J. Phys. C: Solid St. Phys., 13(1980) 435–9. Printed in Great Britain

On the mathematical structure of the Lindhard dielectric tensor

B N J Persson

Institute of Theoretical Physics, Chalmers University of Technology, Fack, S-402 20 Göteborg 5, Sweden

Received 23 April 1979

Abstract. The way in which the branch cuts of the Lindhard dielectric tensor are located in the complex-wavenumber plane is shown. Some of its physical implications are discussed.

1. Introduction

The infinite and uniform electron-gas system is an important model when trying to understand a large number of physical processes such as the optical properties of simple metals (Kliewer and Fuchs 1968, Fuchs and Kliewer 1969, Mukhopadhyay and Lundqvist 1978) or the slowing down of a charged particle when passing through a metal (Lindhard 1954). The dielectric tensor $\epsilon_{ij}(\boldsymbol{k}, \omega)$ of the electron gas is of crucial importance in many of these discussions. For a homogeneous and isotropic system this tensor can be written as

$$\epsilon_{ij}(\boldsymbol{k}, \omega) = \delta_{ij}\epsilon_{\mathrm{T}} + (k_i k_j/k^2)(\epsilon_{\mathrm{L}} - \epsilon_{\mathrm{T}}) \tag{1}$$

where ϵ_{L} (the longitudinal dielectric function) and ϵ_{T} (the transverse dielectric function) are functions of the wavenumber $|\boldsymbol{k}|$ and frequency ω.

In this paper we shall take ϵ_{ij} to be the Lindhard dielectric tensor (Lindhard 1954). We shall consider ϵ_{L} and ϵ_{T} as analytical functions in the complex k plane and we will show how the branch cuts of these functions move in the k plane when the frequency ω is varied. In particular, we will find that there is a discontinuous change in one of these branch cuts when ω changes from $\omega_{\mathrm{F}} - 0^+$ to $\omega_{\mathrm{F}} + 0^+$, where ω_{F} is the Fermi frequency of the electron gas.

2. The branch cuts of ϵ_{L} and ϵ_{T}

Let k_{F} be the Fermi wavenumber and ω_{F} the Fermi frequency of an electron gas at zero temperature. We define

$$q = k/k_{\mathrm{F}} \qquad \text{and} \qquad \Omega = \omega/\omega_{\mathrm{F}}.$$

The Lindhard dielectric tensor is given by equation (1) with

$$\epsilon_{\mathrm{L}} = 1 + \tfrac{3}{8}\left(\frac{\omega_{\mathrm{P}}}{\omega_{\mathrm{F}}}\right)^2 \frac{1}{q^2}\left\{1 - \frac{1}{8q^3}F\right\} \tag{2}$$

$$\epsilon_{\mathrm{T}} = 1 - \left(\frac{\omega_{\mathrm{P}}}{\omega_{\mathrm{F}}}\right)^2 \left[\tfrac{3}{8}\left(\frac{q^2}{4} + \frac{3}{4}\frac{\Omega^2}{q^2} + 1\right) + \frac{1}{64q}F\right] \tag{3}$$

where

$$F = (q-a)(q+a)(q-b)(q+b)\ln[(q-a)(q+b)/(q+a)(q-b)]$$
$$+ (q-a')(q+a')(q-b')(q+b')\ln[(q-a')(q+b')/(q+a')(q-b')] \tag{4}$$

where

$$a = -1 + (1+\Omega)^{1/2} \qquad b = 1 + (1+\Omega)^{1/2}$$

$$\left.\begin{array}{l} a' = -1 + \mathrm{i}(\Omega - 1)^{1/2} \\ b' = 1 + \mathrm{i}(\Omega - 1)^{1/2} \end{array}\right\} \qquad \text{if } \Omega > 1$$

$$\left.\begin{array}{l} a' = -1 - (1 - \Omega)^{1/2} \\ b' = 1 - (1 - \Omega)^{1/2} \end{array}\right\} \qquad \text{if } \Omega < 1.$$

ω_{P} in equations (2) and (3) is the plasma frequency.

In these formula it should be implicitly understood that $\Omega = \Omega + \mathrm{i}0^+$ and that the ln function is the principal branch of the logarithmic function. The ϵ_{L} and ϵ_{T} functions are considered as analytical functions in the complex q plane. Associated with the first ln function in equation (4) will be one branch cut from $q = a$ to $q = b$ and another from $q = -a$ to $q = -b$. The second ln function gives one branch cut from $q = a'$ to $q = b'$ and another from $q = -a'$ to $q = -b'$. Since a, b, a' and b' are functions of Ω, it follows that these branch cuts will move around in the q plane when Ω is varied.

Let us denote the branch cut from $q = a$ to $q = b$ by $\mathcal{M}$ and the branch cut from a' to b' by $\mathcal{N}$ (figure 1). We now discuss in detail how $\mathcal{M}$ and $\mathcal{N}$ are located in the q plane and how they move when Ω is varied. For all Ω the branch cut $\mathcal{M}$ is a straight line between $q = a$ and $q = b$, located just above the Re(q) axis (for technical reasons we have drawn $\mathcal{M}$ a finite distance above the Re(q) axis in all figures). The 'length' of $\mathcal{M}$ is equal to $b - a = 2$ and is independent of Ω. When $\Omega \to \infty$ then $a \to -1 + \sqrt{\Omega}$ and $b \to 1 + \sqrt{\Omega}$ so that the centre of $\mathcal{M}$ is located very far from $q = 0$. When Ω decreases $\mathcal{M}$ will move towards $q = 0$ and when $\Omega = 0$, then it is a line segment from $q = 0$ to $q = 2$.

The branch cut $\mathcal{N}$ behaves in a slightly more complicated manner. Assume first that $\Omega > 1$. Since $\mathrm{Re}(a') = -1$ and $\mathrm{Re}(b') = 1$ for $\Omega > 1$, it follows that $\mathcal{N}$ will have one endpoint located on the line $\mathrm{Re}(q) = -1$ and another on $\mathrm{Re}(q) = 1$. However, $\mathcal{N}$ is not a straight line between a' and b' but instead a segment of a circle with its centre at $q = 0$. The radius of the circle is $|a'| = |b'| = \sqrt{\Omega}$. It follows that when $\Omega \to \infty$ then $\mathcal{N}$ will also move towards infinity while it looks more and more like a straight line. When $\Omega \to 1$ then $a' \to -1$ and $b' \to 1$ and $\mathcal{N}$ becomes a half circle with radius $|q| = 1$. It is most interesting that when Ω changes from $1 + 0^+$ to $1 - 0^+$ then $\mathcal{N}$ makes a discontinuous change of shape. The half circle with endpoints at $q = \pm 1$ will change into a straight line between the same endpoints (figure 1). For $\Omega < 1$ then $b' - a' = 2$ so that $\mathcal{N}$ has the same length as $\mathcal{M}$ for these Ω. When $\Omega \to 0$ then $\mathcal{N}$ moves to the left in the q plane and when $\Omega = 0$ it is a line segment from $q = -2$ to $q = 0$. Obviously, for $\Omega = 0$ then $\mathcal{M} + \mathcal{N}$ constitute one single line segment from $q = -2$ to $q = 2$ (figure 1).

The movement of branch cut $\mathcal{M}$ when Ω is varied is usually shown as in figure 2.

In many applications there are integrals of the following type

$$Q = \int_{-\infty}^{\infty} \mathrm{d}q \, \frac{F(q)}{\epsilon(q, \omega)} \tag{5}$$

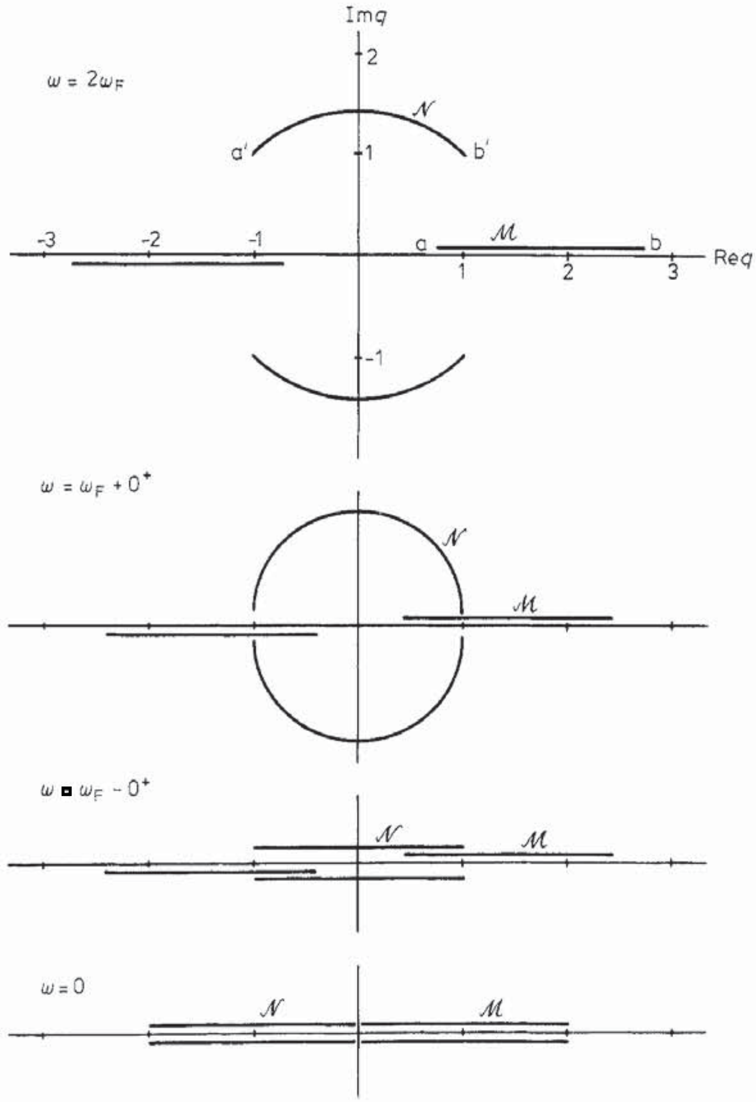

Figure 1. The branch cuts of Lindhard dielectric tensor are shown for four different frequencies ω. All the 'straight line' branch cuts are located an infinitesimal distance from the Re(q) axis.

where ϵ could be either ϵ_L or ϵ_T and where

$$F^*(q) = F(q^*) \qquad \text{and} \qquad F(q) = F(-q).$$

If it is assumed that F is a 'well-behaved function', then it is possible to close the integration contour in the upper half-plane. From the theory of analytical functions it then follows that we can replace the integral in equation (5) with an integral around all branch cuts and poles of the integrand

$$Q = \oint_{\mathcal{M}} \mathrm{d}q \; \frac{F(q)}{\epsilon(q, \omega)} + \oint_{\mathcal{N}} \mathrm{d}q \frac{F(q)}{\epsilon(q, \omega)} + (\text{pole contribution from } F \text{ and } \epsilon^{-1}).$$

Let us assume that $\Omega > 1$. The branch cut $\mathcal{N}$ is located in the q plane as shown in figure 1. Let us denote by $\mathcal{N}_+$ and $\mathcal{N}_-$ respectively those parts of $\mathcal{N}$ which are located in the half-planes $\mathrm{Re}(q) > 0$ and $\mathrm{Re}(q) < 0$. We then have (note $\mathcal{N}_- \to -\mathcal{N}_+$ when $q \to -q^*$)

$$\oint_{\mathcal{N}} \mathrm{d}q \, \frac{F(q)}{\epsilon(q,\omega)} = \oint_{\mathcal{N}_-} \mathrm{d}q \, \frac{F(q)}{\epsilon} + \oint_{\mathcal{N}_+} \mathrm{d}q \, \frac{F(q)}{\epsilon} = \oint_{\mathcal{N}_+} \left(\mathrm{d}q \, \frac{F(q)}{\epsilon} + \mathrm{d}q^* \, \frac{F^*(q)}{\epsilon^*} \right)$$

$$= 2\,\mathrm{Re} \oint_{\mathcal{N}_+} \mathrm{dq} \, \frac{F(q)}{\epsilon}. \tag{6}$$

Consequently, the integral around the branch cut $\mathcal{N}$ is a real number when $\Omega > 1$. The integral around the branch cut $\mathcal{M}$, however, is a complex number. Physically we may say that energy dissipation, due to excitation of electron–hole pairs, can take place (for

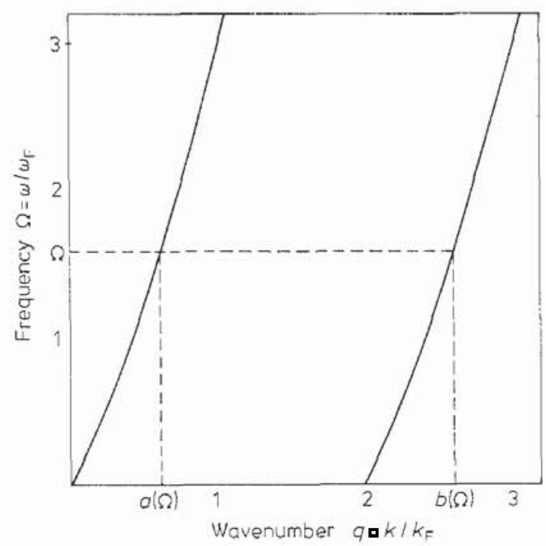

Figure 2. Electron–hole pairs can be excited (for a fixed Ω) with wavenumber $a(\Omega) < q < b(\Omega)$.

$\Omega > 1$) at the branch cut $\mathcal{M}$ but not at the branch cut $\mathcal{N}$. When $\Omega < 1$ then the integral around $\mathcal{N}$ is also complex. Note, however, that when $\Omega = 0$ then $\mathcal{M} + \mathcal{N}$ is a line segment from $q = -2$ to $q = 2$ and it follows that the integral around $\mathcal{M} + \mathcal{N}$ is a real number. From a physical point of view this result is trivial: it just states that no energy dissipation can take place when $\omega = 0$.

3. A simple application

Assume that we have an oscillating monopole located at $\boldsymbol{x} = \boldsymbol{0}$ in an infinite electron gas. Using the Maxwell equation

$$\nabla \,.\, \hat{\epsilon}\boldsymbol{E} = 4\pi q \delta(\boldsymbol{x}) \exp(-\mathrm{i}\omega t)$$

it can be shown that the induced charge density is given by

$$\Delta\rho = \frac{q \exp(-\mathrm{i}\omega t)}{4\pi^2 \mathrm{i}|\boldsymbol{x}|} \int_{-\infty}^{\infty} \mathrm{d}k \, k \exp(\mathrm{i}k|\boldsymbol{x}|) \left(\frac{1}{\epsilon_{\mathrm{L}}(k,\omega)} - 1 \right)$$

and so

$$\Delta\rho = \frac{q \exp(-\mathrm{i}\omega t)}{4\pi^2 \mathrm{i}|\boldsymbol{x}|} \left(\oint_{\mathcal{M}} \mathrm{d}k \, k \, \frac{\exp(\mathrm{i}k|\boldsymbol{x}|)}{\epsilon_{\mathrm{L}}} + \oint_{\mathcal{N}} \mathrm{d}k \, k \, \frac{\exp(\mathrm{i}k|\boldsymbol{x}|)}{\epsilon_{\mathrm{L}}} + R \exp(\mathrm{i}k_{\mathrm{p}}|\boldsymbol{x}|) \right) \tag{7}$$

where

$$\epsilon_L(k_P, \omega) = 0 \qquad \text{and} \qquad \frac{1}{R} = \frac{1}{k_P}\frac{\partial \epsilon_L}{\partial k}\bigg|_{k=k_P}.$$

The last term in equation (7) is the plasmon part of the induced charge density. The asymptotic behaviour (for large $|\boldsymbol{x}|$) of the integrals around the branch cuts $\mathcal{M}$ and $\mathcal{N}$ is determinated by the endpoints of $\mathcal{M}$ and $\mathcal{N}$:

$$\oint_{\mathcal{M}} + \oint_{\mathcal{N}} \sim (1/|\boldsymbol{x}|^2)[\mathcal{M}_1 \exp(\mathrm{i}a|\boldsymbol{x}|) + \mathcal{M}_2 \exp(\mathrm{i}b|\boldsymbol{x}|) + \mathcal{N}_1 \exp(\mathrm{i}a'|\boldsymbol{x}| + \mathcal{N}_2 \exp(\mathrm{i}b'|\boldsymbol{x}|)]$$

$$\text{as} \qquad |\boldsymbol{x}| \to \infty$$

where $\mathcal{M}_1$, $\mathcal{M}_2$, $\mathcal{N}_1$ and $\mathcal{N}_2$ are functions of ω. It is now possible to give a qualitative discussion of the spatial behaviour of $\Delta\rho$ as function of ω:

(i) $\omega = 0$. As we have shown above, $\mathcal{M} + \mathcal{N}$ is a line segment from $k = -2k_F$ to $k = 2k_F$ and so

$$\Delta\rho\,(\text{from } \mathcal{M} + \mathcal{N}) \sim (1/|\boldsymbol{x}|^3) \cos 2k_F|\boldsymbol{x}|$$

i.e. the branch cut contribution to $\Delta\rho$, when $\omega = 0$, correspond to the ordinary Friedel oscillations in the electron gas.

(ii) $0 < \omega < \omega_F$. We now have oscillations in the electron gas density with four different wavelengths $2\pi/a$, $2\pi/b$, $2\pi/a'$ and $2\pi/b'$. The envelope to these oscillations decreases as $|\boldsymbol{x}|^{-3}$ with increasing $|\boldsymbol{x}|$.

(iii) $\omega > \omega_F$. The branch cut $\mathcal{M}$ again gives an oscillatory contribution to $\Delta\rho$ but the branch cut $\mathcal{N}$ will now make a contribution which is both oscillatory and exponential decaying (because a' and b' are complex when $\omega > \omega_F$) with increasing $|\boldsymbol{x}|$.

Acknowledgment

I would like to thank G Mukhopadhyay for a useful discussion and S Lundqvist for reading the manuscript.

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