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ON PHONONS IN SIMPLE METALS

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Synopsis

The dynamical matrix for simple metals is derived in a local ion-electron potential approximation. In order to get a consistent expression for the dynamical matrix in the weak potential limit it is shown to be necessary to include effects from the lattice potential on the electron response-function. The lowest order corrections to the free particle expression are calculated for zero temperature in the R.P.A.-approximation of the polarization operator.

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I. Introduction

The improved experimental technique for determining phonon dispersion curves in crystals has made it possible to investigate them in great detail. The experiments have also revealed many interesting features of these curves, particularly in metals [1], [2], which (at low temperatures) are believed mostly to be effects from the conduction electrons. A proper understanding of these effects may, therefore, give valuable information about the microscopic processes in these crystals.

The theoretical situation, however, is not so encouraging. The origin of of the major difficulty seems to be the splitting of the electrons into two physically quite different groups of either core electrons or conduction electrons, which already makes the electron problem difficult to treat in any kind of approximation. And since the energy associated with a lattice wave is a very tiny quantity (in the electron energy scale), the prospect of getting an accurate estimate of it is very uncertain. For instance, an extension to the lattice dynamics of commonly used theoretical techniques [3] for calculating the electron band structure in the perfect lattice becomes very complicated. For that reason it seems to be inevitable that when doing phonon calculations, we have to rely on the construction of models at the very start, which generally is a very delicate problem indeed. An outstanding exception from this rule, however, is the so called simple metals [4]. In these metals the core electrons form closed shells around the nuclei and the radii of these shells are so small that the nuclei plus the closed shells can be treated in this problem as rigid point particles– the ions. The only dynamically important electrons in the problem are then the conduction electrons. This simplification has, however, to be paid for in terms of a complicated interaction between the ions and the electrons [5]. Still, it is possible in simple cases accurately to replace this complicated interaction by a suitable chosen local potential [6], [7]. Although a purely formal device, this potential can be constructed to reproduce the essential properties of the conduction bands.

In section II we briefly discuss the dynamical matrix for normal metals with simple lattices in this model, i. e. we assume that the ion-electron interaction is given by a local potential $v_e(\boldsymbol{r}) = v_e(-\boldsymbol{r})$. A more complete discussion of this model can be found in [8], [9]. The response-function for the electrons is expanded in section III and the most important terms in the dynamical matrix are discussed for the case where the effective periodic potential in the lattice is weak. In IV the R. P. A. – or Hartree – approximation of the polarization operator is discussed and the first corrections to the Lindhard free particle expression are derived. The paper is concluded in section V with a brief discussion of the characteristic functions for these corrections.

II. The Dynamical Matrix

The Hamiltonian for the metal consists of three parts. First we have a purely ionic part for point ions with mass M and charge Ze interacting via a potential $Ze^2V_i(\boldsymbol{r})$.

$$H_i = \sum_R \frac{P_R^2}{2M} + Z^2e^2 \sum_{R,R'}{}' V_i(\boldsymbol{R} + \boldsymbol{u}(R,t) - \boldsymbol{R}' - \boldsymbol{u}(R',t)) \tag{1}$$

where R and $\boldsymbol{R}$ denote the R-th ion with the mean position at the lattice point $\boldsymbol{R}$ and $\boldsymbol{u}(R,t)$ is the instantaneous position relative to this lattice point. $\sum'$ means exclusion of the term $R = R'$ in the sum.

The second part in the Hamiltonian is a purely electronic part ($\hbar = 1$)

$$\left.\begin{aligned} H_e = \int \frac{d\boldsymbol{r}}{2m} \nabla \psi^+(\boldsymbol{r},t) \nabla \psi(\boldsymbol{r},t) + \frac{e^2}{2}\int \psi^+(\boldsymbol{r}'t)\psi^+(\boldsymbol{r},t)\, v(|\boldsymbol{r}-\boldsymbol{r}'|)\,\cdot \\ \cdot\, \psi(\boldsymbol{r},t)\psi(\boldsymbol{r}'t)\, d\boldsymbol{r}\, d\boldsymbol{r}' \end{aligned}\right\} \tag{2}$$

where $\psi(\boldsymbol{r}, t)$ is the field operator for the dynamically important electrons and $e^2v(|\boldsymbol{r}-\boldsymbol{r}'|)$ is their interaction, typically equal to $|\boldsymbol{r}-\boldsymbol{r}'|^{-1}. e^2$

Finally we have the interaction between the electrons and ions given by

$$H_{ie} = -Ze^2 \sum_R \int d\boldsymbol{r}\, v_e(\boldsymbol{R} + \boldsymbol{u}(\mathrm{R}, t) - \boldsymbol{r})\, \varrho(\boldsymbol{r}, t) \tag{3}$$

in this approximation. ($\varrho(\boldsymbol{r},t) = \psi^+(\boldsymbol{r},\mathrm{t})\psi(\boldsymbol{r},\mathrm{t})$).

The total Hamiltonian is the sum of the three parts

$$H = H_i + H_e + H_{ie}. \tag{4}$$

Standard methods [9] give the following equation of motion for the R-th ion.

$$\left.\begin{aligned} M\ddot{\boldsymbol{u}}(R,t) = &-\left\{Z^2e^2\sum_{R'}{}' T_i(\boldsymbol{R}-\boldsymbol{R}') - Ze^2\int d\boldsymbol{r}\, T_e(\boldsymbol{R}-\boldsymbol{r})\varrho(\boldsymbol{r},t)\right\}\boldsymbol{u}(R,t) + \\ &+ Z^2e^2\sum_{R'}{}' T_i(\boldsymbol{R}-\boldsymbol{R}')\boldsymbol{u}(R',t) + Ze^2\int \mathrm{d}\boldsymbol{r}\, t_e(\boldsymbol{R}-\boldsymbol{r})\,\varrho(\boldsymbol{r},t) \end{aligned}\right\} \quad (5)$$

where in terms depending explicitly on the ionic displacements we only kept terms linear in $\boldsymbol{u}$.

In Eq. (5) means

$$T_i(\boldsymbol{r}) = \nabla\nabla\, V_i(\boldsymbol{r});\, t_e(\boldsymbol{r}) = \nabla\, v_e(\boldsymbol{r});\; T_e(\boldsymbol{r}) = \nabla\nabla\, v_e(\boldsymbol{r}).$$

In order to get a consistent equation for the harmonic motion we have to find the electron density operator $\varrho(\boldsymbol{r},t)$ up to terms linear in the displacements $\boldsymbol{u}(R,t)$ also. This is formally easily done with use of response techniques [10], [11]. When the ions are moving the term H_{ie} in the Hamiltonian causes an external time-depending perturbation on the electron system

$$\left.\begin{aligned} \delta U(\boldsymbol{r},t) &= -Ze^2\sum_{R}\{v_e(\boldsymbol{R}+\boldsymbol{u}(R,t)-\boldsymbol{r}) - v_e(\boldsymbol{R}-\boldsymbol{r})\} = \\ &= Ze^2\sum_{R} t_e(\boldsymbol{r}-\boldsymbol{R})\cdot\boldsymbol{u}(R,t) \end{aligned}\right\} \quad (6)$$

to terms linear in $\boldsymbol{u}(R,t)$.

This perturbation gives to linear terms in $\boldsymbol{u}$ a response in $\varrho(\boldsymbol{r},t)$

$$\left.\begin{aligned} \delta\varrho(\boldsymbol{r},t) = \varrho(\boldsymbol{r},t) - \varrho_0(\boldsymbol{r},t) = &-iZe^2\sum_{R}\int d\boldsymbol{r}'\,dt'\,[\varrho_0(\boldsymbol{r},t),\varrho_0(\boldsymbol{r}',t')]\cdot \\ &\cdot t_e(\boldsymbol{r}'-\boldsymbol{R})\cdot\boldsymbol{u}(R,t') \end{aligned}\right\} \quad (7)$$

where $\varrho_0(\boldsymbol{r},t)$ is the density operator in the case all $\boldsymbol{u}(R,t) = 0$, i.e. in the ideal lattice.

By multiplying Eq. (5) from the right with $\boldsymbol{u}(R_0,t_0)$ and forming the statistical average, we arrive at the following equation

$$\left.\begin{aligned} &M\frac{d^2}{dt^2}\langle\boldsymbol{u}(R,t)\,\boldsymbol{u}(R_0,t_0)\rangle = \\ &= -\{Z^2e^2\sum_{R'}{}' T_i(\boldsymbol{R}-\boldsymbol{R}') - Ze^2\int d\boldsymbol{r}\, T_e(\boldsymbol{R}-\boldsymbol{r})\,\langle\varrho_0(\boldsymbol{r})\rangle\} \\ &\langle\boldsymbol{u}(R,t)\,\boldsymbol{u}(R_0,t_0)\rangle + Z^2e^2\sum_{R'}{}' T_i(\boldsymbol{R}-\boldsymbol{R}')\,\langle\boldsymbol{u}(R',t)\,\boldsymbol{u}(R_0,t_0)\rangle + \\ &+ Z^2e^4\sum_{R'}\int d\boldsymbol{r}\,d\boldsymbol{r}'\,dt'\,t_e(\boldsymbol{R}-\boldsymbol{r})\,h(\boldsymbol{r},t;\boldsymbol{r}',t')\,t_e(\boldsymbol{r}'-\boldsymbol{R}')\,\}\cdot \\ &\cdot\langle\boldsymbol{u}(R',t')\,\boldsymbol{u}(R_0,t_0)\rangle \end{aligned}\right\} \quad (8)$$

to terms linear in $\boldsymbol{u}$. In Eq. (8) we have used the fact that

$$\int t_e(\boldsymbol{R}-\boldsymbol{r})\langle\varrho_0(\boldsymbol{r})\rangle\, d\boldsymbol{r} = 0$$

from the lattice symmetry. In Eq. (8) we have also introduced the linear response function in the ideal lattice

$$\left.\begin{aligned} h(\boldsymbol{r},t;\boldsymbol{r}',t') &= -i\langle[\varrho_0(\boldsymbol{r},t),\varrho_0(\boldsymbol{r}',t')]\rangle\,\theta(t-t') \\ &\left(\theta(x) = \begin{matrix} 1\,; x>0 \\ 0\,; x<0 \end{matrix}\right). \end{aligned}\right\} \tag{9}$$

Since $h(\boldsymbol{r},t,\boldsymbol{r}',t')$ is a quantity determined in the ideal lattice it is a function only of the time difference $t-t$ and has the full symmetry of the lattice in its spatial indices. In particular this means that

$$h(\boldsymbol{r}+\boldsymbol{R},\boldsymbol{r}'+\boldsymbol{R}) = h(\boldsymbol{r},\boldsymbol{r}'). \tag{10}$$

Before leaving this point we want to stress one property of the electron system which is important in practical applications. Since the change in the electron density is generally governed by Eq. (7), we get in particular for an infinitely slow uniform translation of all ions a (small) distance $\boldsymbol{u}$

$$\left.\begin{aligned} \langle\varrho(\boldsymbol{r})\rangle - \langle\varrho_0(\boldsymbol{r})\rangle &= -\boldsymbol{u}\cdot\nabla\langle\varrho_0(\boldsymbol{r})\rangle = \\ &= \sum_R Ze^2\int d\boldsymbol{r}'\,dt'\,h(\boldsymbol{r},t;\boldsymbol{r}',t')\cdot t_e(\boldsymbol{r}'-\boldsymbol{R})\cdot\boldsymbol{u} \end{aligned}\right\} \tag{11}$$

which implies

$$\nabla\langle\varrho_0\rangle = -Ze^2\sum_R\int d\boldsymbol{r}'\,dt'\,h(\boldsymbol{r},t;\boldsymbol{r}',t')\,t_e(\boldsymbol{r}'-\boldsymbol{R}). \tag{12}$$

By the aid of this expression the second term on the R.H.S. in Eq. (8) can be transformed to

$$\left.\begin{aligned} \int d\boldsymbol{r}\,T_e(\boldsymbol{R}-\boldsymbol{r})\langle\varrho_0(\boldsymbol{r})\rangle &= -e^2\sum_{R'}\int t_e(\boldsymbol{R}-\boldsymbol{r})\,h(\boldsymbol{r},t;\boldsymbol{r}',t')\cdot \\ &\quad\cdot t_e(\boldsymbol{r}'-\boldsymbol{R}')\,d\boldsymbol{r}\,d\boldsymbol{r}'\,dt'. \end{aligned}\right\} \tag{13}$$

In case $\langle\varrho_0(\boldsymbol{r})\rangle$ is independent of $\boldsymbol{r}$, its gradient is equal zero, which means completely vanishing of this term. Toya has demonstrated [12] that this is a quite reasonable approximation in the simpler alkali metals. An inclusion of the effect from the periodic electron distribution gives only minor corrections in these cases [13]. In a more general simple metal, however, there is no hope of expecting that it is so. When estimating this effect it is, then, important to fulfil Eq. (13) in order to get sensible results.

By Fourier transforming Eq. (8) and by using the property of $\langle \boldsymbol{u}(R,t\ \boldsymbol{u}(R_0, t_0))\rangle$ to be a function of $t-t$ and $\boldsymbol{R}-\boldsymbol{R}$ only one obtains the equation

$$[\omega^2 I - \omega_p^2 D(\boldsymbol{q},\omega)]\langle \boldsymbol{u}(\boldsymbol{q},\omega)\,\boldsymbol{u}(\boldsymbol{q},\omega)\rangle = 0 \tag{14}$$

where $D(\boldsymbol{q},\omega)$ is the dimensionless dynamical matrix. It is naturally split into two parts.

$$D(\boldsymbol{q},\omega) = D_I(\boldsymbol{q},\omega) + D_E(\boldsymbol{q},\omega) \tag{15}$$

where D_I stands for the part due to the direct ion-ion interaction and is independent of ω, since we assumed an instantaneous ion-ion interaction.

$$\left.\begin{aligned} D_I(\boldsymbol{q}) &= -\frac{1}{4\pi N}\sum_{R'}{}'\{T_i(\boldsymbol{R}-\boldsymbol{R}')\,e^{-i\boldsymbol{q}(\boldsymbol{R}-\boldsymbol{R}')} - T_i(\boldsymbol{R}-\boldsymbol{R}')\} = \\ &= \frac{1}{4\pi}\sum_{K}\{V_i(\boldsymbol{K}+\boldsymbol{q})(\boldsymbol{K}+\boldsymbol{q})(\boldsymbol{K}+\boldsymbol{q}) - V_i(\boldsymbol{K})\boldsymbol{K}\boldsymbol{K}\} \end{aligned}\right\} \tag{16}$$

with $\boldsymbol{K}$ a vector in the reciprocal lattice. The term $V_i(\boldsymbol{K})\boldsymbol{K}\boldsymbol{K}$ with $\boldsymbol{K} = 0$ in Eq. (16) is so far not defined, but we can think of it as the limit $q \to 0$ of $V_i(\boldsymbol{q})\boldsymbol{q}\boldsymbol{q}$. We shall later see that it is exactly cancelled by a corresponding term in $D_E(\boldsymbol{q},\omega)$. In Eq. (16) N is the ion density and $\omega_p^2 = \dfrac{4\pi Z^2 e^2 N}{M}$ is the classical plasma frequency for the ions. With the ion-ion interaction known, this part of the dynamical matrix is readily calculated and no particular attention is paid to it in the following.

Similarly the electronic part of $D(\boldsymbol{q},\omega)$ is written

$$\left.\begin{aligned} D_E(\boldsymbol{q},\omega) = -\frac{1}{4\pi N}\sum_{R'}\int d\boldsymbol{r}\,d\boldsymbol{r}'\{&e^{-i\boldsymbol{q}(\boldsymbol{R}-\boldsymbol{R}')}\,t_e(\boldsymbol{R}-\boldsymbol{r})\,h(\boldsymbol{r},\boldsymbol{r}',\omega)\,t_e(\boldsymbol{r}'-\boldsymbol{R}') - \\ &- t_e(\boldsymbol{R}-\boldsymbol{r})\,h(\boldsymbol{r},\boldsymbol{r}',0)\,t_e(\boldsymbol{r}'-\boldsymbol{R}')\} \end{aligned}\right\} \tag{17}$$

where $h(\boldsymbol{r},\boldsymbol{r}',\omega)$ is the Fourier transform in time of the response function h.

For subsequent use we introduce the function

$$\Phi(\boldsymbol{r},\boldsymbol{r}',t) = \langle[\varrho_0(\boldsymbol{r},t),\varrho_0(\boldsymbol{r}',0)]\rangle = \int\frac{d\omega}{2\pi}\,\Phi(\boldsymbol{r},\boldsymbol{r}',\omega)\,e^{-i\omega t}. \tag{18}$$

It is readily seen that $\Phi(\boldsymbol{r},\boldsymbol{r}',\omega)$ is real, odd in ω and symmetric in its spatial indices. From the spectral representation of the stepfunction

$$\theta(t) = i\int \frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega + i\delta} \quad (\delta = 0^+) \tag{19}$$

and the formal identity

$$\frac{1}{\omega + i\delta} = P\frac{1}{\omega} - i\pi\delta(\omega), \tag{20}$$

where P means the Cauhy principal value, the function $\Phi(\boldsymbol{r},\boldsymbol{r}',\omega)$ enables us to write the response-function $h(\boldsymbol{r},\boldsymbol{r}',\omega)$ in the following form

$$h(\boldsymbol{r},\boldsymbol{r}',\omega) = P\int \frac{d\omega'}{2\pi}\frac{\Phi(\boldsymbol{r},\boldsymbol{r}',\omega)}{\omega - \omega'} - \frac{i}{2}\Phi(\boldsymbol{r},\boldsymbol{r}',\omega). \tag{21}$$

For real ω we have in Eq. (21) $h(\boldsymbol{r},\boldsymbol{r}',\omega)$ written in a real part even in ω and an imaginary part odd in ω.

When dealing with the strongly screening electron system it is in practice convenient to introduce another response-function H instead of h. This can be done by defining the effective potential δU_{eff} acting on the electron system

$$\delta U_{\text{eff}} = \delta U + e^2 v\delta\langle\varrho\rangle \tag{22}$$

and by defining H from

$$\delta\langle\varrho\rangle = H\delta U_{\text{eff}} = h\delta U, \tag{23}$$

which implies

$$h = H\{I - e^2 vH\}^{-1}. \tag{24}$$

So defined, $H(\boldsymbol{r},\boldsymbol{r}',\omega)$ is related to the local polarizability of the electron system and the dielectric operator of the system (with the ions fixed at their lattice sites) is given by

$$\varepsilon(\boldsymbol{r},\boldsymbol{r}',\omega) = I - e^2 vH(\boldsymbol{r},\boldsymbol{r}',\omega). \tag{25}$$

The properties of h found earlier and the symmetry of v give to H the following features

$$\left.\begin{aligned} \operatorname{Re} H(\omega) &= \operatorname{Re} H(-\omega) \\ \operatorname{Im} H(\omega) &= -\operatorname{Im} H(-\omega) \\ H(\boldsymbol{r},\boldsymbol{r}') &= H(\boldsymbol{r}',\boldsymbol{r}) = H(\boldsymbol{r}+\boldsymbol{R},\boldsymbol{r}'+\boldsymbol{R}). \end{aligned}\right\} \tag{26}$$

In order to preserve the symmetric form of $D_E(\boldsymbol{q},\omega)$ in Eq. (17), we shall make a small adjustment in Eq. (24). By writing

$$v = Q\cdot Q \tag{27}$$

and

$$\varkappa = -QHQ \tag{28}$$

(the minus sign is only for convenience) Eq. (24) is transformed to

$$h = -Q^{-1}\frac{\varkappa}{1+e^2\varkappa}Q^{-1} \tag{29}$$

$D_E(\boldsymbol{q},\omega)$ can now be written in the symmetric form

$$\left.\begin{aligned} D_E(\boldsymbol{q},\omega) = -\frac{1}{4\pi}\sum_{\boldsymbol{K},\boldsymbol{K}'}\Bigg\{&\frac{v_e(\boldsymbol{K}+\boldsymbol{q})(\boldsymbol{K}+\boldsymbol{q})}{\sqrt{v(\boldsymbol{K}+\boldsymbol{q})}}\cdot\\ &\cdot\langle\boldsymbol{K}+\boldsymbol{q}|\frac{e^2\varkappa(\omega)}{1+e^2\varkappa(\omega)}|\boldsymbol{K}'+\boldsymbol{q}\rangle\frac{v_e(\boldsymbol{K}'+\boldsymbol{q})(\boldsymbol{K}'+\boldsymbol{q})}{\sqrt{v(\boldsymbol{K}'+\boldsymbol{q})}} -\\ &-\frac{v_e(\boldsymbol{K})\boldsymbol{K}}{\sqrt{v(\boldsymbol{K})}}\langle\boldsymbol{K}|\frac{e^2\varkappa(0)}{1+e^2\varkappa(0)}|\boldsymbol{K}'\rangle\frac{v_e(\boldsymbol{K}')\boldsymbol{K}'}{\sqrt{v(\boldsymbol{K}')}}\Bigg\}\end{aligned}\right\} \tag{30}$$

where again we may define the terms containing $\boldsymbol{q} = 0$; $\boldsymbol{K}$ and/or $\boldsymbol{K}' = 0$ by a limiting procedure. We have in Eq. (30) used Eq. (10), which tells us that h (and $\varkappa$) has the following form in Fourier space

$$h(\boldsymbol{r},\boldsymbol{r}') = \sum_{\boldsymbol{K},\boldsymbol{K}'}\int\frac{d\boldsymbol{q}}{(2\pi)^3}\langle\boldsymbol{K}+\boldsymbol{q}|h|\boldsymbol{K}'+\boldsymbol{q}\rangle\, e^{i(\boldsymbol{K}+\boldsymbol{q})\boldsymbol{r}-i(\boldsymbol{K}'+\boldsymbol{q})\boldsymbol{r}'} \tag{31}$$

where the integration is only over the first Brillouin zone.

In metals we expect the element $\langle\boldsymbol{q}|H(0)|\boldsymbol{q}\rangle$ to be finite when $\boldsymbol{q}$ tends toward zero. This gives a singularity of order $\frac{1}{q^2}$ in the element $\langle\boldsymbol{q}|\varkappa(0)|\boldsymbol{q}\rangle$ and of order $\frac{1}{q}$ in the elements $\langle\boldsymbol{K}+\boldsymbol{q}|\varkappa(0)|\boldsymbol{q}\rangle$ $(\boldsymbol{K}\neq 0)$, all other elements staying finite. Clearly this is a manifestation of the complete screening of a static, macroscopic long wave external perturbation we have in a metal. The singularity of order $\frac{1}{q^2}$ in $\langle\boldsymbol{q}|\varkappa(0)|\boldsymbol{q}\rangle$ is seen to give one eigenvalue h_0 of the matrix $\varkappa(0)$ of order $\frac{1}{q^2}$ and the corresponding eigenfunction $\psi_0 \xrightarrow[q\to 0]{} e^{i\boldsymbol{q}\boldsymbol{r}}$. This result implies that all terms in the second sum in Eq. (30) with $\boldsymbol{K} = 0$, $\boldsymbol{K}' \neq 0$ or vice versa are equal to zero, since all other factors stay finite when q tends toward zero. The term with both $\boldsymbol{K}$ and $\boldsymbol{K}'$ equal to zero, however, gives $\lim_{q\to 0}\langle\boldsymbol{q}|\frac{e^2\varkappa(0)}{1+e^2\varkappa(0)}|\boldsymbol{q}\rangle = 1$ and since all potentials (including V_i) have

Fourier-transforms tending to $\frac{4\pi}{q^2}$ for small q, we get from this term a contribution to D_E equal 1 which exactly cancels the corresponding contribution to D_I in Eq. (16).

If we try to find non-trivial solutions to Eq. (14) as it stands, we observe two disturbing difficulties not present in a Born- von Kármán treatment of this problem. Primarily, we have the dynamical matrix in Eq. (14) not Hermitian and it also depends on the eigenvalue we are trying to find in the equation. Our solutions are no longer the three real roots in a cubic algebraic equation. We know, however, that in actual cases there are three solutions to Eq. (14) which we associate with the phonon vibrations. Now, the obvious way of obtaining only three solutions to Eq. (14) is to completely neglect the ω-dependency in $D_E(\boldsymbol{q},\omega)$ and thus to discard all possible other solutions to it. But putting $\omega = 0$ in $D(\boldsymbol{q},\omega)$ means adopting the adiabatic approximation and this seems, thus, to be the natural starting point when dealing with the phonon problem (low ω case). Since $D(\boldsymbol{q},0)$ is real, this means that the peaks in the correlation function $\langle \boldsymbol{u}(\omega)\ \boldsymbol{u}(\omega)\rangle$ in that case become δ-functions and, consequently, are quite non-physical. We may, however, improve upon the adiabatic solution by treating corrections to it as a kind of perturbation in the low ω case. To lowest order this correction means including an imaginary part (linear in the adiabatic ω) in the dynamical matrix, thus introducing a finite lifetime of the excitations or a width of the peaks (even in the harmonic approximation). One part of our problem is, accordingly, to investigate to what extent this procedure is practical to follow, i.e. to show that the non-adiabatic corrections are small.

There is also another difficulty in Eq. (30) not present in the simplest Born- von Kármán treatment. We have even in $D_E(\boldsymbol{q},0)$ in Eq. (30) to deal with a double sum in the reciprocal space. This means in particular that we cannot in general find a local effective ion-ion interaction to use in a Born- von Kármán calculation.

III. Expansion of the Response-Function

In connection with Eq. (13) we mentioned that – even in simple metals – we are not generally allowed to neglect the effect from the periodic part of the undisturbed electron density $\langle \varrho_0(\boldsymbol{r})\rangle$. This implies that $\varkappa(\boldsymbol{r},\boldsymbol{r}')$ is not generally a function of $\boldsymbol{r}-\boldsymbol{r}'$ only. The problem of calculating $D_E(\boldsymbol{q})$ becomes then much more difficult. Experimental and theoretical results indicate [14],

[15], however, that in some cases of interest the matrix $\varkappa$ is quite close to being diagonal in a plane wave representation. In such cases an expansion of the matrix h seems to be feasible and the problem is to find out which terms in the expansion are of most importance in $D_E(\boldsymbol{q})$.

By writing

$$\varkappa = A + B, \tag{32}$$

where A is the part of the matrix diagonal in a Fourier representation and B is the supposed small purely non-diagonal part, we get formally

$$\frac{e^2\varkappa}{1 + e^2\varkappa} = I - \sum_{n=0}^{\infty} \frac{1}{1 + e^2 A}\left(-e^2 B \frac{1}{1 + e^2 A}\right)^n. \tag{33}$$

In order to judge which terms in this expansion are of most importance in $D_E(\boldsymbol{q})$, we need some kind of expansion parameter in our problem and then to collect all terms of a certain order in this parameter. A natural choice of this parameter seems to be to consider the periodic part of $\langle \varrho_0(\boldsymbol{r}) \rangle$ as small (say, of first order) compared to the mean (uniform) value of $\langle \varrho_0(\boldsymbol{r}) \rangle = NZ$. This means that the periodic potential in the ideal lattice acting on the electron system is small (of the same order) compared to the kinetic energy of the electrons. For all important Fourier components $V(\boldsymbol{K})$ of this potential we then must have

$$V(\boldsymbol{K}) \ll E_F \approx \frac{k_F^2}{2m} \tag{34}$$

(E_F is the Fermi energy of the electron system). But from Eq. (12) we find that this means

$$Ze^2 N v_e(\boldsymbol{K}) \ll E_F. \tag{35}$$

This inequality implies that the function $v_e(\boldsymbol{k})$ decreases more rapidly for increasing $k \leq$ any K than the function $v(\boldsymbol{k})$, since for metals of interest $\left(\text{with } v(r) \sim \frac{1}{r}\right)$ we have $Ze^2 N v(\boldsymbol{K})$ of the same order as E_F for the first (and most important) reciprocal vectors $\boldsymbol{K}$. For a small q we can from these observations find the most important terms in the series in Eq. (33), when it is used in Eq. (30).

In case $n = 0$ only the diagonal part A enters. When combined with the unit matrix the contribution to $D_E(\boldsymbol{q})$ from the term $\boldsymbol{K} = 0$ is very large and gives mainly a cancellation of the corresponding term in $D_I(\boldsymbol{q})$ in Eq. (16). The remaining part of this contribution is, however, very important and is in a certain model of the metal entirely responsible for the sound velocity (Bohm and Staver [16]). Their value for this rest is $\approx \frac{E_F}{Ze^2N}\cdot q^2$. For terms with $\boldsymbol{K} \neq 0$ in the diagonal part we get corrections to this value of order $\left(\frac{V(\boldsymbol{K})}{E_F}\right)^2$ compared to 1. Thus, this is the order of the corrections we can expect from the non-uniform electron distribution in the perfect crystal.

From the term with $n = 1$ in Eq. (33) and with B containing a factor $\frac{V(\boldsymbol{K})}{E_F}$ we get clearly contributions to $\mathrm{D}_E(\boldsymbol{q})$ of this order from elements with either $\boldsymbol{K}$ or $\boldsymbol{K}'$ equal to zero. All other terms (both $\boldsymbol{K}$ and $\boldsymbol{K}' \neq 0$) are a factor $\frac{V(\boldsymbol{K})}{E_F}$ smaller.

Similarly, we find contributions to $D_E(\boldsymbol{q})$ of this order in the term with $n = 2$ in Eq. (33) in case both $\boldsymbol{K}$ and $\boldsymbol{K}'$ are equal 0. All other terms in the sum are at least a factor $\frac{V(\boldsymbol{K})}{E_F}$ smaller. So is also the case for all contributions from terms with $n \geqslant 3$.

Consequently, in order to take a consistent step beyond the approximation of Bohm-Staver (and Toya) regarding the electron distribution in the crystal we have to include all terms of the same order discussed above (at least for small q). This means that for small q we have at least to consider the first "row" and "column" in the matrix $\langle \boldsymbol{K}+\boldsymbol{q}|B|\boldsymbol{K}'+\boldsymbol{q}\rangle$ (corresponding to either $\boldsymbol{K}$ or $\boldsymbol{K}' = 0$). So much about the small q case. But what happens when $\boldsymbol{q}$ increases and approaches any zone boundary? This is a more difficult question to answer. However, the crucial point in the arguments above is the behaviour of the function $v_e(\boldsymbol{k})$. For $\boldsymbol{k}$ equal to any of the important reciprocal lattice vectors we have assumed the value of this function to be so small that the ratio

$$\frac{Ze^2Nv_e(\boldsymbol{k})}{E_F} \approx \frac{Ze^2Nv_e(\boldsymbol{k})}{E_F(1+e^2A(\boldsymbol{k}))} \approx \frac{V(\boldsymbol{K})}{E_F}$$

is a suitable expansion parameter. But for $\boldsymbol{k}$ tending to zero the expression $\frac{Ze^2Nv_e(\boldsymbol{k})}{E_F(1+e^2A(\boldsymbol{k}))}$ tends to order 1. Of importance is then for what value of $\boldsymbol{k}$ this change of order takes place. If it happens for a $\boldsymbol{k}$ well inside the first zone the arguments above hold for any $\boldsymbol{q}$ in the first zone. Although this is – so far – an unsettled point, we shall in the following as a proviso assume that this is the case and consequently assume that the terms kept in $D_E(\boldsymbol{q})$ for small q contain uniformly in the whole zone all terms of importance. That means we are extrapolating the condition in Eq. (35) to the more general

$$Ze^2 N\, v_e(\boldsymbol{K}+\boldsymbol{q}) \ll E_F \tag{36}$$

($\boldsymbol{K} \neq 0$ and any $\boldsymbol{q}$ in the first zone).

Then, the tentative form of $D_E(\boldsymbol{q})$ becomes as follows

$$\left.\begin{aligned} D_E(\boldsymbol{q}) = -\frac{1}{4\pi}\Bigg\{ & \sum_{\boldsymbol{K}} \frac{v_e^2(\boldsymbol{K}+\boldsymbol{q})\,(\boldsymbol{K}+\boldsymbol{q})\,(\boldsymbol{K}+\boldsymbol{q})}{v(\boldsymbol{K}+\boldsymbol{q})} \frac{e^2 A(\boldsymbol{K}+\boldsymbol{q})}{1+e^2 A(\boldsymbol{K}+\boldsymbol{q})} - \\ & - \sum_{\boldsymbol{K}}{}' \frac{v_e^2(\boldsymbol{K})\boldsymbol{K}\boldsymbol{K}}{v(\boldsymbol{K})} \frac{e^2 A(\boldsymbol{K})}{1+e^2 A(\boldsymbol{K})} + \\ & + \sum_{\boldsymbol{K}}{}' \frac{v_e(\boldsymbol{K}+\boldsymbol{q})v_e(\boldsymbol{q})}{[v(\boldsymbol{K}+\boldsymbol{q})v(q)]^{1/2}} \frac{\boldsymbol{q}(\boldsymbol{K}+\boldsymbol{q})+(\boldsymbol{K}+\boldsymbol{q})\boldsymbol{q}}{1+e^2 A(\boldsymbol{K}+\boldsymbol{q})} \frac{e^2\langle \boldsymbol{K}+\boldsymbol{q}|B|\boldsymbol{q}\rangle}{1+e^2 A(\boldsymbol{q})} - \\ & - \sum_{\boldsymbol{K}}{}' \frac{v_e^2(\boldsymbol{q})\boldsymbol{q}\boldsymbol{q}}{v(\boldsymbol{q})} \frac{e^4|\langle \boldsymbol{K}+\boldsymbol{q}|B|\boldsymbol{q}\rangle|^2}{[1+e^2A(\boldsymbol{q})]^2[1+e^2A(\boldsymbol{K}+\boldsymbol{q})]}\Bigg\} = D_{E0}+D_{E1}+D_{E2} \end{aligned}\right\} \tag{37}$$

where we have suppressed the ω-dependency. In Eq. (37) we have also discarded the term $\boldsymbol{K} = 0$ (indicated by $\sum'$) in the second sum due to the cancellation from D_I discussed earlier. The symmetry of the matrix B is also used and an obvious notation for the diagonal elements is introduced. We observe that in Eq. (37) the contribution to $D_E(\boldsymbol{q})$ from the static electron distribution $\langle \varrho_0 \rangle$ (the second sum) contains only the diagonal part of $\varkappa$. We further note in Eq. (37) that the periodic property in the reciprocal lattice of the complete $D_E(\boldsymbol{q})$ in Eq. (30) is lost when doing this small q approximation. In order to reensure this property one needs consider the complete matrix B in the contribution from the $n = 1$ part (the third sum in Eq. (37)) and at least an extension of the last sum in Eq. (37) (contributions from $n = 2$) by replacing $\boldsymbol{q}$ with $\boldsymbol{K}'+\boldsymbol{q}$ and do the sum over $\boldsymbol{K}'$. If we make these extensions in Eq. (37), we have, however, to adjust the contribution from $\langle \varrho_0 \rangle$ in order to satisfy Eq. (13).

IV. Approximation of the Polarizability Matrix

In Eq. (23) we introduced the irreducible polarization operator for the electron system in the ideal lattice. In order to make an explicit calculation we have to know this quantity. However, no closed form for it is known even in the fairly simple model of the metal we have adopted here. Consequently, we have to rely on more or less realistic approximations. The simplest nontrivial approximation we can adopt is the R.P.A. or Hartre approximation [17], [18], [9], which is the first term in an expansion [19]. In that case we have (ω real)

$$\left.\begin{aligned} H(\boldsymbol{r},\boldsymbol{r}',\omega) &= \sum_{i,j} \varphi_i(\boldsymbol{r})\,\varphi_i^*(\boldsymbol{r}')\varphi_j(\boldsymbol{r}')\varphi_j^*(\boldsymbol{r}) \cdot \left\{\frac{f(E_i)-f(E_j)}{E_i-E_j+\omega+i\delta}\right\} \\ &\qquad (\delta = 0^+) \end{aligned}\right\} \tag{38}$$

where $f(E_i) = \{1+e^{\beta(E_i-\mu)}\}^{-1}\left(\beta = \dfrac{1}{k_B T}\right)$ is the Fermi factor and $\varphi_i(\boldsymbol{r})$ is the wavefunction for the single particle electron state with energy E_i. It satisfies an equation

$$\left\{-\frac{\Delta}{2m} - V(\boldsymbol{r})\right\}\varphi_i(\boldsymbol{r}) = E_i\varphi_i(\boldsymbol{r}). \tag{39}$$

Although this seems to be a rather crude approximation, since not even exchange effects between the electrons are properly considered, its effect in Eq. (25) can be substantially improved by a proper choice of the potential $v(\boldsymbol{r})$. So it is possible in this way to cover the commonly used approximate inclusions of exchange and correlation effects [12], [13], [20], [21] and [22]. $V(\boldsymbol{r})$ is in Eq. (39) the effective one-electron potential in the ideal lattice and has to be consistently chosen. It has the full symmetry of the lattice and can be written

$$V(\boldsymbol{r}) = \sum_{\boldsymbol{K}}{}' V(\boldsymbol{K})e^{i\boldsymbol{K}\cdot\boldsymbol{r}} \quad \text{with} \quad V(\boldsymbol{K}) = V(-\boldsymbol{K}) \tag{40}$$

in the cases considered here.

We have in Eq. (40) ignored the uniform part, since it has no dynamical effect and can be subtracted in Eq. (39). With $\langle\varrho_0(\boldsymbol{r})\rangle$ supposed to be almost uniform, we are led to make a perturbation expansion of E_i and φ_i in eigenfunctions $e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \langle\boldsymbol{r}|\boldsymbol{k}\rangle$ to the free electron operator $H_0 = -\dfrac{\Delta}{2m}$. In an extended zone scheme we get (neglecting spin)

$$\varphi(\boldsymbol{k},\boldsymbol{r}) = \frac{1}{N(\boldsymbol{k})^{1/2}}\{1+\sum_{\boldsymbol{K}}{}' c(\boldsymbol{k},\boldsymbol{K})e^{i\boldsymbol{K}\cdot\boldsymbol{r}}\}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tag{41}$$

with [23] and [19]

$$c(\boldsymbol{k},\boldsymbol{K}) = \sum_{n=1}^{\infty} \langle \boldsymbol{K}+\boldsymbol{k} | \left\{ \frac{|\boldsymbol{k}\rangle\langle\boldsymbol{k}| - 1}{E(\boldsymbol{k}) - H_0} V \right\}^n |\boldsymbol{k}\rangle \tag{42}$$

and

$$\left. \begin{aligned} E(\boldsymbol{k}) &= \varepsilon(k) - \sum_{n=1}^{\infty} \langle \boldsymbol{k} | V \left\{ \frac{|\boldsymbol{k}\rangle\langle\boldsymbol{k}| - 1}{E(\boldsymbol{k}) - H_0} V \right\}^n |\boldsymbol{k}\rangle \\ &\left(\varepsilon(k) = \frac{k^2}{2m} \right). \end{aligned} \right\} \tag{43}$$

In Eq. (41), $N(\boldsymbol{k})$ is the normalization factor and with $\varphi(\boldsymbol{k},\boldsymbol{r})$ normalized in a unit cube, we get

$$N(\boldsymbol{k}) = 1 + \sum_{\boldsymbol{K}}{}' |c(\boldsymbol{k},\boldsymbol{K})|^2. \tag{44}$$

The reason why we have used this Wigner-Brillouin expansion in this case rather than a Rayleigh-Schrödinger expansion is because in the latter we get singularities for states close to the Bragg planes.

The zero order terms in these expansions give the usual LINDHARD [17] expression for $\varkappa_0$. It is of interest to find corrections to low order in V to this function. In order to do this we have to study quantities as

$$\left. \begin{aligned} \langle \boldsymbol{K}+\boldsymbol{q} | M(\boldsymbol{k},\boldsymbol{k}') | \boldsymbol{K}'+\boldsymbol{q} \rangle = \langle \varphi(\boldsymbol{k}) | e^{-i(\boldsymbol{K}+\boldsymbol{q})\boldsymbol{r}} | \varphi(\boldsymbol{k}') \rangle \cdot \\ \cdot \langle \varphi(\boldsymbol{k}') | e^{i(\boldsymbol{K}'+\boldsymbol{q})\boldsymbol{r}} | \varphi(\boldsymbol{k}) \rangle. \end{aligned} \right\} \tag{45}$$

To zero order in V, with $\varphi(\boldsymbol{k})$ and $\varphi(\boldsymbol{k}')$ equal plane waves, these quantities obey a simple momentum conservation rule and are equal to $\delta_{\boldsymbol{k}'}^{\boldsymbol{K}+\boldsymbol{k}+\boldsymbol{q}} \delta_{\boldsymbol{K}'}^{\boldsymbol{K}}$. In other words, all non-zero elements of M_0 are equal to one and then assume the biggest possible value, due to the simple dynamical properties of a free electron when acted upon by an external plane wave. For more general states $|\varphi(\boldsymbol{k})>$, $|\varphi(\boldsymbol{k}')>$, however, we get a more complicated conservation rule and the non-zero elements are no longer constants. With the state $|\varphi(\boldsymbol{k})> = |\boldsymbol{k}> + \sum_{\boldsymbol{K}}{}' \delta(\boldsymbol{k},\boldsymbol{K}) |\boldsymbol{K}+\boldsymbol{k}>$, where $\delta(\boldsymbol{k},\boldsymbol{K})$ is of order V, it is seen that to first order in V this effect sets in only in case $\boldsymbol{K} \neq \boldsymbol{K}'$ in Eq. (45). The first order correction to the Lindhard matrix $\varkappa_0$ is consequently purely non-diagonal, while the first correction to the diagonal elements is of higher order in V. But from the discussion of the approximate dynamical matrix in Eq. (37) it is obvious that what we consistently need there is just the part of B linear in V. Furthermore, it is clear that the only place in Eq. (37) in which we have to consider the first correction to the diagonal elements is in the important term with $\boldsymbol{K} = 0$ in the first sum, i.e. in the term containing $\frac{e^2 A(\boldsymbol{q})}{1 + e^2 A(\boldsymbol{q})}$. We shall in the following include the correction of this term in the second order part D_{E2} in Eq. (37) and thus by D_{E0} mean the expression where $\varkappa_0$ is used throughout.

In the following we concentrate on the real part of H and get, by using the expansion in Eq. (42), the following expression for the non-diagonal element.

$$\left.\begin{aligned} \langle \boldsymbol{q}|H(\omega)|\boldsymbol{K}+\boldsymbol{q}\rangle = 2P\sum_{\boldsymbol{k},\boldsymbol{k}'}\frac{f(E(\boldsymbol{k}))-f(E(\boldsymbol{k}'))}{E(\boldsymbol{k})-E(\boldsymbol{k}')+\omega}\cdot \\ \cdot\frac{1}{N(\boldsymbol{k})N(\boldsymbol{k}')}\{[c^*(\boldsymbol{k}',\boldsymbol{K})+c(\boldsymbol{k},-\boldsymbol{K})]\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}+[c(\boldsymbol{k}',-\boldsymbol{K})+c^*(\boldsymbol{k},\boldsymbol{K})]\cdot \\ \cdot\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{K}+\boldsymbol{q}}\} \end{aligned}\right\} \quad (46)$$

where the factor 2 is from the trace over the spin states. We have in Eq. (46) only kept terms that can possibly give lowest order contributions at least in cases where $\boldsymbol{q}$ is not close to a Bragg plane $2\boldsymbol{K}'\cdot\boldsymbol{q}+\boldsymbol{K}'^2 = 0$ with $\boldsymbol{K}'$ parallel to $\boldsymbol{K}$. This restriction on $\boldsymbol{q}$ appears, because we have in Eq. (46) neglected terms of the second and third degrees in the $c(\boldsymbol{k},\boldsymbol{K})$:s. These neglected terms can, however, be of order 1 for states $\boldsymbol{k}$ and $\boldsymbol{k}'$ in narrow intervals of thickness $\frac{mV(\boldsymbol{K})}{K}$ around Bragg planes and the sum over these states may then give contributions of order $V(\boldsymbol{K})$ in case $f(E(\boldsymbol{k})) \neq 0$ and $f(E(\boldsymbol{k}')) = 0$ (or vice versa) in these regions. Therefore, the restriction is of importance only in cases where the Fermi surface is intersected by any Bragg plane. But even in these cases, we are going to neglect the restrictions and consider the expression in Eq. (46) as generally valid for all values on $\boldsymbol{q}$, since the corrections for $\boldsymbol{q}$ within a narrow region close to the Bragg planes discussed can be expected to be quite small. Effects of this kind are obviously to be expected, since the matrix H has a zone-structure in the periodic lattice and a representation of this zone-structure in the extended scheme leads to "rounding off" effects at the Bragg planes, which give a smooth function in the reduced scheme, when the pieces are brought together.

From Eq. (47) we get the desired part of the matrix B linear in $V(\boldsymbol{K})$

$$\left.\begin{aligned} e^2\langle \boldsymbol{q}|B(\omega)|\boldsymbol{K}+\boldsymbol{q}\rangle \simeq e^2\langle \boldsymbol{q}|\varkappa_1(\omega)|\boldsymbol{K}+\boldsymbol{q}\rangle = \frac{k_0}{\pi^2 a_0}[v(\boldsymbol{q})v(\boldsymbol{K}+\boldsymbol{q})]^{1/2}\frac{V(\boldsymbol{K})}{\varepsilon_0}\cdot u_1(\boldsymbol{K},\boldsymbol{q},\omega) \\ \left(\frac{k_0}{\pi^2 a_0} = \frac{Ze^2N}{\frac{2}{3}\varepsilon_0}\right) \end{aligned}\right\} \quad (47)$$

where a_0 is the first Bohr radius in hydrogen and $\varepsilon_0 = \dfrac{k_0^2}{2m}$ is the free electron Fermi energy at $T = 0$. In Eq. (47) u_1 is the characteristic first order function of order 1, which is given in the appendix in zero T case.

From the expansion in Eq. (42) we also get the following expression for the diagonal element of H

$$\left.\begin{aligned}\langle \boldsymbol{q}|H(\omega)|\boldsymbol{q}\rangle &= 2P\sum_{\boldsymbol{k},\boldsymbol{k}'}\frac{f(E(\boldsymbol{k}))-f(E(\boldsymbol{k}'))}{E(\boldsymbol{k})-E(\boldsymbol{k}')+\omega}\cdot\\ &\cdot\left\{\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}-\sum_{\boldsymbol{K}}{}'\frac{\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}}{N(\boldsymbol{k})N(\boldsymbol{k}')}|c(\boldsymbol{k},\boldsymbol{K})-c(\boldsymbol{k}',\boldsymbol{K})|^2+\right.\\ &\left.+\sum_{\boldsymbol{K}}{}'\frac{\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{K}+\boldsymbol{q}}}{N(\boldsymbol{k})N(\boldsymbol{k}')}|c(\boldsymbol{k},\boldsymbol{K})+c^*(\boldsymbol{k}',-\boldsymbol{K})|^2\right\}.\end{aligned}\right\}\quad(48)$$

Again this expression contains all effects of the desired order except possibly when $\boldsymbol{q}$ is close to a Bragg plane.

In Eq. (48) the first $\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}$ gives in the free electron case the Lindhard formula. It is, therefore, convenient to subtract this part and get the necessary corrections explicitly. We write

$$\left.\begin{aligned}2P\sum_{\boldsymbol{k},\boldsymbol{k}'}\frac{f(E(\boldsymbol{k}))-f(E(\boldsymbol{k}'))}{E(\boldsymbol{k})-E(\boldsymbol{k}')+\omega}\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}} &= 2P\sum_{\boldsymbol{k},\boldsymbol{k}'}\left\{\frac{f(k)-f(k')}{\varepsilon(k)-\varepsilon(k')+\omega}+\right.\\ &+[f(k)-f(k')]\left[\frac{1}{E(\boldsymbol{k})-E(\boldsymbol{k}')+\omega}-\frac{1}{\varepsilon(k)-\varepsilon(k')+\omega}\right]+\\ &\left.+\frac{g(\boldsymbol{k})-g(\boldsymbol{k}')}{E(\boldsymbol{k})-E(\boldsymbol{k}')+\omega}\right\}\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}\end{aligned}\right\}\quad(49)$$

where $f(k) = f(\varepsilon(k)) = \{1+e^{\beta(\varepsilon(k)-\mu_0)}\}^{-1}$ and $g(\boldsymbol{k}) = f(E(\boldsymbol{k})) - f(k)$. The first term in the curly bracket on the R.H.S. in Eq. (49) gives obviously the Lindhard formula and the remaining parts are corrections to this value due to corrections of the energies in the denominator (but with still the free electron Fermi factors) and the corrections of the Fermi factors respectively.

The element $\langle \boldsymbol{q}|\varkappa|\boldsymbol{q}\rangle$ can now to second order in $V(\boldsymbol{K})$ be written (with the restrictions on $\boldsymbol{q}$ mentioned in connection with Ep. (48))

$$\left.\begin{aligned}e^2\langle \boldsymbol{q}|\varkappa(\omega)|\boldsymbol{q}\rangle &= \frac{k_0}{\pi^2 a_0}v(q)\left\{u_0(q,\omega)+\sum_{\boldsymbol{K}}{}'\left(\frac{V(\boldsymbol{K})}{\varepsilon_0}\right)^2 u_2(\boldsymbol{K},\boldsymbol{q},\omega)\right\} =\\ &= e^2\langle q|\varkappa_0|q\rangle + e^2\langle \boldsymbol{q}|\varkappa_2|\boldsymbol{q}\rangle\end{aligned}\right\}\quad(50)$$

where the dimensionless function $u_2(\boldsymbol{K},\boldsymbol{q},\omega)$ is the characteristic function for the correction to the Lindhard formula that is characterized by $u_0(q,\omega)$. In the appendix we have determined the function u_2 in the zero T case.

It now only remains to relate consistently the potential $V(\boldsymbol{r})$ to the interaction $v_e(\boldsymbol{r})$. This is easily done, since in the tentative dynamical matrix in Eq. (37) we shall put in the zero order matrix $\varkappa_0$ in the terms containing the static electron distribution $\langle\varrho_0\rangle$ (the second sum). From Eq. (22) this immediately gives with $\delta U(\boldsymbol{K}) = -Ze^2Nv_e(\boldsymbol{K})$ and $\delta U_{\text{eff}}(\boldsymbol{K}) = -V(\boldsymbol{K})$

$$V(\boldsymbol{K}) = \frac{Ze^2Nv_e(\boldsymbol{K})}{1+e^2\varkappa_0(\boldsymbol{K})}. \tag{51}$$

The simple form of Eq. (51) is naturally only valid for the form of $D_E(\boldsymbol{q})$ given in Eq. (37). If we alter this form, for instance by including terms in order to preserve the periodic property of $D_E(\boldsymbol{q})$ in the reciprocal lattice, we have to alter Eq. (51) as well.

V. Discussion

In this section we shall briefly discuss the functions u_1 and u_2 obtained in the appendix in the zero T limit. For simplicity we only consider the adiabatic expressions in the two cases, which – as we indicated in the appendix – is quite sufficient to do in connection with phonons.

The symmetry of the dielectric matrix gives the following general structure for u_1

$$u_1(\boldsymbol{K},\boldsymbol{q}) = w_1(\boldsymbol{K},\boldsymbol{q}) + w_1(\boldsymbol{K},-(\boldsymbol{K}+\boldsymbol{q})) \tag{52}$$

Since $\boldsymbol{K}$ is an axis of symmetry in u_1, it follows from Eq. (52) that u_1 has the following symmetry plane

$$2\boldsymbol{K}\cdot\boldsymbol{q}+K^2 = 0. \tag{53}$$

It is therefore sufficient to investigate the function u_1 for $\boldsymbol{K}$ and $\boldsymbol{q}$ in a half-plane. In this plane the intersection with the plane in Eq. (53) generates a line of symmetry.

It is of particular interest to observe the difference between the two cases $Z_0 > 1$ and $Z_0 < 1$. This difference is already emphasized in the definition of the function u_1. The integrals I_{ij} in Eq. (A 13) have two different functional forms depending on whether the functions $R_i(Z_j)$ are negative or positive. And as is seen in Eq. (A 31) all these functions $R_i(Z_j)$ are essentially equal

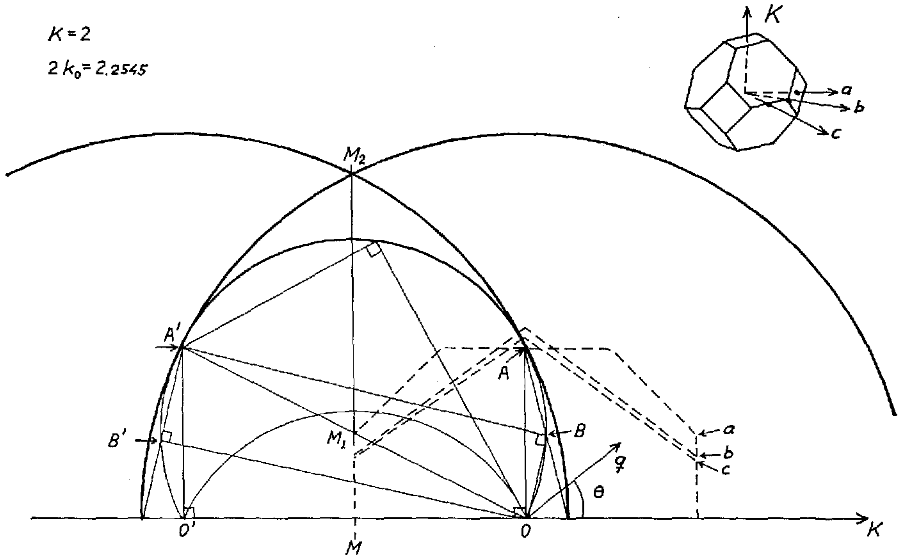

Fig. 1. Figure showing the intersection in the $\boldsymbol{K}-\boldsymbol{q}$-plane of the surfaces where u_1 (and u_2) have nonregular behaviour (heavy lines). The dashed figures show the intersection with the zone as indicated in the inset.

in the adiabatic limit. But, for instance, $R_1(Z_0) < 0$ means that the intersection between the singularity planes $2\boldsymbol{K}\cdot\boldsymbol{k} - K^2 = 0$ and (for $\omega = 0$) $2\boldsymbol{k}\cdot\boldsymbol{q} + q^2 = 0$ in Eq. (A 5) penetrates the Fermi sphere. Accordingly we cannot have $R_1(Z_0)$ negative in case $Z_0 > 1$, since $Z_0 > 1$ means that the plane $2\boldsymbol{K}\cdot\boldsymbol{k} - K^2 = 0$ is entirely outside the Fermi sphere. There is consequently an important qualitative difference between metals with a Fermi sphere extending outside the first zone and those with the Fermi sphere completely inside the zone. This is one reason why the polyvalent metals is felt to be much more interesting than, for instance, a metal such as *Na*.

In order to demonstrate easily the behaviour of the function u_1, some relevant curves have been drawn in Fig. 1 for the case $K = 2$ and $2k_0 = 2.2545$ in $\frac{2\pi}{a}$, which is a value appropriate for Al.

$\boldsymbol{K}$ is here the axis of symmetry and the circles around O and O' are the traces in the $\boldsymbol{K}-\boldsymbol{q}$-plane of the "Fermi spheres" (radii $2k_0$) around O and O'. M is the intersection with the plane in Eq. (53). The locus for points making $\mathrm{R}_i(Z_j) = 0$ is also shown. This locus is a circle with diameter OA' and centre at M_1 which thus touches the "Fermi spheres" at the points A and A' (note the folded part). The heavy parts of the circles in the figure give the loci for points where there are infinities in the derivative of u_1. The parts along the "Fermi circles" are to be expected, but it is interesting to note that along the circle around M_1 there are also such points between A and A' and moreover with stronger infinities. The formal reason for these singularities is easily located. Approaching the circle M_1 from the inside means that the functions $R_i(Z_j)$ tend to -0. Then all cyclometric functions approach the values $+\frac{\pi}{2}$ or $-\frac{\pi}{2}$. On the arc between A and A' all functions I_{ij} give a contribution $+\pi$ to the sum in Eq. (A 32). When the factors are considered, a rapid increase is found in the contribution from the sum of I_{ij} there. On the circle the contribution is zero. If, however, the circle is approached from outside, then $R_i(Z_j)$ tends to $+0$ and the integral are given by hyperbolic area functions which themselves go to zero on the circle. These arguments apply for all points on the circle between A and A', since there is no change in sign for the contributions from the cyclometric functions along $A - A'$. This can be seen to be the case, since for any of the integrals the following sum rule applies for the arguments involved in I_{ij}.

$$R_i(Z_j) - (c_i + Z_i Z_j)^2 = -(1 - Z_j^2)(1 - Z_j^2). \tag{54}$$

Eq. (54) demonstrates that on the circle around M_1 where $R_i(Z_j) = 0$, the quantity $(c_i + Z_i Z_j)$ cannot become zero unless Z_i or Z_j equals ± 1. This never happens between A and A': at A (or A'), however, Z_3(or Z_1) equals 1 and there is a change in the sign of I_{30} and I_{32} (or I_{10} and I_{12}). Along $A0$ and $A'0'$, and also along the folded continuation, this edge effect therefore disappears. I_{32} and I_{12} change signs again at B (or B') where $|Z_2| = 1$, but these sign changes cancel, making the function smooth there.

Physically this edge-effect arises from the discontinuity in the expansion coefficients of the electron wave function at the Bragg planes. In the present treatment these discontinuities are infinitely large, since for the integrations, the finite coefficients (in a Wigner Brillouin expansion) have de facto been replaced by the singular coefficients in a Schrödinger expansion. Consequently the form of u_1 used does not give a correct reproduction of the real behaviour of the matrix element $\langle \boldsymbol{q} | \varkappa_1 | \boldsymbol{K} + \boldsymbol{q} \rangle$ for values of $\boldsymbol{q}$ close to this edge. This form of u_1 can only be expected to give the correct behaviour of the true function up to a distance of order $\Delta q = \frac{V(\boldsymbol{K})}{\varepsilon_0} \cdot k_0$ from the edge. The approximation made here yields a function connecting continuously (but with infinite slope at the edge) points on both sides of this edge. However, even in the real case a rapid variation in the nondiagonal terms of the dielectric matrix can be expected for values of q in that region. It is therefore of interest to find out whether or not this property is observable in the experimental measurements. What makes the situation so interesting is that points on this edge are not in general close to any "ordinary" KOHN point, where the following should apply [24].

$$(\boldsymbol{K}+\boldsymbol{q})^2 - 4k_0^2 = 0. \tag{55}$$

Instead the relationship is of the form [25]

$$(\boldsymbol{K}+\boldsymbol{q})^2 - s^2 4k_0^2 = 0: \quad \text{with} \quad s^2 = \frac{|\boldsymbol{K}\times\boldsymbol{q}|^2}{K^2q^2}. \tag{56}$$

Although this condition is identical with the condition given by TAYLOR in the limit of vanishing deformation of the Fermi sphere, the reason for the effect is entirely different in this case. In his treatment TAYLOR considers the matrix elements as slowly varying functions and attributes the effect to the shape of the Fermi surface (through the energy of the one-particle states), but here to lowest order the effect is seen to be due to the rapid variation of the matrix element and present even for a spherical Fermi surface.

In Fig. 1 some traces in the $\boldsymbol{K}-\boldsymbol{q}$-plane of the first zone in a f.c.c. lattice have been drawn. It can be seen that the curve $A-A'$ is rather far out from 0, in a region where the influence on the dynamical matrix from elements $\langle\boldsymbol{q}|\varkappa_1|\boldsymbol{K}+\boldsymbol{q}\rangle$ is expected to be small. In any case it is clear from Fig. 1 that the regions of particular interest are those around A (or A') and also around the intersection M_2, where two singularities are added. It is also of interest to observe the detailed shape of the function u_1 close to the edge along $A-A'$. In Fig. 2 some results of an accurate computation are shown for some values of the angle between $\boldsymbol{K}$ and $\boldsymbol{q}$. In Fig. 3 results are shown of a more extensive computation of u_1 close to A'. The edge-effect is seen to set in for

$$c_1 = \cos\theta > -\frac{K}{2k_0} \approx -0.8871.$$

Around M_2 the function is found to be quite smooth. It is almost impossible to detect the logarithmic infinities in the slope, even in a very detailed computation. However, in both these regions around A' (and A) and M_2 the influence from the neglected terms in Eq. (46) can be expected to give comparatively large "rounding off" effects and the results given here have for that reason to be interpreted with some care.

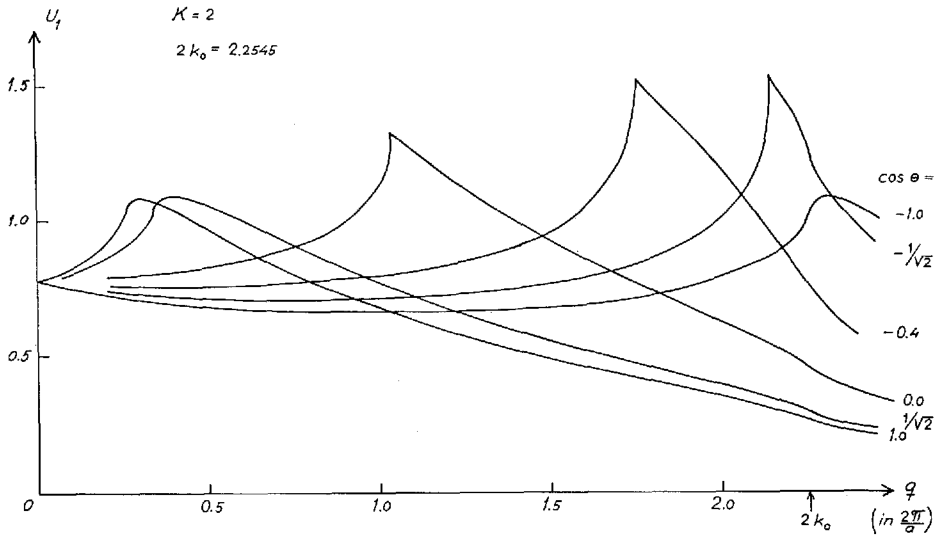

Fig. 2.

Fig. 2, 3 and 4. $u_1(\mathbf{K},\mathbf{q})$ as a function of q for some K and $\cos\theta = \dfrac{\mathbf{K}\cdot\mathbf{q}}{Kq}$.

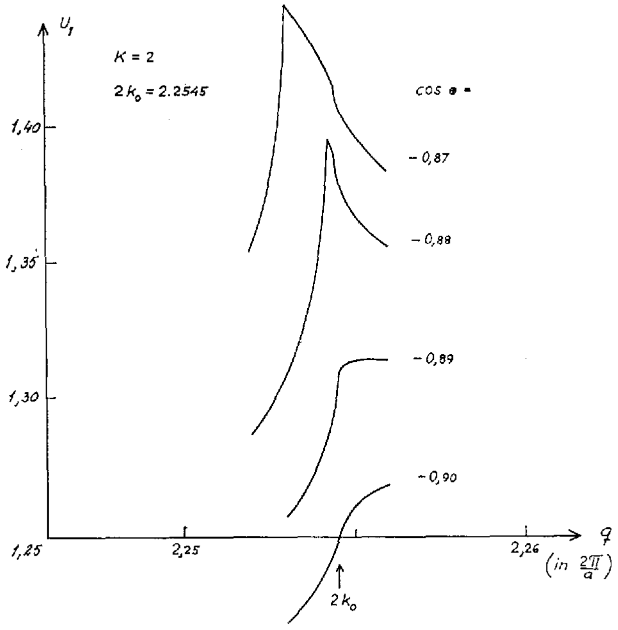

Fig. 3.

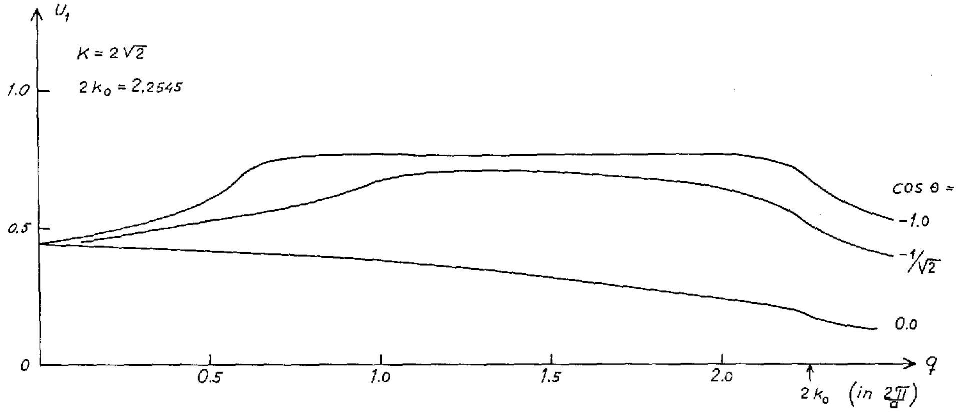

Fig. 4.

In the case $Z_0 > 1$, the function u_1 becomes much less dramatic. In this case the point $0'$ in Fig. 1 lies outside the circle $q = 2k_0$, and $R_i(Z_j) > 0$ for all values of $\boldsymbol{q}$. Hence the edge-effect does not appear in this case and only the logarithmic infinities appear in the slope on the circles $q = 2k_0$ and $|\boldsymbol{K} + \boldsymbol{q}| = 2k_0$. In Fig. 4 the result is shown of a computation for Al in the case $K = 2\sqrt{2}$.

There is a third possibility, namely $Z_0 > 2$: the two circles at 0 and $0'$ in Fig. 1 then lie completely outside each other. This alternative has not been investigated in detail, but nothing of importance is expected to happen in this case either.

In the appendix the function $u_2(\boldsymbol{K},\boldsymbol{q})$ is split into two parts so that the trivial effect from the change in the Fermi energy is treated separately. We write

$$u_2(\boldsymbol{K},\boldsymbol{q}) = u_2'(\boldsymbol{K},\boldsymbol{q}) + u_2''(\boldsymbol{K},\boldsymbol{q}) \qquad (57)$$

where $u_2''(\boldsymbol{K},\boldsymbol{q})$ gives the isotropic effect from the decrease in the Fermi energy and is given in Eq. (A 30). The more interesting part $u_2'(\boldsymbol{K},\boldsymbol{q})$ is in the appendix written as follows

$$u_2'(\boldsymbol{K},\boldsymbol{q}) = \tfrac{1}{2}\{w_2(\boldsymbol{K},\boldsymbol{q}) + w_2(-\boldsymbol{K},\boldsymbol{q})\} \qquad (58)$$

and is also given in Eq. (A 30). Due to the axial symmetry of u_2' around the direction $\boldsymbol{K}$ and its evenness in q it is again only necessary to consider $\boldsymbol{K}$ and $\boldsymbol{q}$ in a plane, and this time only for values of c_1 satisfying $0 \leq c_1 \leq 1$. Of interest to us here is the behaviour of $u_2(\boldsymbol{K},\boldsymbol{q})$ for rather small values of q: say for q within a sphere inscribed in the first zone, since it is only for such q:s the corrections from u_2 are expected to be significant. This restriction is important because both the expressions in Eq. (A 30) are singular for q:s outside this sphere. The singularity in u_2'' is obvious at $Z_1 = 1$, which means

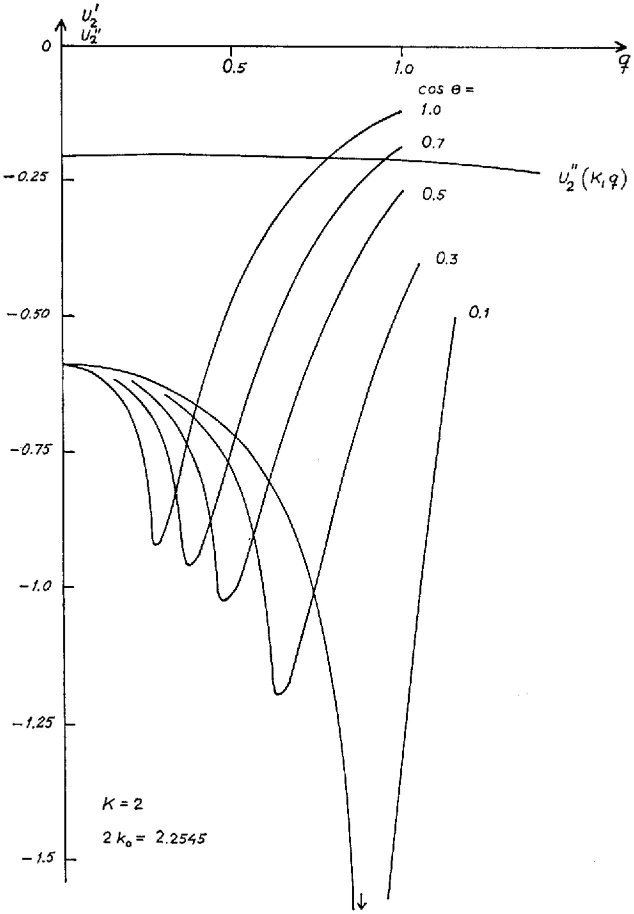

Fig. 5.

Fig. 5 and 6. The second order functions u_2' and u_2'' for some values of K and the angle θ.

when $q = 2k_0$. In u_2 the factor $\frac{1}{\sqrt{R_{10}}}$ produces singularities along the arc of the circle at M_1 denoted by $A - A'$ in Fig. 1. This arc also has to be reflected in the line $A - O$ in order to give the total picture in this case. The singularities are naturally quite non-physical, and indicate that the element $\langle \boldsymbol{q}|\varkappa|\boldsymbol{q}\rangle$ cannot be expanded in a power series in $V(\boldsymbol{K})$ at zero temperature, which might be expected from Lindhard's formula. They have to be removed if the function u_2 is to be defined all over the $\boldsymbol{K} - \boldsymbol{q}$-plane. This removal requires among other things a more careful investigation of the contributions to u_2 from states

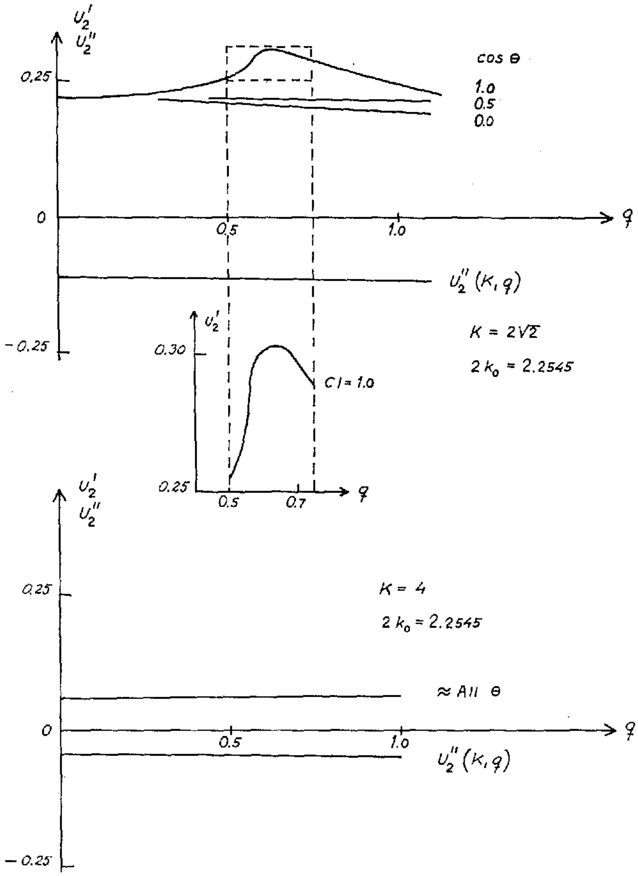

Fig. 6.

close to the zone boundary. At any rate, the expression given would suffice here because the correction is only being considered for small q well inside the first zone.

The qualitative difference between the cases $Z_0 < 1$ and $Z_0 > 1$ is more marked here than in the first order case. In Figs. 5 and 6 some results of a calculation for $K = 2$ and $K = 2\sqrt{2}$; 4; have been collected, using the value of $2k_0 = 2.2545$.

The significant difference between the two cases is this that for $Z_0 < 1$, $u_2'(\boldsymbol{K},\boldsymbol{q})$ is comparatively large and negative for the relevant values of $\boldsymbol{q}$ (it becomes positive for larger q) whereas for $Z_0 > 1$, $u_2'(\boldsymbol{K},\boldsymbol{q})$ is positive. This means that in the $Z_0 < 1$ case there is a comparatively strong reduction of the dielectric function for small q. The effect from terms with $Z_0 < 1$ is then to increase the frequency of the longitudinal phonons, contrary to what might be expected for the effect from the lattice potential. For $Z_0 < 1$ there are also interesting peaks with infinities in the slope to the left, at points where $|\boldsymbol{K} + \boldsymbol{q}| = 2k_0$. The infinities are here of the same logarithmic kind as those found in the function $u_1(\boldsymbol{K},\boldsymbol{q})$ at these points.

In the case $Z_0 > 1$, however, the function u_2 contains little of interest. For all relevant values of q, $u_2 > 0$, and as in the case of u_1 there is a weak singularity in the slope at $Z_3 = 1$. (Seen in Fig. 6 for $K = 2\sqrt{2}$.) For still larger K the function u_2' becomes practically isotropic for all values of q of interest. This is also seen in Fig. 6 for $K = 4$. There it can also be observed how fast the physically interesting quantity $u_2' + u_2''$ goes to zero. For $K = 2$, this quantity is numerically of the order 1 at $q = 0$. But already for $K = 4$ it has decreased to about 0.01, and for $K = 6$ it has gone down to about 0.002. This rapid convergency even in the function u_2 indicates that no practical problem will arise in the performance of the sum in Eq. (50).

The model developed in this paper has been applied to aluminium by the present author and A Westin. The results of the calculations are collected in: On Phonons in Simple Metals II, AB Atomenergi, Studsvik, Nyköping, Sweden, Report AE-365 (1969).

Acknowledgement

I wish to thank Prof. Bernard Goodman, on visit in Sweden at the time of this investigation (1962–63), for many valuable suggestions during the course of the work. I am also indebted to Prof:s A. Sjölander and H. Højgaard-Jensen for kindly reading the manuscript and suggesting some improvements. Finally, I thank the members and staff at NORDITA for a pleasant time in Copenhagen and AB Atomenergi for financial support.

Appendix

Our problem is to find explicit expressions for the various functions u_i introduced in the text.

For completeness we include also the LINDHARD [17] expression for $u_0(q)$.

From Eq. (49) we have (**q** an arbitrary vector in the following)

$$\left.\begin{aligned} e^2\varkappa_0(\boldsymbol{q},\omega) &= -\,e^2 v(q) 2P \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{f(k)-f(k')}{\varepsilon(k)-\varepsilon(k')+\omega}\,\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}} = \frac{k_0}{\pi^2 a_0}\,\cdot \\ &\quad \cdot v(q)\, u_0(q,\omega) \end{aligned}\right\} \tag{A 1}$$

where

$$u_0(q,\omega) = \frac{1}{2\pi k_0} P \int \frac{f(k)d\boldsymbol{k}}{2\boldsymbol{k}\cdot\boldsymbol{q} + q^2 \pm 2m\omega} \tag{A 2}$$

which gives

$$u_0(q,\omega) = \frac{1}{8Z_1}\left\{(1-Z_{1\pm}^2)\ln\left|\frac{1+Z_{1\pm}}{1-Z_{1\pm}}\right| + 2Z_{1\pm}\right\} \tag{A 3}$$

in the zero T case. We have in Eq. (A 3) put $Z_1 = \dfrac{q}{2k_0}$; $Z_\pm = Z_1 \pm \dfrac{\omega}{4\varepsilon_0 Z_1}$ and shall add the expression for Z_{1+} and Z_{1-}.

For the first order element we get from Eq. (46) after removing a factor $V(\boldsymbol{K})$ in the coefficients $c(\boldsymbol{k},\boldsymbol{K})$ in Eq. (42) and passing to the limit $V = 0$ in the remaining expression

$$e^2\langle \boldsymbol{q}\,|\,\varkappa_1(\omega)\,|\,\boldsymbol{K}+\boldsymbol{q}\rangle = \frac{k_0}{\pi^2 a_0}\,\frac{V(\boldsymbol{K})}{\varepsilon_0}\left[v(q)v(\boldsymbol{K}+\boldsymbol{q})\right]^{1/2} u_1(\boldsymbol{K},\boldsymbol{q},\omega) \tag{A 4}$$

where

$$\left.\begin{aligned} u_1(\boldsymbol{K},\boldsymbol{q},\omega) = -\frac{k_0}{2\pi} P \int f(k)\, d\boldsymbol{k} \Bigg\{ \frac{1}{2\boldsymbol{k}\cdot\boldsymbol{q} + q^2 \pm 2m\omega} \cdot \\ \cdot \left[\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k} - K^2} - \frac{1}{2\boldsymbol{K}(\boldsymbol{k}+\boldsymbol{q}) + K^2}\right] - \frac{1}{2\boldsymbol{k}(\boldsymbol{K}+\boldsymbol{q}) + (\boldsymbol{K}+\boldsymbol{q})^2 \pm 2m\omega} \cdot \\ \cdot \left[\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k} + K^2} - \frac{1}{2\boldsymbol{K}(\boldsymbol{k}+\boldsymbol{q}) + K^2}\right]\Bigg\} \end{aligned}\right\} \tag{A 5}$$

with the P symbol extended to all singularity planes.

In order to integrate this expression in the zero T limit we choose axes and variables as follows

$$\left.\begin{aligned} \boldsymbol{K} &= K(0,0,1); \; \boldsymbol{q} = q(s_1, 0, c_1) \\ \boldsymbol{K}+\boldsymbol{q} &= |\boldsymbol{K}+\boldsymbol{q}|(s_3, 0, c_3) \\ \boldsymbol{k} &= k_0(\varrho\cos\varphi, \varrho\sin\varphi, Z); \; d\boldsymbol{k} = k_0^3\, dZ \varrho\, d\varrho\, d\varphi \end{aligned}\right\} \tag{A 6}$$

and are also going to use the following notations

$$\left.\begin{aligned} Z_0 &= \frac{K}{2k_0}; \; Z_{1\pm} = Z_1 \pm \frac{\omega}{4\varepsilon_0 Z_1} \quad \text{as earlier} \\ Z_2 &= \frac{\boldsymbol{K}(\boldsymbol{K}+\boldsymbol{q})}{4k_0^2 Z_0} = Z_0 + 2c_1 Z_1 \\ Z_3 &= \frac{|\boldsymbol{K}+\boldsymbol{q}|}{2k_0}; \; Z_{3\pm} = Z_3 \pm \frac{\omega}{4\varepsilon_0 Z_3}. \end{aligned}\right\} \tag{A 7}$$

From (A 6) and (A 7) we get the relationships

$$s_3^2 = \left(\frac{Z_1}{Z_3}\right)^2 s_1^2; \; c_3 = \frac{Z_0 + c_1 Z_1}{Z_3}. \tag{A 8}$$

After performing some simple integrations, we get for $T = 0$

$$\left.\begin{aligned} u_1(\boldsymbol{K},\boldsymbol{q},\omega) = \frac{1}{16 Z_0}\Bigg\{\frac{1}{Z_1 s_1^2}\Bigg[(c_1 Z_0 + Z_{1\pm})\ln\left|\frac{1+Z_0}{1-Z_0}\right| \\ + P\int_{-1}^{1} dZ \sqrt{R_{1\pm}(Z)}\left(\frac{1}{Z - Z_0} - \frac{1}{Z + Z_2}\right)\Bigg] - \frac{1}{Z_3 s_3^2}\Bigg[(c_3 Z_0 - Z_{3\pm}) \cdot \\ \cdot \ln\left|\frac{1+Z_0}{1-Z_0}\right| + P\int_{-1}^{1} dZ\sqrt{R_{3\pm}(Z)}\left(\frac{1}{Z + Z_0} - \frac{1}{Z + Z_2}\right)\Bigg]\Bigg\} \end{aligned}\right\} \tag{A 9}$$

where

$$\left.\begin{aligned} R_{1\pm}(Z) &= Z^2 + 2c_1 Z_{1\pm} Z + Z_{1\pm}^2 - s_1^2 \\ R_{3\pm}(Z) &= Z^2 + 2c_3 Z_{3\pm} Z + Z_{3\pm}^2 - s_3^2. \end{aligned}\right\} \quad \text{(A 10)}$$

The integrations in Eq. (A 9) are only over real values of the square-roots which are interpreted in these intervals as follows

$$\left.\begin{aligned} \sqrt{R_{1\pm}(Z)} &= \operatorname{sgn}(c_1 Z + Z_{1\pm}) \, |R_{1\pm}(Z)|^{1/2} \\ \sqrt{R_{3\pm}(Z)} &= \operatorname{sgn}(c_3 Z + Z_{3\pm}) \, |R_{3\pm}(Z)|^{1/2}. \end{aligned}\right\} \quad \text{(A 11)}$$

By writing the integrand

$$\begin{aligned} \frac{\sqrt{R_{1\pm}(Z)}}{Z - Z_0} = \frac{1}{\sqrt{R_{1\pm}(Z)}(Z - Z_0)} \{ & R_{1\pm}(Z_0) + R_{1\pm}'(Z_0)(Z - Z_0) + \\ & + (Z - Z_0)^2 \} \quad \text{where} \quad R_{1\pm}'(Z_0) = \left(\frac{dR_{1\pm}}{dZ} \right)_{Z_0} \end{aligned}$$

and similarly for the others, we get after performing the integrations and some reductions.

$$\left.\begin{aligned} u_1(\boldsymbol{K}, \boldsymbol{q}, \omega) = \frac{1}{16 Z_0 Z_1 s_1^2} \Bigg\{ & 2(Z_0 + c_1 Z_1) \ln \left| \frac{1 + Z_{1\pm}}{1 - Z_{1\pm}} \right| \\ & + 2(c_1 Z_0 + Z_{1\pm}) \ln \left| \frac{1 + Z_0}{1 - Z_0} \right| - 2 c_1 Z_3 \ln \left| \frac{1 + Z_{3\pm}}{1 - Z_{3\pm}} \right| \\ + \operatorname{sgn}(R_{1\pm}(Z_0)) \sqrt{R_{10}^{\pm}} (I_{10}^{\pm} - I_{30}^{\pm}) & - \operatorname{sgn}(R_{1\pm}(-Z_2)) \cdot \sqrt{R_{12}^{\pm}} (I_{12}^{\pm} - I_{32}^{\pm}) \Bigg\} \end{aligned}\right\} \quad \text{(A 12)}$$

where $I_{ij}^{\pm}$ means

$$\left.\begin{aligned} I_{10}^{\pm} &= \sqrt{R_{10}^{\pm}} P \int_{-1}^{1} \frac{dZ}{(Z - Z_0)\sqrt{R_{1\pm}(Z)}} = \begin{cases} \ln \left| \dfrac{c_1 + Z_0 Z_{1\pm} - \sqrt{R_{10}^{\pm}}}{c_1 + Z_0 Z_{1\pm} + \sqrt{R_{10}^{\pm}}} \right| & \text{if } R_{1\pm}(Z_0) > 0 \\ 2 \operatorname{arctg} \left(\dfrac{c_1 + Z_0 Z_{\pm 1}}{\sqrt{R_{10}^{\pm}}} \right) & \text{if } R_{1\pm}(Z_0) < 0 \end{cases} \\ I_{12}^{\pm} &= \sqrt{R_{12}^{\pm}} P \int_{-1}^{1} \frac{dZ}{(Z + Z_2)\sqrt{R_{1\pm}(Z)}} = \begin{cases} \ln \left| \dfrac{c_1 - Z_2 Z_{1\pm} - \sqrt{R_{12}^{\pm}}}{c_1 - Z_2 Z_{1\pm} + \sqrt{R_{12}^{\pm}}} \right| & \text{if } R_{\pm 1}(-Z_2) > 0 \\ 2 \operatorname{arctg} \left(\dfrac{c_1 - Z_2 Z_{1\pm}}{\sqrt{R_{12}^{\pm}}} \right) & \text{if } R_{1\pm}(-Z_2) < 0 \end{cases} \end{aligned}\right\} \quad \text{(A 13)}$$

$$\left.\begin{aligned} I_{30}^{\pm} &= \sqrt{R_{30}^{\pm}}\,P\int_{-1}^{1}\frac{dZ}{(Z+Z_0)\sqrt{R_{1\pm}(Z)}} = \\ I_{32}^{\pm} &= \sqrt{R_{32}^{\pm}}\,P\int_{-1}^{1}\frac{dZ}{(Z+Z_2)\sqrt{R_{3\pm}(Z)}} = \end{aligned}\right\}\text{similar expressions}\quad\left.\vphantom{\int_{-1}^{1}}\right\}\quad (\text{A }13)$$

where in Eq. (A 13) $\sqrt{R_{10}^{\pm}} = |R_{1\pm}(Z_0)|^{1/2}$, and similarly for the others. The evaluation of the integrals $I_{ij}^{\pm}$ is a little bit tricky, at least in case $R_{i\pm}(Z_j) < 0$. We have to consider the two distinct cases possible (depending on whether $R_{i\pm}(\pm 1)$ have the same sign or not) with the sign rule in Eq. (A 11) in mind and to keep track of which branch of the cyclometric function we deal with. In Eq. (A 13), however, all angles are in the interval $-\pi \leq I_{ij}^{\pm} \leq \pi$. When doing the reduction in Eq. (A 13) we have also used the following relationsships

$$\left.\begin{aligned} R_{1\pm}(Z_0) &= \left(\frac{Z_3}{Z_1}\right)^2 R_{3\pm}(-Z_0) \\ R_{1\pm}(-Z_2) &= \left(\frac{Z_3}{Z_1}\right)^2 R_{3\pm}(-Z_2). \end{aligned}\right\}\quad (\text{A }14)$$

The corrections to the Lindhard value of the diagonal part of $\varkappa$ had in Eq. (48) and Eq. (49) three different sources. Considering first the contribution from the change in the matrix M in Eq. (45). We get this part after removing a factor $V(\boldsymbol{K})^2$ and passing to the limit $V = 0$ in the remaining expression.

$$\left.\begin{aligned} e^2\langle \boldsymbol{q}|\varkappa_2^M|\boldsymbol{q}\rangle &= e^2 v(q)\sum_{\boldsymbol{K}}{}' |V(\boldsymbol{K})|^2\cdot 2P\sum_{\boldsymbol{k},\boldsymbol{k}'} \\ \frac{f(k)-f(k')}{\varepsilon(k)-\varepsilon(k')+\omega} &\left\{\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{q}}\left[\frac{1}{\varepsilon(k)-\varepsilon(\boldsymbol{k}+\boldsymbol{K})}-\frac{1}{\varepsilon(k')-\varepsilon(\boldsymbol{k}'+\boldsymbol{K})}\right]^2 - \right. \\ &\left. -\,\delta_{\boldsymbol{k}'}^{\boldsymbol{k}+\boldsymbol{K}+\boldsymbol{q}}\left[\frac{1}{\varepsilon(k)-\varepsilon(\boldsymbol{k}+\boldsymbol{K})}+\frac{1}{\varepsilon(k')-\varepsilon(\boldsymbol{k}'-\boldsymbol{K})}\right]^2\right\} \end{aligned}\right\}\quad (\text{A }15)$$

with again the P symbol extended to all singularity planes. This contribution – and as we will see later, the others too – is made up of a sum over all $\boldsymbol{K} \neq 0$. This fact may be used to simplify the calculations by a proper choice of the terms in this sum. Of interest to us is to find the function $u_2(\boldsymbol{K},\boldsymbol{q})$ having the same symmetry as the lattice, which means a function even in q in this case. Thus, with

$$e^2 \langle \boldsymbol{q} | \varkappa_2^M | \boldsymbol{q} \rangle = \frac{k_0}{\pi^2 a_0} \sum_{\boldsymbol{K}}' \left(\frac{V(\boldsymbol{K})}{\varepsilon_0} \right)^2 v(q)\, u_2^M(\boldsymbol{K}, \boldsymbol{q}, \omega), \tag{A 16}$$

we write

$$\left.\begin{aligned} u_2^M(\boldsymbol{K}, \boldsymbol{q}, \omega) = -\frac{k_0^3}{2\pi} P \int \Bigg\{ \frac{f(k) d\boldsymbol{k}}{2\boldsymbol{K}\cdot\boldsymbol{q} + q^2 \pm 2m\omega} \cdot \\ \cdot \left[\left(\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k} - K^2} \right)^2 + \left(\frac{1}{2\boldsymbol{K}(\boldsymbol{k}+\boldsymbol{q}) + K^2} \right)^2 \right] - \frac{f(k) d\boldsymbol{k}}{2\boldsymbol{k}(\boldsymbol{K}+\boldsymbol{q}) + (\boldsymbol{K}+\boldsymbol{q})^2 \pm 2m\omega} \cdot \\ \cdot \left[\left(\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k} + K^2} \right)^2 + \left(\frac{1}{2\boldsymbol{K}(\boldsymbol{k}+\boldsymbol{q}) + K^2} \right)^2 \right] \Bigg\} - \frac{1}{4 Z_0 Z_1 c_1} u_1(\boldsymbol{K}, \boldsymbol{q}, \omega) \end{aligned} \right\} \tag{A 17}$$

where we have made a substitution $\boldsymbol{K} \rightarrow -\boldsymbol{K}$ in appropriate terms. Similar calculations as in the previous case give in the zero T limit

$$\left.\begin{aligned} u_2^M(\boldsymbol{K}, \boldsymbol{q}, \omega) = \frac{1}{64 Z_0} \Bigg(\Bigg\{ \frac{c_1}{Z_1 s_1^2} \ln \left| \frac{1+Z_0}{1-Z_0} \right| - \frac{c_1}{Z_1 s_1^2} \cdot \\ \cdot \ln \left| \frac{1+Z_2}{1-Z_2} \right| + \frac{c_3}{Z_3 s_3^2} \ln \left| \frac{1+Z_0}{1-Z_0} \right| + \frac{c_3}{Z_3 s_3^2} \ln \left| \frac{1+Z_2}{1-Z_2} \right| + \\ + P \int_{-1}^{1} dZ \frac{\sqrt{R_{1\pm}(Z)}}{Z_1 s_1^2} \left[\frac{1}{(Z-Z_0)^2} + \frac{1}{(Z+Z_2)^2} \right] - P \int_{-1}^{1} dZ \frac{\sqrt{R_{3\pm}(Z)}}{Z_3 s_3^2} \cdot \\ \cdot \left[\frac{1}{(Z+Z_0)^2} + \frac{1}{(Z+Z_2)^2} \right] \Bigg\} - \frac{1}{4 Z_0 Z_1 c_1} u_1(\boldsymbol{K}, \boldsymbol{q}, \omega) \end{aligned} \right\} \tag{A 17}$$

where we have exposed the integrals, which are singular in case $|Z_0| < 1$ or/and $|Z_2| < 1$, if the integrations are over these Z-values. With

$$\int dZ \frac{\sqrt{R_{1\pm}(Z)}}{(Z-Z_0)^2} = -\frac{\sqrt{R_{1\pm}(Z)}}{(Z-Z_0)} + \int \frac{dZ\, R_{1\pm}'(Z)}{2(Z-Z_0)\sqrt{R_{1\pm}(Z)}} \tag{A 18}$$

and similar expressions for the others, we get from Eqs. (A 7), (A 8), (A 11) and (A 14) a cancellation of the dangerous terms; in fact all integrated parts in Eq. (A 18) and the similar expressions for the others are seen to completely cancel. Performing the remaining integrations, gives

$$\left.\begin{aligned} u_2^M(\boldsymbol{K},\boldsymbol{q},\omega) &= \frac{1}{64Z_0^2Z_1^2s_1^2}\left\{Z_2\ln\left|\frac{1+Z_0}{1-Z_0}\right| + \right.\\ &\left. + 2Z_1\ln\left|\frac{1+Z_{1\pm}}{1-Z_{1\pm}}\right| + Z_0\ln\left|\frac{1+Z_2}{1-Z_2}\right| - 2Z_3\ln\left|\frac{1+Z_{3\pm}}{1-Z_{3\pm}}\right|\right\}\\ &+ \frac{1}{64Z_0^2}\left\{\frac{(Z_0+c_1Z_{1\pm})}{s_1^2Z_1\sqrt{R_{10}^\pm}}I_{10}^\pm - \frac{(Z_2-c_1Z_{1\pm})}{s_1^2Z_1\sqrt{R_{12}^\pm}}I_{12}^\pm\right.\\ &\left.+\frac{(Z_0-c_3Z_{3\pm})}{s_3^2Z_3\sqrt{R_{30}^\pm}}I_{30}^\pm + \frac{(Z_2-c_3Z_{3\pm})}{s_3^2Z_3\sqrt{R_{32}^\pm}}I_{32}^\pm\right\} - \frac{1}{4Z_0Z_1c_1}u_1(\boldsymbol{K},\boldsymbol{q},\omega) \end{aligned}\right\} \tag{A 15}$$

where again we may reduce the expression by use of the relationships given earlier. We leave, however, this to a later stage in this case.

Next we consider the lowest order contribution to $\langle\boldsymbol{q}|\varkappa_2|\boldsymbol{q}\rangle$ from the correction of the energy denominator in Eq. (49). By a similar procedure as in the previous case, we get

$$\left.\begin{aligned} u_2^E(\boldsymbol{K},\boldsymbol{q},\omega) &= \frac{k_0^3}{2\pi}P\int d\boldsymbol{k}\frac{f(k)}{(2\boldsymbol{k}\cdot\boldsymbol{q}+q^2\pm 2m\omega)^2}\left\{\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k}-K^2}+\right.\\ &\left.+\frac{1}{2\boldsymbol{K}(\boldsymbol{k}+\boldsymbol{q}+K^2)}\right\} \end{aligned}\right\} \tag{A 20}$$

where the second order singularity clearly must be interpreted as the limit of two nearby first order singularities, then giving zero contribution when the principal value is taken.

Similar calculations as those already shown give in the zero T limit

$$\left.\begin{aligned} u_2^E(\boldsymbol{K},\boldsymbol{q},\omega) &= \frac{1}{64\,Z_0Z_1^2s_1^2}\left\{2c_1\ln\left|\frac{1+Z_{1\pm}}{1-Z_{1\pm}}\right|+\right.\\ &\left.+\ln\left|\frac{1+Z_0}{1-Z_0}\right| - \ln\left|\frac{1+Z_2}{1-Z_2}\right| + \frac{(c_1Z_0+Z_{1\pm})}{\sqrt{R_{10}^\pm}}I_{10}^\pm - \frac{(c_1Z_2-Z_{1\pm}}{\sqrt{R_{12}^\pm}}I_{12}^\pm\right\}. \end{aligned}\right\} \tag{A 21}$$

In this case it is practical to use axes with $\boldsymbol{q} = q(0, 0, 1)$ and $\boldsymbol{K} = K(s_1, 0, c_1)$ and, then, to introduce functions $R_0(Z) = Z^2 - 2c_1Z_0Z + Z_0^2 - s_1^2$ and $R_2(Z) = Z^2 + 2c_1Z_2Z + Z_2^2 - s_1^2$, which lead to integrals as

$$\int_{-1}^{1}\frac{dZ}{(Z+Z_{1\pm})\sqrt{R_0(Z)}} = \int_{-1}^{1}\frac{dZ}{(Z-Z_0)\sqrt{R_{1\pm}(Z)}} = \frac{I_{10}^\pm}{\sqrt{R_{10}^\pm}}.$$

Finally we consider the effect from the change in the Fermi factors in Eq. (49).

To lowest order we have

$$g(\boldsymbol{k}) = \frac{\partial f(k)}{\partial \varepsilon}\{E(\boldsymbol{k}) - \varepsilon(k) - (\mu - \mu_0)\} \tag{A 22}$$

and then a contribution to u_2

$$u_2^F(\boldsymbol{K},\boldsymbol{q},\omega) = \frac{k_0^3}{4m\pi} P\int d\boldsymbol{k} \frac{\dfrac{\partial f(k)}{\partial \varepsilon}}{2\boldsymbol{k}\cdot\boldsymbol{q} + q^2 \pm 2m\omega} \cdot \left\{\frac{1}{2\boldsymbol{K}\cdot\boldsymbol{k} - K^2} - \frac{\eta(\boldsymbol{K})}{k_0^2}\right\} \tag{A 23}$$

where we have written

$$\mu - \mu_0 = \frac{1}{\varepsilon_0}\sum_{\boldsymbol{K}}{}' |V(\boldsymbol{K})|^2 \eta(\boldsymbol{K}). \tag{A 24}$$

In the zero T limit is $\dfrac{\partial f(k)}{\partial \varepsilon} = -\delta(\varepsilon - \varepsilon_0) = -\dfrac{m}{k_0}\{\delta(k - k_0) + \delta(k + k_0)\}$.

In that case we get from the condition $\sum_{\boldsymbol{K}} g(\boldsymbol{k}) = 0$ the following expression for $\eta(\boldsymbol{K})$

$$\eta(\boldsymbol{K}) = -\frac{1}{8Z_0}\ln\left|\frac{1 + Z_0}{1 - Z_0}\right|, \tag{A 25}$$

which finally gives

$$u_2^F(\boldsymbol{K},\boldsymbol{q},\omega) = -\frac{1}{64\,Z_0 Z_1}\left\{\frac{2}{\sqrt{R_{10}^{\pm}}} I_{10}^{\pm} + \ln\left|\frac{1 + Z_0}{1 - Z_0}\right| \cdot \ln\left|\frac{1 + Z_{1\pm}}{1 - Z_{1\pm}}\right|\right\}. \tag{A 26}$$

Collecting all contributions gives the following cumbersome expression (where the first two terms cancel when the sum over $\boldsymbol{K}$ is performed)

$$\left.\begin{aligned} u_2^M + u_2^E + u_2^F = &-\frac{1}{32\,Z_0^2 Z_1 c_1}\ln\left|\frac{1 + Z_0}{1 - Z_0}\right| - \\ &-\frac{1}{32\,Z_0 Z_1^2 c_1}\ln\left|\frac{1 + Z_{1\pm}}{1 - Z_{1\pm}}\right| + \frac{1}{64 Z_0^2 Z_1^2 c_1 \sqrt{R_{10}^{\pm}}} \\ &\left\{\frac{[c_1 Z_1(Z_0 + c_1 Z_{1\pm}) + c_1 Z_0(c_1 Z_0 + Z_{1\pm}) - 2s_1^2 c_1 Z_0 Z_1 - R_{1\pm}(Z_0)]}{s_1^2}\cdot\right. \\ &\left.\cdot I_{10}^{\pm} + \frac{[c_1 Z_1(Z_0 - c_3 Z_{3\pm}) + R_{3\pm}(-Z_0)]}{s_3^2} I_{30}^{\pm}\right\} - \end{aligned}\right\} \tag{A 27}$$

$$\left.\begin{aligned} - \frac{1}{64 Z_0^2 Z_1^2 c_1 \sqrt{R_{12}^{\pm}}} \Bigg\{ & \frac{[c_1 Z_1 (Z_2 - c_1 Z_{1\pm}) + c_1 Z_0 (c_1 Z_2 - Z_{1\pm}) - R_{1\pm}(- Z_2)]}{s_1^2} \cdot I_{12}^{\pm} \\ & - \frac{[c_1 Z_1 (Z_2 - c_3 Z_{3\pm}) - R_{3\pm}(- Z_2)]}{s_3^2} I_{32}^{\pm} \Bigg\} + u_2'' \end{aligned}\right\} \quad \text{(A 27)}$$

with $u_2''(\boldsymbol{K}, \boldsymbol{q}, \omega)$ the last part of u_2^F in Eq. (A 26), i.e. the contribution from the change in the Fermi energy caused by the periodic potential.

As mentioned earlier, we are in this case interested in the function $u_2(\boldsymbol{K}, \boldsymbol{q}, \omega)$ which is even in q. For this reason we define the function

$$u_2 = u_2' + u_2''. \quad \text{(A 28)}$$

With u_2'' already of the desired form and with

$$u_2'(\boldsymbol{K}, \boldsymbol{q}, \omega) = \tfrac{1}{2} [u_2^M(\pm c_1) + u_2^E(\pm c_1) + u_2^F(\pm c_1)] - u_2''. \quad \text{(A 29)}$$

We have here consequently dragged along the ω-dependency of the various functions u_i in order to explicitly show how unimportant (in this case) the non-adiabatic corrections are in the real part of $\varkappa$. The ω-dependency comes in via quantities like $Z_{1\pm} = Z_1 \pm \frac{\omega}{4 \varepsilon_0 Z_1}.$ In the phonon case $Z_{1\pm}$ is thus almost identical with Z_1 except when Z_1 is very small. In this limit $\frac{\omega}{4 \varepsilon_0 Z_1}$ tends to a constant $\frac{c}{v_0}$ = (sound velocity/Fermi velocity at zero T for the free electrons) $\approx 10^{-3}$. In almost all practical calculations it is, therefore, quite safe to neglect the non-adiabatic corrections completely in the real part of $\varkappa$. And in the adiabatic limit the expression containing the integrals $I_{ij}^{\pm}$ in Eq. (A 27) becomes surprisingly simple. We get in that case

$$\left.\begin{aligned} u_2'(\boldsymbol{K}, \boldsymbol{q}, 0) &= - \frac{1}{64 Z_0^2 Z_1^2} \left\{ \frac{(Z_3^2 - 1)}{c_1 \sqrt{R_{10}}} [I_{10} - I_{12} - I_{30} + I_{32}] \right\}_{\pm c_1} \\ u_2''(\boldsymbol{K}, \boldsymbol{q}, 0) &= - \frac{1}{32 Z_0 Z_1} \cdot \ln \left| \frac{1 + Z_0}{1 - Z_0} \right| \cdot \ln \left| \frac{1 + Z_1}{1 - Z_1} \right| \end{aligned}\right\} \quad \text{(A 30)}$$

where we shall add the two expressions with $\pm c_1$. In the adiabatic limit we have

$$\left.\begin{aligned} R_{1\pm}(Z_0) = R_1(Z_0) = R_1(- Z_2) &= (Z_3^2 - s_1^2); \\ R_{3\pm}(- Z_0) = R_3(- Z_0) = R_3(- Z_2) = (Z_1^2 - s_3^2) &= \left(\frac{Z_1}{Z_3} \right)^2 (Z_3^2 - s_1^2). \end{aligned}\right\} \quad \text{(A 31)}$$

The expression for $u_1(\boldsymbol{K},\boldsymbol{q},\omega)$ in Eq. (A 12) becomes also somewhat simpler in the adiabatic limit. We get from Eq:s (A 12) and (A 31)

$$\left.\begin{aligned} u_1(\boldsymbol{K},\boldsymbol{q},0) &= \frac{1}{8Z_0Z_1s_1^2}\left\{2(Z_0+c_1Z_1)\cdot\ln\left|\frac{1+Z_1}{1-Z_1}\right|+\right.\\ &+2(c_1Z_0+Z_1)\cdot\ln\left|\frac{1+Z_0}{1-Z_0}\right|-2c_1Z_3\cdot\ln\left|\frac{1+Z_3}{1-Z_3}\right|+\\ &\left.+\operatorname{sgn}(R_{10})\sqrt{R_{10}}\left[I_{10}-I_{12}-I_{30}+I_{32}\right]\right\}\end{aligned}\right\} \quad (A\ 32)$$

where in Eq:s (A 30) and (A 32)

$$\sqrt{R_{10}} = |R_{10}|^{1/2}.$$

There is one point worth noticing in connection with the performance of the integrations above. The expressions found for u_1 and u_2 are both singular in case $Z_0 = 1$ and this value for Z_0 is consequently not allowed. We can physically understand this situation by remembering that $Z_0 = 1$ means that the free electron Fermi sphere is just touching a Bragg plane. The principal value calculation close to this plane then breaks down, since this calculation assumes an (essentially continuous) distribution of occupied states on both sides of the plane. In order safely to obtain such a distribution, we must require that Z_0 is sufficiently different from 1, which in physical terms means that we require for any $k = 2k_0Z_0 = \frac{K}{2}$

$$|\varepsilon(k)-\varepsilon_0| > |V(\boldsymbol{K})|.$$

This condition is no serious restriction in actual cases.

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