} \cdot \vec{\eta}_{Qj} \right|^2 \;\equiv\; 1 + \Gamma_\mu \quad . \tag{A.3}$$

Appendix B

Equation (25) is derived as follows. Following ref. 13 the matrix ϵ^{-1} can be written in the form

$$\epsilon^{-1} = \begin{pmatrix} \left(\epsilon^{-1}_{QQ}\right) & \left(\epsilon^{-1}_{Q,Q+G}\right) \\ \left(\epsilon^{-1}_{Q+G,Q}\right) & \left(\epsilon^{-1}_{Q+G,Q+G'}\right) \end{pmatrix} \tag{B.1}$$

where $\left(\epsilon^{-1}_{QQ}\right)$ is a 1×1 matrix, $\left(\epsilon^{-1}_{Q,Q+G}\right)$ is a $1 \times n$ matrix where there are n non-zero values of G, and $\left(\epsilon^{-1}_{Q+G,Q+G'}\right)$ is a $n \times n$ matrix. Use of Eq. (5.11) from Ref. 13 yields

$$\left(\epsilon^{-1}_{Q+G,Q+G'}\right) = \left(S^{-1}_{Q+G,Q+G'} + \epsilon^{-1}_{Q+G,Q} \frac{1}{\epsilon^{-1}_{QQ}} \epsilon^{-1}_{Q,Q+G'}\right) \tag{B.2}$$

where S^{-1} is defined immediately after Eq. (23) in our text. Using Eqs. (B.1) and (B.2) in Eq. (23), and the fact that ϵ^{-1} is Hermitian yields Eq. (25).

Appendix C: Derivation of the Translational Sum Rule

To derive the translational sum rule (Eq. 27), suppose that the entire lattice is rigidly translated by a small amount η in the $\hat{\beta}$ direction. For the present purposes we consider only a primitive lattice, however the results are easily generalized to a lattice with a basis. The resulting perturbation in the lattice potential,

$$V(\vec{r}) = \sum_l \frac{Ze^2}{|\vec{r} - \vec{R}_l|} \quad , \tag{C.1}$$

where Z is the nuclear charge and $\vec{R}_l$ is a lattice vector, is given by

$$\delta V(\vec{r}) = V(\vec{r} - \eta\hat{\beta}) - V(\vec{r}) = -\eta \frac{\delta V}{\delta r_\beta} \quad . \tag{C.2}$$

Since the perturbation is (trivially) periodic in the lattice, we may Fourier transform both sides of Eq. (C.2) to give

$$\delta V(\vec{G}) = -i\, G_\beta\, \eta\, V(\vec{G}) \quad , \tag{C.3}$$

where $\vec{G}$ is a vector in the reciprocal lattice. The electronic charge density $\rho(\vec{r})$ will also be rigidly translated by $\eta\hat{\beta}$ so that, in analogy with Eq. (C.3),

$$\delta\rho(\vec{G}) = -i\, G_\beta\, \eta\, \rho(\vec{G}) \quad . \tag{C.4}$$

The perturbation $\delta\rho(\vec{G})$ is a response to the perturbation $\delta V(\vec{G})$, and therefore the two quantities are related, within linear response theory, by

$$\delta\rho(\vec{G}) = \sum_{\vec{G}'} \chi(\vec{G}, \vec{G}')\, \delta V(\vec{G}') \quad , \tag{C.5}$$

where χ is the electronic susceptibility. Combining Eqs. (C.3)– (C.5) yields

$$G_\beta\, \rho(\vec{G}) = \sum_{\vec{G}'} \chi(\vec{G}, \vec{G}')\, G'_\beta\, V(\vec{G}') = \sum_{\vec{G}'} \chi(\vec{G}, \vec{G}')\, \frac{4\pi Ze^2}{G'^2}\, G'_\beta \quad . \tag{C.6}$$

For reduced wave vector $Q = 0$, only the $\vec{G}, \vec{G}' \neq 0$ components of the response functions are relevant, and

$$S_{\rm el}^{-1}(\vec{G}, \vec{G}') = \delta_{\vec{G},\vec{G}'} + \frac{4\pi e^2}{G^2}\, \chi(\vec{G}, \vec{G}') \quad , \tag{C.7}$$

where $S_{\rm el}^{-1}$ is related to $\epsilon_{\rm el}^{-1}$ as described in the text following Eq. (23). Thus, Eq. (C.6) becomes

$$\left(1 - \frac{\rho(\vec{G})}{\rho(0)}\right) \frac{G_\beta}{G^2} = \sum_{\vec{G}'} S_{\rm el}^{-1}(\vec{G}, \vec{G}')\, \frac{G'_\beta}{G'^2} \quad , \tag{C.8}$$

where we have made use of the fact that $Z = -\rho(0)$ (*i.e.*, charge neutrality). Finally, if symmetric notation is used (see section 2.B), the translational sum rule as given in Eq. (27) results.

Appendix D: Re-write Sum Rules in Terms of ϵ

The acoustic and translational sum rules (Eqs. (26) and (27), respectively) are written in terms of $\epsilon^{-1}_{S,\mathrm{el}}$. Since model calculations usually define the dielectric function and not its inverse, it is convenient to recast the sum rules in terms of $\epsilon_{S,\mathrm{el}}$. Before doing this it is useful to express $\epsilon_{S,\mathrm{el}}$ and $\epsilon^{-1}_{S,\mathrm{el}}$ as

$$\epsilon_{S,\mathrm{el}}(Q+G,Q+G') = \begin{pmatrix} P & R \\ Q & S \end{pmatrix} \tag{D.1}$$

and

$$\epsilon^{-1}_{S,\mathrm{el}}(Q+G,Q+G') = \begin{pmatrix} W & Y \\ X & Z \end{pmatrix} \quad , \tag{D.2}$$

where P, Q, R, and S are 1×1, $n\times1$, $1\times n$, and $n\times n$ arrays, respectively, corresponding to $\epsilon_{S,\mathrm{el}}(Q,Q)$, $\epsilon_{S,\mathrm{el}}(Q+G,Q)$, $\epsilon_{S,\mathrm{el}}(Q,Q+G')$, and $\epsilon_{S,\mathrm{el}}(Q+G,Q+G')$, $(G,G' \neq 0)$, respectively. W, X, Y, and Z are similarly defined. This is the same notation used by Pick, *et al.* [13] in their Eq. (5.9).

If we now define two $n\times1$ vectors $|u_\alpha\rangle$ and $|c_\alpha\rangle$ such that

$$|u_\alpha\rangle_i = \widehat{(Q+G_i)}_\alpha \quad \text{and} \quad |c_\alpha\rangle_i = \left(1 - \frac{\rho(G_i)}{\rho(0)}\right) \widehat{(Q+G_i)}_\alpha \tag{D.3}$$

for $G_i \neq 0$, then it is clear that the acoustic and translational sum rules can be written, in the limit $Q \to 0$, as

$$W\hat{Q}_\alpha + \langle Y|u_\alpha\rangle = 0 \tag{D.4}$$

and

$$S^{-1}\,|u_\alpha\rangle = |c_\alpha\rangle \quad , \tag{D.5}$$

respectively. Inverting Eq. (D.5) gives $|u_\alpha\rangle = S|c_\alpha\rangle$, or

$$\sum_{G'\neq0} \left(\epsilon_{S,\mathrm{el}}(\vec{G},\vec{G}') \cdot \left(1 - \frac{\rho(G')}{\rho(0)}\right) \cdot \widehat{G'}_\alpha\right) = \hat{G}_\alpha \quad , \quad (G \neq 0) \quad . \tag{D.6}$$

It is easy to verify (see Eq. (5.10) of Ref. 13) that

$$\langle Y| = -W\langle R|S^{-1} \quad . \tag{D.7}$$

Substituting this into Eq. (D.4) and applying the translational sum rule yields

$$\lim_{Q\to0}\left[W\hat{Q}_\alpha - W\langle R|S^{-1}|u_\alpha\rangle\right] = \lim_{Q\to0}\left[W\cdot(\hat{Q}_\alpha - \langle R|c_\alpha\rangle)\right] = 0 \quad . \tag{D.8}$$

If the system is metallic, then $W \to 0$ as $Q \to 0$, and Eq. (D.8) contains no additional information. However, for an insulator, W remains finite as $Q \to 0$, and therefore Eq. (D.8) states that $\langle R|c_\alpha\rangle \to 1$ as $Q \to 0$, or

$$\lim_{Q\to 0} \sum_{G\neq 0} \left(\epsilon_{S,\mathrm{el}}(Q, Q+G) \cdot \left(1 - \frac{\rho(G)}{\rho(0)}\right) \cdot \widehat{(Q+G)}_\alpha\right) = \widehat{Q}_\alpha \tag{D.9}$$

Equations (D.6) and (D.9) are the sum rules recast in terms of $\epsilon_{S,\mathrm{el}}$.

Appendix E: Proof of Theorem about Sign of Eigenvalues of $\epsilon^{-1}_{S,\mathrm{TOT}}$

In this Appendix we prove the theorem described in section 2.G (here referred to as Theorem I); namely, that the $\omega = 0$ value of $\epsilon^{-1}_{S,\mathrm{TOT}}$ has an odd number of negative eigenvalues for one and three spatial dimensions (or, for that matter, any odd number of dimensions) and zero or an even number of negative eigenvalues for two (or any even number) dimensions. It is sufficient to prove that

$$\det(\epsilon^{-1}_{S,\mathrm{TOT}}) = (-1)^d \det(\epsilon^{-1}_{S,\mathrm{el}}) \cdot \frac{\det(-K^0)}{\det(K)} \quad , \tag{E.1}$$

where $\epsilon^{-1}_{S,\mathrm{TOT}}$ and $\epsilon^{-1}_{S,\mathrm{el}}$ are, in general, countably-infinite dimensional matrices labeled by the reciprocal lattice vectors, $\vec{G}$ and $\vec{G}'$, and K (the dynamical matrix) and K^0 are $d\times d$ matrices labeled by d-dimensional Cartesian coordinates. Theorem I then follows from Eq. (E.1). Both $\det(K)$ and $\det(-K^0)$ are positive because their eigenvalues must all be positive. This follows from the stability of the lattice. Furthermore, within the random phase approximation (RPA), the eigenvalues of $\epsilon^{-1}_{S,\mathrm{el}}$ are all positive [4], and thus $\det(\epsilon^{-1}_{S,\mathrm{el}})$ is positive. Therefore, Eq. (E.1) says that the RPA value of $\det(\epsilon^{-1}_{S,\mathrm{TOT}})$ is negative (positive) if d is odd (even), from which we conclude that $\epsilon^{-1}_{S,\mathrm{TOT}}$ has an odd (zero or even) number of negative eigenvalues.

The most straightforward approach is to prove Eq. (E.1) for one dimension (d=1) and then generalize to higher dimensions. We start by defining some convenient notation. Define an $n\times n$ matrix B so that $B^2 = \epsilon^{-1}_{S,\mathrm{el}}$ (n is the dimension of $\epsilon^{-1}_{S,\mathrm{el}}$) and also an $n\times 1$ vector $|u\rangle$ whose ith component is

$$|u\rangle_i = (\widehat{Q + G_i}) \quad , \tag{E.2}$$

where G_i is the ith reciprocal lattice vector. From these we define another $n\times 1$ vector $|v\rangle$ by $|v\rangle = B|u\rangle$, and, finally, a symmetric $n\times n$ matrix N by

$$N = I - \left(\frac{4\pi e^2 Z^2}{\Omega}\right) |v\rangle K^{-1} \langle v| \quad , \tag{E.3}$$

where I is the $n\times n$ identity matrix. Using these definitions, $\epsilon^{-1}_{S,\mathrm{TOT}}$ and K can be written succinctly as [see Eqs. (19), (21), (23), and (28)]

$$\epsilon^{-1}_{S,\mathrm{TOT}} = B\,N\,B \tag{E.4}$$

$$K = \left(\frac{4\pi e^2 Z^2}{\Omega}\right) \langle v|v\rangle + K^0 \quad . \tag{E.5}$$

Taking the determinant of both sides of Eq. (E.4) gives

$$\det(\epsilon^{-1}_{S,\mathrm{TOT}}) = [\det(B)]^2 \cdot \det(N) = \det(\epsilon^{-1}_{S,\mathrm{el}}) \cdot \det(N) \tag{E.6}$$

Therefore, we must examine $\det(N)$ in order to prove Eq. (E.1). Using Eqs. (E.3) and (E.5) it is evident that $|v\rangle$ is an eigenvector of N with eigenvalue K^0/K. Furthermore, all other eigenvalues of N are unity. This follows from the fact that all eigenvectors of N are mutually orthogonal since N is symmetric. Thus, if $|w\rangle$ is an eigenvector of N other than $|v\rangle$, then

$$N|w\rangle = |w\rangle - \frac{\langle v|w\rangle}{K}|v\rangle = |w\rangle \quad . \tag{E.7}$$

This implies that

$$\det(N) = \left(\frac{K_0}{K}\right) \cdot 1 \cdot \cdots \cdot 1 = \left(\frac{K_0}{K}\right) \quad , \tag{E.8}$$

which, with Eq. (E.6), proves Eq. (E.1) for d=1.

Extending this proof to multiple spatial dimensions introduces the complication of having to deal with two different vector spaces — the n-dimensional Fourier space in which the dielectric function is represented and the d-dimensional Cartesian space. In particular, K and K^0 are now $d\times d$ matrices and not numbers. We now must define $|u\rangle$ and $|v\rangle$ to be $n\times d$ arrays, where the component $|u\rangle_{i\alpha}$ is

$$|u\rangle_{i\alpha} = \widehat{(Q+G)}_\alpha \tag{E.9}$$

and Q and G are the αth Cartesian component of $\vec{Q}$ and $\vec{G}_i$, respectively. The definition $|v\rangle = B|u\rangle$ still holds. With these new definitions of $|u\rangle$ and $|v\rangle$, Eqs. (E.3)–(E.6) remain formally the same, and the task of proving Eq. (E.1) again reduces to examining $\det(N)$.

It is straightforward to show using Eq. (E.3) that

$$N|v\rangle = -|v\rangle\, K^{-1}\,(-K^0) = -|v\rangle\, T \quad , \tag{E.10}$$

where T is the $d\times d$ matrix $T = K^{-1}\,(-K^0)$. Suppose U is the matrix that diagonalizes T. Multiplying both sides of Eq. (E.10) on the right by U leads to

$$N|v'\rangle = -|v'\rangle\, U^{-1}\, T\, U = -|v'\rangle \begin{pmatrix} \tau_1 & & \\ & \ddots & \\ & & \tau_d \end{pmatrix} \quad , \tag{E.11}$$

where $|v'\rangle = |v\rangle\, U$, and $\tau_1, \ldots, \tau_d$ are the eigenvalues of T. This implies that the columns of $|v'\rangle$ are eigenvectors of N with eigenvalues $-\tau_1, \ldots, -\tau_d$, respectively. Furthermore, as before, all other eigenvalues of N are unity. Thus, $\det(N)$ is given by

$$\begin{aligned} \det(N) &= (-\tau_1)\cdot\cdots\cdot(-\tau_d)\cdot 1\cdot\cdots\cdot 1 = (-1)^d\cdot\tau_1\cdot\cdots\cdot\tau_d \\ &= (-1)^d\cdot\det(T) = (-1)^d\cdot\left(\frac{\det(-K^0)}{\det(K)}\right) \quad . \end{aligned} \tag{E.12}$$

This result, with Eq. (E.6), proves Eq. (E.1) and thus proves Theorem I.

Appendix F

Equation (36) is proved in this appendix. Use of Eq. (17) in Eq. (18) in the limit $\omega = 0$ and $Q = 0$ gives

$$\epsilon_{S,\mathrm{TOT}}(\vec{G},\vec{G}') = \epsilon_{\mathrm{el}}(\vec{G},\vec{G}') + \frac{4\pi e^2 Z^2 N}{\Omega} \sum_{\alpha\beta} \hat{G}_\alpha (K^0)^{-1}_{\alpha\beta} \hat{G}'_\beta \quad . \tag{F.1}$$

Multiplying both sides of Eq. (F.1) by $\left(1 - \rho(\vec{G}')/\rho(0)\right) \hat{G}'_\gamma$ and summing over $\vec{G}' \neq 0$ gives

$$\sum_{G'\neq 0} \epsilon_{S,\mathrm{TOT}}(\vec{G},\vec{G}') \left(1 - \frac{\rho(\vec{G}')}{\rho(0)}\right) \hat{G}'_\gamma = \sum_{G'\neq 0} \epsilon_{S,\mathrm{el}}(\vec{G},\vec{G}') \left(1 - \frac{\rho(\vec{G}')}{\rho(0)}\right) \hat{G}'_\gamma$$

$$+ \frac{4\pi e^2 Z^2 N}{\Omega} \sum_{\alpha\beta} (K^0)^{-1}_{\alpha\beta} \hat{G}_\alpha \sum_{G'\neq 0} \hat{G}'_\beta \left(1 - \frac{\rho(\vec{G}')}{\rho(0)}\right) \hat{G}'_\gamma \quad . \tag{F.2}$$

From Eq. (29a) the first term on the right-hand side of Eq. (F.2) is $\vec{G}_\gamma$. Making use of Eq. (28) gives the value $-\vec{G}_\gamma$ for the second term on the right-hand side of Eq. (F.2) which proves Eq. (36).

Appendix G

It is shown that there is an eigenvalue of $\epsilon_{S,\mathrm{TOT}}$ that vanishes at the phonon frequencies. Use of Eq. (17) in Eq. (18) gives

$$\epsilon_{S,\mathrm{TOT}} \;=\; \epsilon_{S,\mathrm{el}} \;-\; \frac{4\pi\, e^2\, Z^2}{\Omega} \sum_{\alpha\beta} |u\rangle_\alpha \, [M\,\omega^2 - K^0]^{-1}_{\alpha\beta} \, \langle u_\beta| \tag{G.1}$$

where $\epsilon_{S,\mathrm{TOT}}$, $\epsilon_{S,\mathrm{el}}$, $|u\rangle_\alpha$, and $|u\rangle_\beta$ are matrices with indices $\vec{Q}+\vec{G}$; ϵ is $(n\times n)$ while $|u\rangle_\alpha$ is $(n\times 1)$ and $|u\rangle_\beta$ is $(1\times n)$. The latter two matrices are defined in Appendix E. Multiplying both sides of Eq. (G.1) by $\epsilon^{-1}_{S,\mathrm{el}}|u\rangle_\gamma$ gives

$$\epsilon_{S,\mathrm{TOT}}\; \epsilon^{-1}_{S,\mathrm{el}}\; |u\rangle_\gamma \;=\; |u\rangle_\gamma \;-\; \sum_{\alpha\beta} |u\rangle_\alpha \, \Big([M\,\omega^2 - K^0]^{-1}\, [K(Q) - K^0] \Big)_{\alpha\gamma} \tag{G.2}$$

where use has been made of Eqs. (23) and (28),

$$K_{\alpha\beta}(Q) \;=\; \frac{4\pi\, e^2\, Z^2}{\Omega} \, \langle u_\alpha|\, \epsilon^{-1}_{S,\mathrm{el}}\, |u_\beta\rangle \;+\; K^0_{\alpha\beta} \quad . \tag{G.3}$$

One can write

$$M\,\omega^2 - K(Q) \;=\; \sum_k \eta^*_j(Q) \, \left(\omega^2 - \omega^2_{Qj}\right) \, \eta_j(Q) \tag{G.4}$$

where $\eta_j(Q)$ and ω^2_{Qj} are the eigenfunctions and eigenvalues of $K(Q)$. Use of Eq. (G.4) in (G.2) gives

$$\epsilon_{S,\mathrm{TOT}}\; \epsilon^{-1}_{S,\mathrm{el}}\; |u\rangle_\gamma \;=\; \sum_\alpha |u_\alpha\rangle \, \left([M\,\omega^2 - K^0]^{-1} \sum_j \eta^*_j(Q) \, \left(\omega^2 - \omega^2_{Qj}\right) \, \eta_j(Q) \right)_{\alpha\gamma} \quad . \tag{G.5}$$

If γ denotes a direction parallel to $\eta_j(Q)$ then $\epsilon_{S,\mathrm{TOT}}\; \epsilon^{-1}_{S,\mathrm{el}}\; |u\rangle_\gamma = 0$ if $\omega^2 = \omega^2_{Qj}$ as stated in Eq. (37), since $\varphi^S_\alpha = \epsilon^{-1}_{S,\mathrm{el}}\; |u\rangle_\alpha$.

Figure Captions

Figure 1: Parameters α and κG_0^2 which satisfy the sum rules and the stability requirements for the truncated, one-dimensional Johnson model (Eq. (54)). Points denoted by blackened squares give eigenvalues of $\epsilon_{S,\mathrm{el}}^{-1}$ which are all between 0 and 1 for all Q. Crosses imply that some eigenvalue of $\epsilon_{S,\mathrm{el}}^{-1}$ is negative, but none are greater than 1, and unblackened boxes imply that, for some range of Q, an eigenvalue of $\epsilon_{S,\mathrm{el}}^{-1}$ exceeds unity. (b) is a higher resolution plot of the boxed region in (a).

Figure 2: Phonon dispersion curves calculated using the parameters (a) $\alpha = 9$, $\kappa G_0^2 = 3.16$ and (b) $\alpha = 4$, $\kappa G_0^2 = 0.22$. The units of frequency are chosen such that $\omega^2 = K$, where K is the dynamical matrix (or number in one-dimension) calculated using Eq. (23). Wave vectors are given in units of $G_0 = 2\pi/a$, where a is the lattice constant.

Figure 3: Eigenvalues of $\epsilon_{S,\mathrm{el}}$ and $\epsilon_{S,\mathrm{TOT}}$ vs. wave vector calculated using the parameters (a) $\alpha = 9$, $\kappa G_0^2 = 3.16$ and (b) $\alpha = 4$, $\kappa G_0^2 = 0.22$, the same as in Fig. 2. Recall that an eigenvalue of ϵ is the reciprocal of an eigenvalue of ϵ^{-1}. Wave vectors are given in units of $G_0 = 2\pi/a$, where a is the lattice constant.

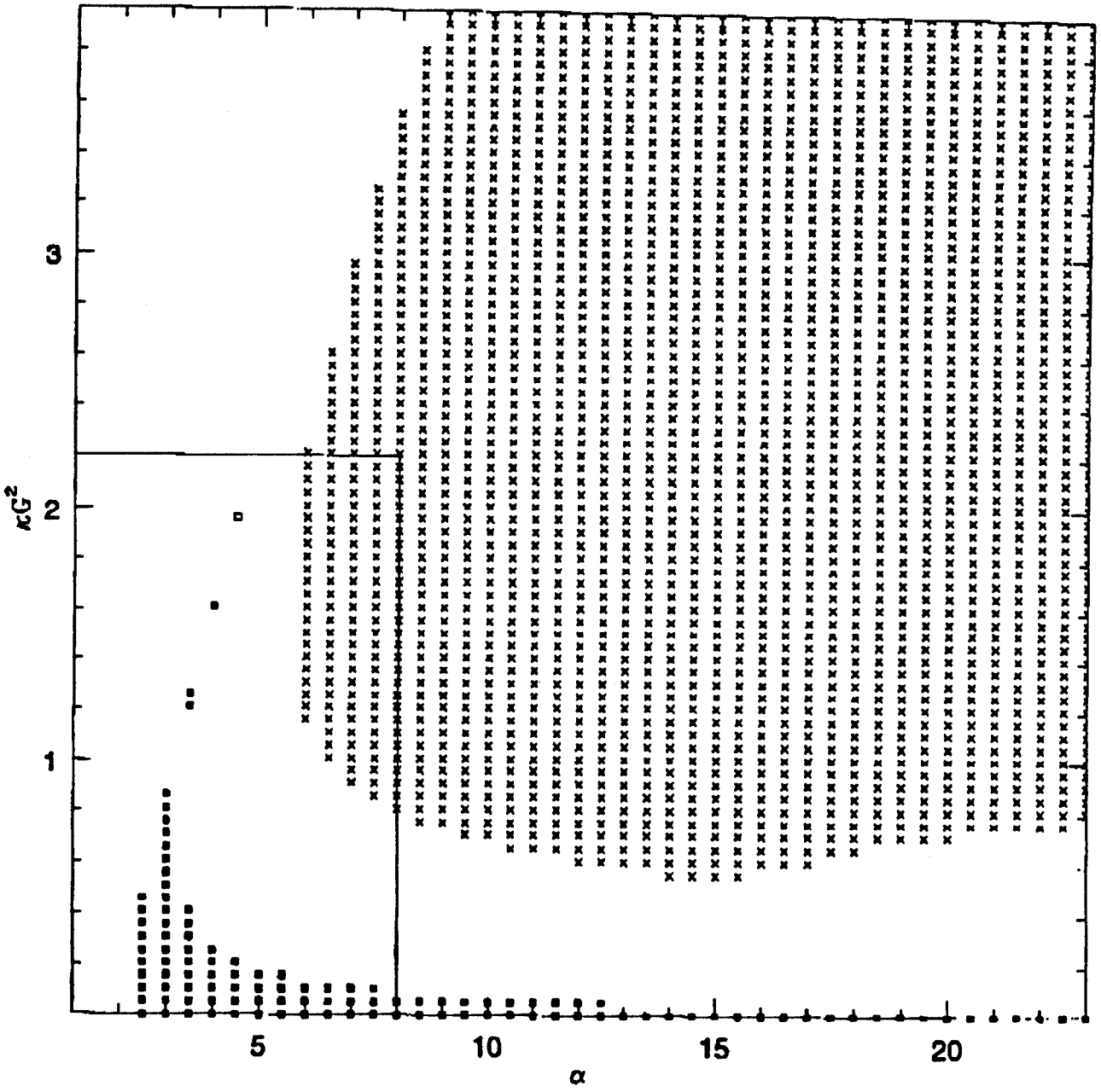

FIG. 1(a)

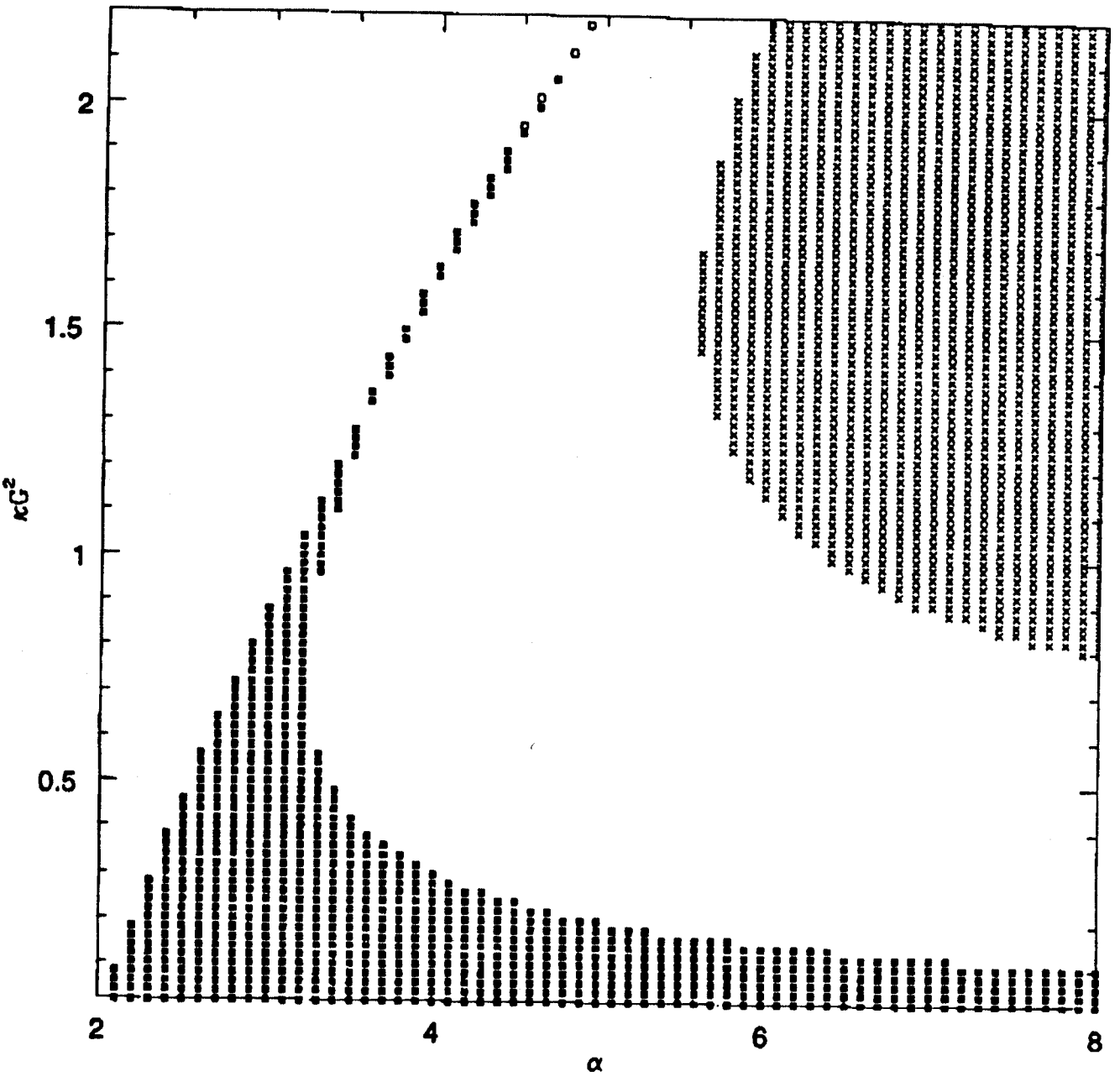

FIG. 1(b)

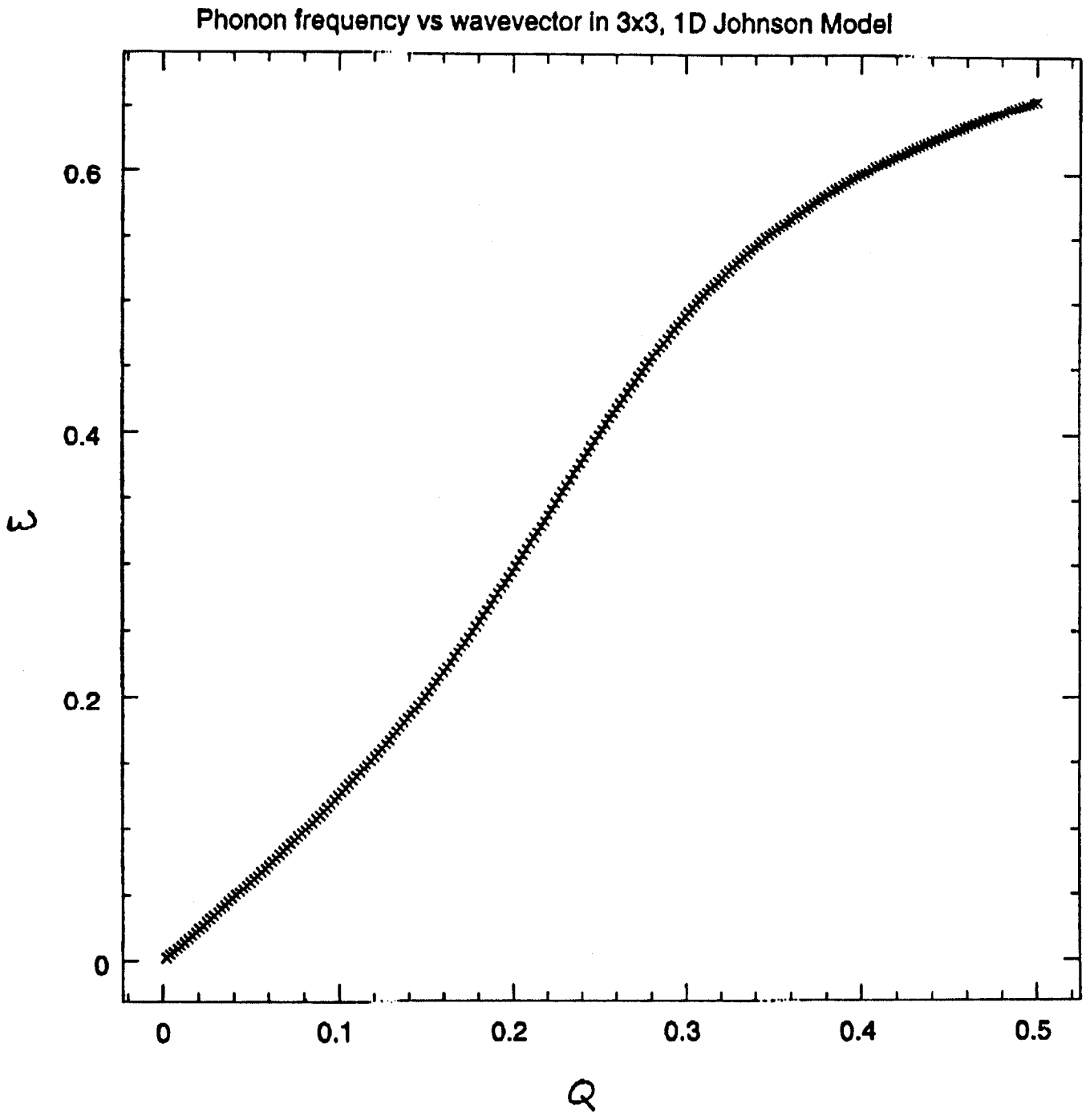

FIG. 2(a)

$\alpha = 9$, $KG^2 = 3.16$

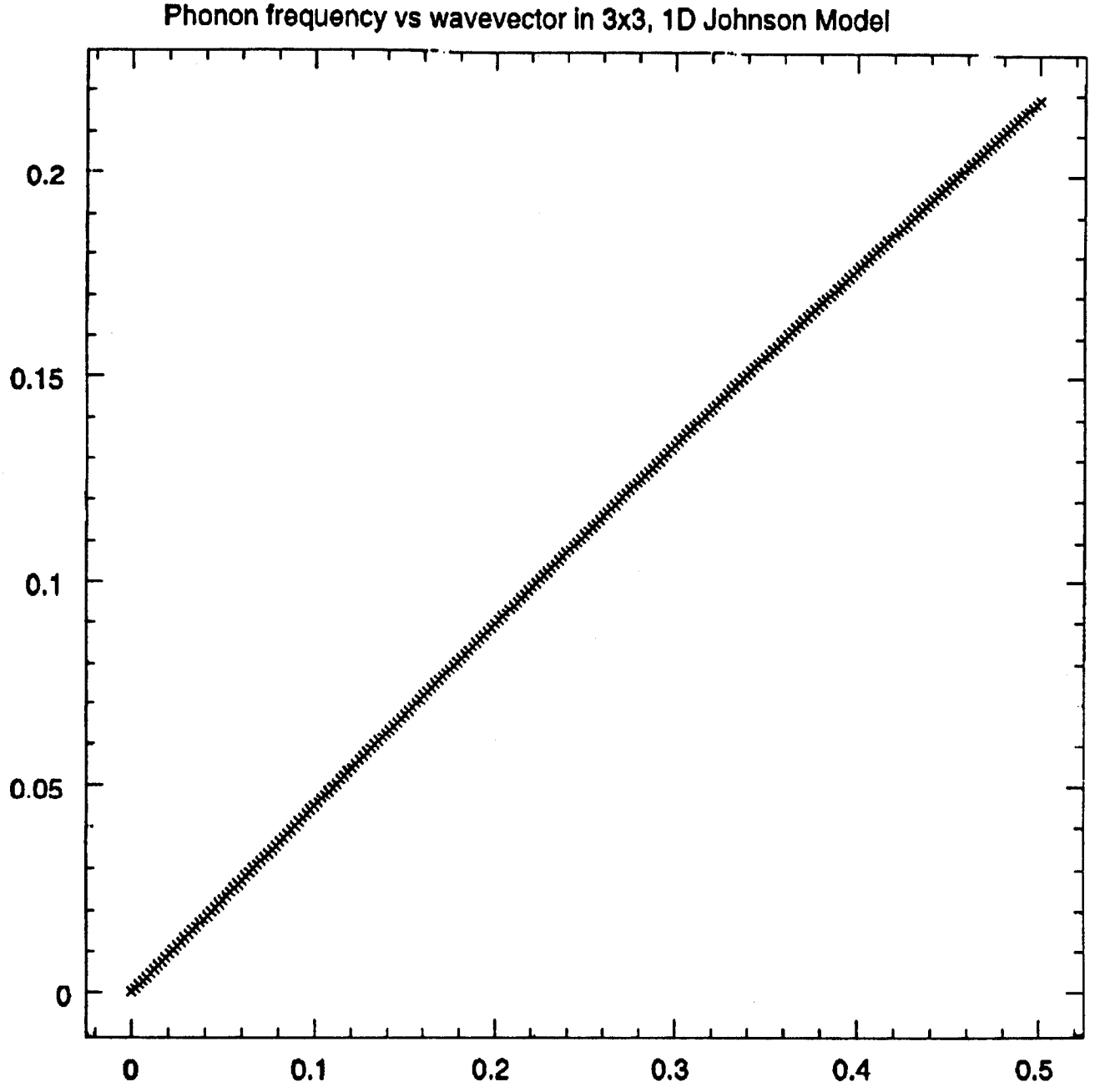

FIG. 2(b)

$\alpha = 4, \quad KG^2 = 0.22$

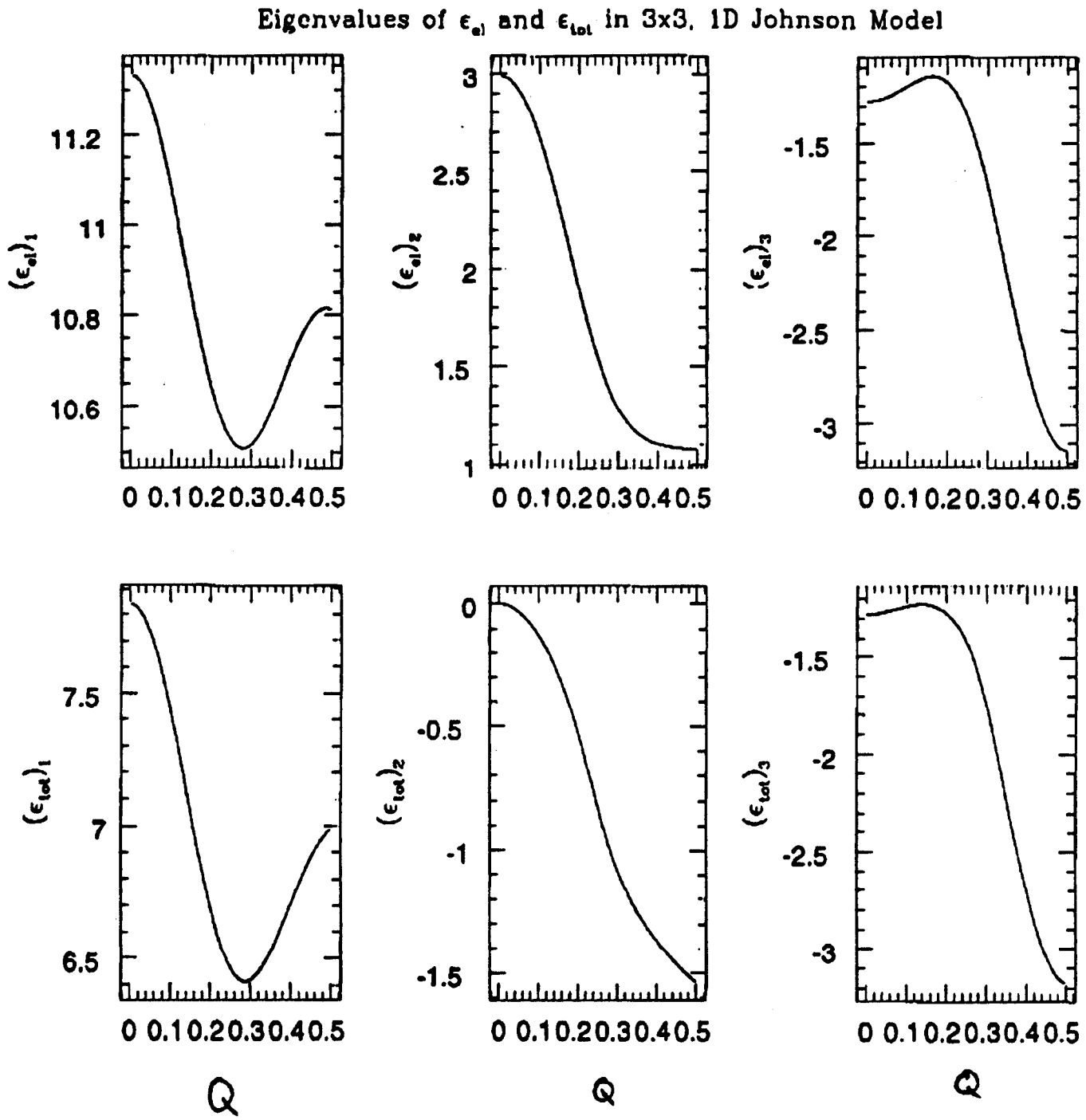
Eigenvalues of ϵ_{el} and ϵ_{tot} in 3x3, 1D Johnson Model
$(\epsilon_{el})_1$
11.2
11
10.8
10.6
0 0.1 0.2 0.3 0.4 0.5
$(\epsilon_{el})_2$
3
2.5
2
1.5
1
0 0.1 0.2 0.3 0.4 0.5
$(\epsilon_{el})_3$
-1.5
-2
-2.5
-3
0 0.1 0.2 0.3 0.4 0.5
$(\epsilon_{tot})_1$
7.5
7
6.5
0 0.1 0.2 0.3 0.4 0.5
Q
$(\epsilon_{tot})_2$
0
-0.5
-1
-1.5
0 0.1 0.2 0.3 0.4 0.5
Q
$(\epsilon_{tot})_3$
-1.5
-2
-2.5
-3
0 0.1 0.2 0.3 0.4 0.5
Q

FIG. 3(a)

Eigenvalues of ϵ_{el} and ϵ_{tot} in 3x3, 1D Johnson Model

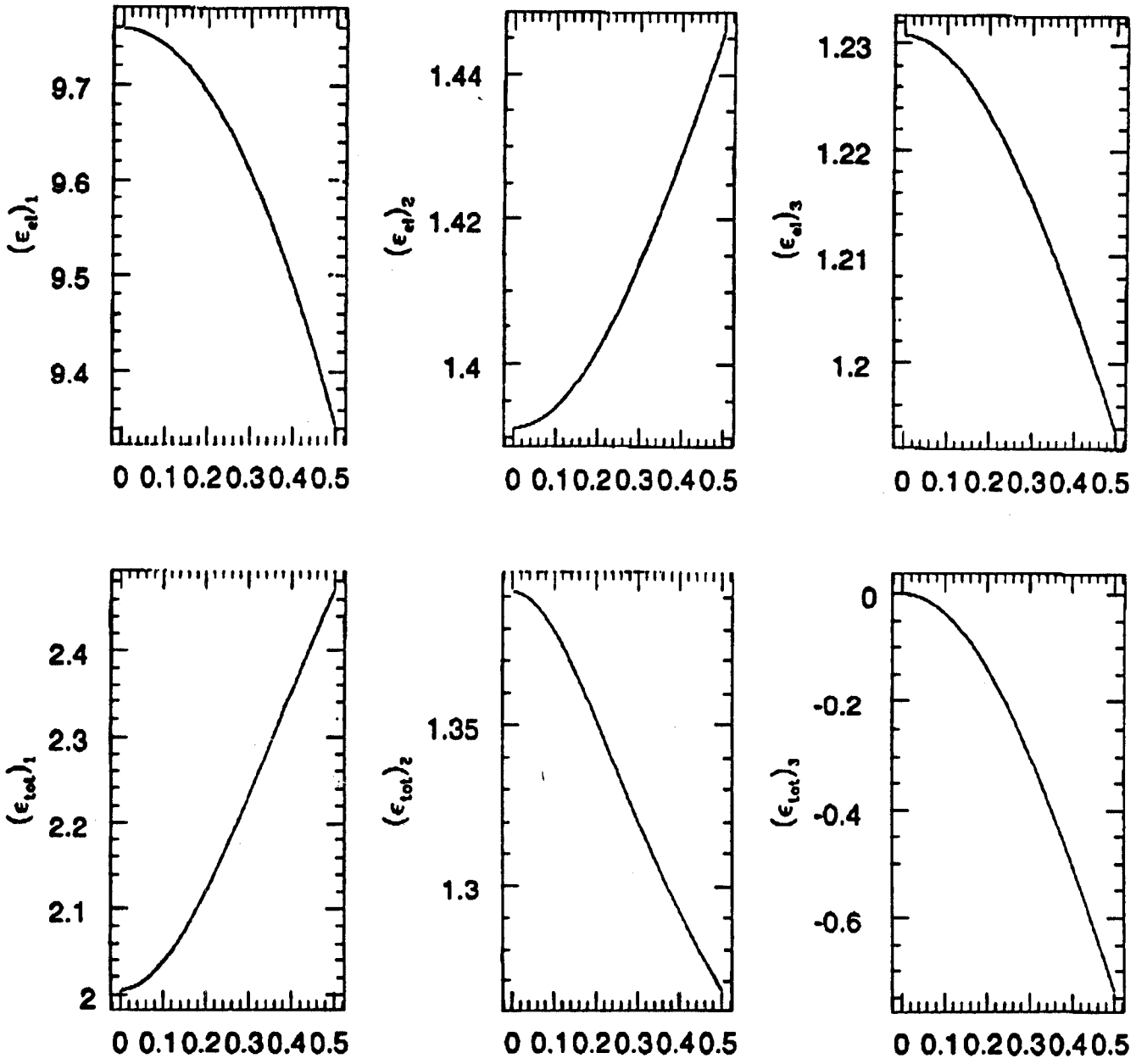

FIG. 3(b)