Electron-Density Oscillations in a General Potential*†

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The asymptotic density of a free noninteracting electron gas is discussed in the presence of a general potential $V(X)$, where $\mathbf{X}$ is a vector in one, two, and three dimensions corresponding, respectively, to the potential of a surface barrier, an edge dislocation, and an impurity. At zero temperature, oscillations in the density have the form $AX^{-\frac{1}{2}(\nu+3)}\cos(2k_fX+\theta)$, where ν is the dimensionality of $\mathbf{X}$, $\mathbf{k}_f$ is the Fermi momentum, and θ is a phase angle. The amplitude A is determined by the backward scattering amplitude at the Fermi energy for the potential $V(X)$. At a finite temperature the amplitude of the oscillations in normal metals is reduced approximately by the factor $\xi/\sinh\xi$, where $\xi=(2\pi/\beta k_f)X$, and β is the reciprocal of the thermal energy KT. In the high-density limit, the results of the dielectric theory become the Born-approximation version of the exact scattering theory. Mild restrictions on the potential to guarantee certain analytical properties of the scattering matrix are imposed.

I. INTRODUCTION

SEVERAL authors[1–3] have recently discussed the possibility of long-range spin polarization in a nonmagnetic metal when it is in contact with a ferromagnetic metal. It was assumed that the electrons of negative z component of the spin (spin-down) see a potential which is constant everywhere, and that the electrons of positive z component of the spin (spin-up) see a step-function potential which is constant in each metallic slab, but assumes a discontinuity at the contact plane of the two media. For this special potential model, Bardasis, Falk, Ferrell, Fullenbaum, Prange, and Mills,[2] and independently Yosida and Okiji,[3] have correctly concluded that the asymptotic electron density for the spin-up component differs from a constant value by terms which are only of oscillatory nature. The original aim of this paper was to show that the results of these authors[2,3] can be established for a general one-dimensional potential by using the scattering-matrix method which we applied earlier to other surface problems.[4] It became clear, however, that some of the basic features of the development transcend the dimensionality of the potential, and to bring out these features clearly we shall discuss the questions of electron density oscillations for two and three-dimensional potentials, and the damping of the oscillations at finite temperatures.

We consider here a free noninteracting electron gas whose motion is perturbed by a static local potential $V(\mathbf{r})$. The problem is to calculate the electron density, $n(\mathbf{r})$, in the region where V is negligible. The single-electron Hamiltonian H is

$$H=-\tfrac{1}{2}\nabla^2+V(\mathbf{r}), \tag{1.1}$$

where Hartree's atomic units $|e|=\hbar=m=1$ have been used. The density is given by the diagonal element of the density matrix at thermal equilibrium, namely,

$$n(\mathbf{r})=\langle\mathbf{r}|F(H)|\mathbf{r}\rangle, \tag{1.2}$$

and the density-matrix operator $F(H)$ is defined by

$$F(H)=[1+\exp\beta(H-\zeta)]^{-1}, \tag{1.3}$$

where β is the reciprocal of the thermal energy KT and ζ is the Fermi energy. By using the complete set of functions $\psi_j(\mathbf{r})$ which are eigenfunctions of H with eigenvalues E_j, the density of (1.2) takes the form

$$n(\mathbf{r})=\sum_b|\psi_b(\mathbf{r})|^2F(E_b)+\sum_i|\psi_i(\mathbf{r})|^2F(E_i), \tag{1.4}$$

where the subscript b denotes bound states, if any, and the subscript i denotes free scattering states. To evaluate $n(\mathbf{r})$ asymptotically we shall insert in (1.4) the asymptotic form of the wave functions $\psi_j(\mathbf{r})$ which is well known from scattering theory, and perform the implied integrations by contour integration methods.

The oscillations are discussed first at zero temperature. In the second section we deal with the general one-dimensional potential studied in I, and show how the results of Refs. 2 and 3 follow as a special case from our general formulas. In Sec. III, the potential is cylindrically symmetric such as that of an edge dislocation, and the amplitude of the oscillations is shown to fall off as $\rho^{-5/2}$, where ρ is the distance from the symmetry axis of the potential. The case of a spherically symmetric potential, such as that of an ionized impurity in a metal, has received considerable attention, and the density oscillations (often known as the Friedel oscillations) were discussed by Friedel,[5] Kohn and Vosko,[6] Langer and Vosko,[7] and others. However, for complete-

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† Some of the basic results of this paper which apply at zero temperature were included in a talk presented at the meeting of the American Physical Society at Kansas City, I. Adawi, Bull. Am. Phys. Soc. **10**, 302 (1965).

[1] B. Dreyfus, R. Maynard, and A. Quattropani, Phys. Rev. Letters **13**, 342a (1964).

[2] A. Bardasis, D. S. Falk, R. A. Ferrell, M. S. Fullenbaum, R. E. Prange, and D. L. Mills, Phys. Rev. Letters **14**, 298 (1965).

[3] K. Yosida and A. Okiji, Phys. Rev. Letters **14**, 301 (1965).

[4] I. Adawi, Phys. Rev. **134**, A788 (1964). This paper will be referred to as I.

[5] J. Friedel, Nuovo Cimento Suppl. **2**, 287 (1958).

[6] W. Kohn and S. H. Vosko, Phys. Rev. **119**, 912 (1960).

[7] J. S. Langer and S. H. Vosko, J. Phys. Chem. Solids **12**, 196 (1960).

ness and to introduce the discussion of Sec. V, we shall discuss this case briefly from the general point of view of this paper.

In all cases considered, the perturbed electron density approaches its asymptotic constant value in an oscillatory fashion. The absence of long-range terms is due to the behavior of the backward scattering amplitude at zero energy.

In Sec. IV we consider a "rigid"-charge distribution to be embedded in a solid, and study the density oscillations in the screening charge of the free electrons of the crystal, with the object of relating the results of the dielectric theory to those of the exact theory by using two methods. In the Fourier-transform method, previously used by Langer and Vosko,[7] the density oscillations in all dimensions can be treated by one formulation. In the second method we work directly in position space and show that the asymptotic form of the kernel in the integral representation of the screening charge density reflects the character of the oscillations, and again brings out the intimate connection between the results in different dimensions. By either method it is shown that in the high-density limit, which is characterized by $\pi k_f \gg 1$, the amplitude of the density oscillations given by the dielectric theory follows from the exact theory by making the Born approximation in calculating the backward scattering amplitude of the potential.

In Sec. V the oscillations are discussed at finite temperatures, and the damping brought about by the thermal spread in the Fermi surface is described. It is shown that for all potentials considered, the oscillations in normal metals decay exponentially with distance. This agrees with the qualitative remark by Kohn and Vosko,[6] but disagrees with the "empirical" considerations of March and Murray.[8] The analysis leads naturally to a new derivation of the Sommerfeld formula for the Fermi-Dirac integrals.

II. ONE-DIMENSIONAL POTENTIAL

Consider two metallic slabs joined at $x=0$ and extending over the interval $-L_2<x<L_1$. Let the potential energy V of a free electron of spin down ($s_z=-\frac{1}{2}$) be zero in this interval. For a spin up electron ($s_z=\frac{1}{2}$), let V vary only in the x direction, and assume that

$$V(x)=-\tfrac{1}{2}\alpha^2, \quad -L_2<x<0, \tag{2.1}$$

and that $V(x)$ rises to zero in a distance much less than L_1. The problem is to calculate the asymptotic electron densities of spin-up electrons $n_1(x)$ and $n_2(x)$ for large positive and negative x, respectively.

The electron motion in the y and z directions is described by a plane wave $\exp[i(k_y y+k_z z)]$ normalized to one per unit area and obeying cyclic boundary conditions. The x motion is given by solutions to Schrödinger's equation,

$$d^2\phi/dx^2+2[\epsilon_x-V(x)]\phi(x)=0, \tag{2.2}$$

where the energy $\epsilon_x=\frac{1}{2}q_x^2$. In the limit that $L_1\to\infty$ and $L_2\to\infty$, the wave functions $u(x)$ and $v(x)$ of I become appropriate solutions of (2.2), and we recall that these functions have the asymptotic form:

$$\begin{aligned} &u(x)\sim[e^{ik_x x}+S_{22}e^{-ik_x x}, S_{12}e^{iq_x x}], \\ &v(x)\sim[S_{21}e^{-ik_x x}, S_{11}e^{iq_x x}+e^{-iq_x x}], \\ &\qquad\qquad \text{for} \quad x\leq 0, \ x\to\infty . \end{aligned} \tag{2.3}$$

Here $k_x^2=q_x^2+\alpha^2$, and S is the scattering matrix with the subscripts 1 and 2 referring to the medium on the right and left, respectively. It was established that

$$S=[f'(q_x)+ik_x f(q_x)]^{-1} \times\begin{pmatrix} -ik_x g(q_x)-g'(q_x) & 2ik_x \\ 2iq_x & -f'(q_x)+ik_x f(q_x) \end{pmatrix}, \tag{2.4}$$

$$SS^*=I, \text{ for } q_x \text{ real}, \quad q_x S_{12}=k_x S_{12}, \tag{2.5}$$

$$\langle u(q_x)\,|\,v(q_x)\rangle=0, \tag{2.6}$$

$$\langle u(q_x)\,|\,u(q_x')\rangle=2\pi\delta(k_x'-k_x)=2\pi(k_x/q_x)\delta(q_x-q_x'), \tag{2.7}$$

$$\langle v(q_x)\,|\,v(q_x')\rangle=2\pi\delta(q_x-q_x'). \tag{2.8}$$

The functions $f(q_x)$ and $g(q_x)$, and their derivatives $f'(q_x)$ and $g'(q_x)$ with respect to x, are the values of the functions $f(q_x,x)$ and $g(q_x,x)$, and their derivatives with respect to x, at $x=0$. These functions[9] are solutions to Eq. (2.2) with the condition that for large x, $f(q_x,x)\sim\exp(iq_x,x)$, and $g(q_x,x)\sim\exp(-iq_x x)$.

In this model there are no true bound states. At temperature $T=0$ the density in (1.4) reduces to an integration of $|u(x)|^2$ and $|v(x)|^2$ over all states below the Fermi surface which is a hemisphere of radius q_f in the first medium and radius k_f in the second medium with the obvious relation $k_f^2=q_f^2+\alpha^2$. To evaluate the asymptotic density $n_1(x)$ we split the integration over $|u(x)|^2$ at $k_x=\alpha$ and set $q_x=ip$ for $k_x<\alpha$. By using (2.3)–(2.8), we obtain after elementary manipulations

$$n_1(x)\sim q_f^3/(6\pi^2)+B+C, \tag{2.9}$$

$$B=\frac{1}{8\pi^2}\int_0^\alpha |S_{12}(ip)|^2 e^{-2px}(q_f^2+p^2)\frac{p}{k_x}dp, \tag{2.10}$$

$$C=\frac{1}{4\pi^2}\,\mathrm{Re}\int_0^{q_f} S_{11}(q_x)e^{2iq_x x}(q_f^2-q_x^2)dq_x, \tag{2.11}$$

where Re (Im) denotes the real (imaginary) part.

[8] N. H. March and A. M. Murray, Proc. Phys. Soc. (London) **79**, 1001 (1962).

[9] The functions $f(q)$ and $g(q)$ are the Jost functions, and they would conventionally be denoted by $f(-q)$ and $f(q)$, respectively.

If we assume that the potential $V(x)$ satisfies the two conditions,

$$\int_0^\infty |V(z)| z e^{2\mu z} dz < \infty , \tag{2.12}$$

$$\int_0^\infty |V(z)| z^2 e^{2\mu z} dz < \infty , \tag{2.13}$$

where μ is positive, then it follows that the scattering matrix S of (2.4) is an analytic function of the complex variable q_x in the strip $|\mathrm{Im} q_x| \leq \mu$, excluding possible branch cuts. Details of the analyticity and the passage to the limits L_1 and $L_2 \to \infty$ are discussed in Appendices A and B.

We can now evaluate C asymptotically by deforming the path of integration in the complex q_x plane so as to pass through the lines of steepest descent[10] which are parallel to the imaginary axis at the points $q_x=0$ and $q_x=q_f$. This is denoted symbolically by

$$\int_0^{q_f} \cdots = \int_0^{i\mu} \cdots + \int_{i\mu}^{i\mu+q_f} \cdots + \int_{i\mu+q_f}^{q_f} \cdots \tag{2.14}$$

and

$$C = C_1 + C_2 + C_3 , \tag{2.15}$$

respectively.

In the integral C_1, $q_x = ip$ and we have

$$C_1 = -\frac{1}{4\pi^2} \mathrm{Im} \int_0^\mu S_{11}(ip) e^{-2px} (q_f^2 + p^2) dp . \tag{2.16}$$

In the asymptotic sense, $\mu x \gg 1$ and $\alpha x \gg 1$, the effective upper limits of the integration in (2.10) and (2.16) are ∞. Since it is simple to derive by using (2.4) the following property:

$$(p/k_x)|S_{12}(ip)|^2 - 2\,\mathrm{Im} S_{11}(ip) = 0 , \tag{2.17}$$

it follows from (2.10) and (2.16) that[11]

$$B + C_1 \sim 0 . \tag{2.18}$$

The path of integration in C_2 can be taken along the line $\mathrm{Im} q_x = \mu$, and we see that C_2 is of order $\exp(-2\mu x)$ which is negligible. We are, therefore, left with the integral C_3 and from (2.9) and the above results we have

$$n_1 - q_f^3/6\pi^2 \equiv \Delta n_1 \sim C_3 , \tag{2.19}$$

where we have defined Δn_1 to be the deviation of the density n_1 from the constant value $q_f^3/(6\pi^2)$.

In the integral C_3 we write $q_x = q_f + iy$, $S_{11}(q_f + iy) \approx S_{11}(q_f)$, and stretch the limit $i\mu$ to $i\infty$ since the main contribution to the integral comes from $y \approx 0$. To lowest order we have the result

$$\Delta n_1(x) \sim -(q_f/8\pi^2 x^2)\, \mathrm{Re}[S_{11}(q_f) e^{2iq_f x}] . \tag{2.20}$$

The asymptotic density $n_2(x)$ at the left is given by

$$n_2(x) \sim \frac{k_f^3}{(6\pi^2)} + \frac{1}{4\pi^2} \mathrm{Re} \int_0^{k_f} S_{22}(q_x) e^{-2ik_x x} (k_f^2 - k_x^2) dk_x . \tag{2.21}$$

To evaluate this integral we shall assume that $\mu > \alpha$, and it follows that S is analytic in a strip, say, $0 \leq \mathrm{Im} k_x \leq \mu'$, $\mathrm{Re} k_x \geq 0$, where μ' for the k_x integration plays the role of μ in (2.14) for the q_x integration. On the path $k_x = iy$, $0 \leq y \leq \mu'$, the integral is pure imaginary and hence does not contribute to n_2. The contribution to n_2 from the path $\mathrm{Im} k_x = \mu'$ is negligible as in the case for n_1, and the main contribution comes from the path $\mathrm{Re} k_x = k_f$, and we have

$$\Delta n_2 \equiv n_2(x) - k_f^3/(6\pi^2) \sim -(k_f/8\pi^2 x^2) \times \mathrm{Re}[S_{22}(q_f) e^{-2ik_f x}] . \tag{2.22}$$

Equations (2.20) and (2.22) state that the asymptotic density deviates from its constant value at ∞ by terms which are sinusoidal in x whose period is equal to half the reciprocal of the Fermi momentum, and whose amplitude is determined by the backward scattering amplitude at the Fermi surface. These features and the method of integration are common to all potentials under consideration. Let us now discuss some applications:

(1) For the step-function potential model discussed in Refs. 2 and 3, $S_{11}(q_f) = (q_f - k_f)/(q_f + k_f) = -S_{22}(q_f)$, and by substituting these values in (2.20) and (2.22) we obtain the results of these authors.

(2) If we take $\alpha > k_f$ the first medium becomes vacuum, q_f becomes pure imaginary, and $|S_{22}| = 1$ in the range of interest. With these modifications Eq. (2.22) gives the asymptotic electron density (for each component of the spin) near the surface barrier of the metal. It is interesting to mention that Makinson[12] had published a graph for this density using a step-function potential for the surface barrier.

(3) If the potential $V(x)$ is modified so that $V(-\infty) = V(\infty)$ then $k_x = q_x$ and Eqs. (2.20) and (2.22) remain valid, although the details of the derivation are altered slightly. If we make the (first) Born approximation (see, for example, Sec. IIB of I) in calculating the backward scattering amplitudes S_{11} and S_{22}, we have

$$\Delta n_{1B}(x) \sim -\frac{1}{8\pi^2 x^2} \int_{-\infty}^{\infty} \sin 2k_f(x - x') V(x') dx' , \tag{2.23}$$

$$\Delta n_{2B}(x) \sim -\frac{1}{8\pi^2 x^2} \int_{-\infty}^{\infty} \sin 2k_f(|x| + x') V(x') dx' , \tag{2.24}$$

where the subscript B denotes the Born approximation. It is obvious that $n_1 = n_2$ if $V(x) = V(-x)$.

[10] A lucid account of the saddle point method is given by B. L. Van der Waerden, Appl. Sci. Res. **B2**, 33 (1951–1952).

[11] If we require that $\mu \geq \alpha$, then μ can be replaced by α in (2.14) and (2.16), and Eq. (2.18) becomes exact.

[12] R. E. B. Makinson, Proc. Roy. Soc. (London) **A162**, 367 (1937).

III. TWO- AND THREE-DIMENSIONAL POTENTIALS

We consider a spherically symmetric potential $V(r)$ and a cylindrically symmetric potential $V(\rho)$, where $\boldsymbol{\rho}=(x,y)$, and calculate the perturbations in the electron densities (for a given spin direction) $\Delta n(r)$ and $\Delta n(\rho)$ at zero temperature. The potentials with which we shall be concerned have at most a finite number of bound states,[13] and we shall first estimate the contribution of these states to Δn. A bound state of finite binding energy

$$-E_b=\tfrac{1}{2}\gamma^2>0$$

contributes to Δn a term of order $\exp(-2\gamma r)$ [or $\exp(-2\gamma\rho)$ in two dimensions] which is negligible for sufficiently large r (or ρ). Bound states of zero binding energy could exist in three dimensions for states of angular momentum $l\geq 1$ (and in two dimensions for states of angular momentum $m\geq 2$). Such states contribute to Δn a term of order $r^{-2(l+1)}$ (and ρ^{-2m}) which can at most be of order r^{-4} (and ρ^{-4}) and this will prove to be small compared to the contribution of the free states.

A free scattering state $\psi(\mathbf{k},\mathbf{r})$ for the potential $V(r)$ is resolved as usual in partial waves, namely,[14]

$$\psi(\mathbf{k},\mathbf{r})\sim e^{i\mathbf{k}\cdot\mathbf{r}}+f(\theta,k)e^{ikr}/r$$
$$=\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)e^{i\delta_l(k)}\frac{1}{kr}\sin\left(kr-\frac{\pi}{2}l+\delta_l\right), \quad (3.1)$$

where θ is the scattering angle, $f(\theta,k)$ the scattering amplitude,[15] and δ_l is the phase shift. To obtain Δn we integrate $|\psi(\mathbf{k},\mathbf{r})|^2$ over $\mathbf{k}$ and subtract the same expression with $\delta_l=0$ to account for the unperturbed density $k_f^3/(6\pi^2)$. Thus

$$\Delta n(r)\sim\sum_l -\frac{2l+1}{4\pi^2r^2}(-1)^l\,\mathrm{Re}\int_0^{k_f} e^{2ikr}(e^{2i\delta_l}-1)dk, \quad (3.2)$$

which can also be written in terms of the backward scattering amplitude $f(\pi,k)$ as follows:

$$\Delta n(r)\sim\frac{1}{2\pi^2r^2}\,\mathrm{Im}\int_0^{k_f} e^{2ikr}f(\pi,k)kdk. \quad (3.3)$$

We shall now assume that the potential $V(r)$ satisfies the conditions (2.12) and (2.13) and this ensures that the scattering matrix $S_l(k)\equiv\exp 2i\delta_l(k)$ is analytic in the strip $|\mathrm{Im}k|\leq\mu$, except for simple poles on the imaginary axis corresponding to bound states.[16,17] The path of integration in (3.2) can now be deformed according to Eq. (2.14), except that the contour must be dented on the imaginary axis to avoid the possible poles of the bound states. The contribution from these dents is negligible being of order $\exp(-2\gamma r)$. Near the origin, $\delta_0(0)$ is an odd multiple of $\pi/2$ if there is a zero-energy s-wave resonance; $\delta_l(k)\propto k^{2l+1}$ if there are no zero-energy bound states, or s-wave resonance and the potential satisfies Carter's condition, $\int_0^\infty|V(r)|r^{2(l+1)}dr<\infty$ [which is consistent with conditions (2.12) and (2.13)]; and $\delta_l(k)\propto k^{2l-1}$ for $l\geq 1$, if there is a zero-energy bound state.[17] In all these approximations the real part of the integral of (4.2) vanishes on the path $k=iy$, and we have no contributions to Δn. If we allow, for example, $\delta_l(k)\approx ak+bk^2$, a and b real, we see that the path $k=iy$ contributes a term of order br^{-5} which we shall neglect. The dominant contribution to Δn comes from the path $k=k_f+iy$, and we have to lowest order the result

$$\Delta n(r)\sim-(k_f/4\pi^2r^3)\,\mathrm{Re}[f(\pi,k_f)e^{2ik_fr}], \quad (3.4)$$

which has been obtained previously by Friedel,[5] and Kohn and Vosko.[6]

For the potential $V(\rho)$, the scattering states are resolved into cylindrical partial waves m, and we have

$$\psi(\mathbf{k},\mathbf{r})\sim[\exp(ik_zz)](e^{i\mathbf{k}_\rho\cdot\boldsymbol{\rho}}+f(\theta,k_\rho)e^{ik_\rho\rho}/\rho^{1/2})$$
$$=e^{ik_zz}\sum_{m=0}^{\infty} i^m\epsilon_m\cos m\theta\left(\frac{2}{\pi k_\rho\rho}\right)^{1/2}e^{i\delta_m(k_\rho)}$$
$$\times\cos[k_\rho\rho-(2m+1)\tfrac{1}{4}\pi+\delta_m], \quad (3.5)$$

where $\epsilon_m=1$ for $m=0$, and $\epsilon_m=2$ for $m>0$, δ_m is a phase shift, θ is the angle between the vectors $\boldsymbol{\rho}$, and $\mathbf{k}_\rho\equiv(k_x,k_y)$, and $f(\theta,k_\rho)$ is the scattering amplitude. By the above procedure, we have

$$\Delta n(\rho)\sim\frac{1}{2\pi^3\rho}\sum_m\epsilon_m(-1)^m\,\mathrm{Im}\int_0^{k_f} e^{2ik_\rho\rho}(e^{2i\delta_m}-1)$$
$$\times(k_f^2-k_\rho^2)^{1/2}dk_\rho, \quad (3.6)$$
$$\Delta n(\rho)\sim\frac{1}{2\pi^3\rho}\,\mathrm{Im}\int_0^{k_f}[2\pi ik_\rho(k_f^2-k_\rho^2)]^{1/2}$$
$$\times f(\pi,k_\rho)e^{2ik_\rho\rho}dk_\rho. \quad (3.7)$$

Imposing the same conditions (2.12) and (2.13) on $V(\rho)$ and examining the behavior of the phase shifts at zero energy,[18] we conclude that the dominant contribution to $\Delta n(\rho)$ comes from the path $k_\rho=k_f+iy$, and we have the result,

$$\Delta n(\rho)\sim-(2^{1/2}k_f/8\pi^2\rho^{5/2})\,\mathrm{Re}[f(\pi,k_f)e^{2ik_f\rho}]. \quad (3.8)$$

[13] The binding in the potential $V(\rho)$ applies only to the motion in the xy plane. The z motion is free and can be described by a plane-wave $\exp(ik_zz)$.

[14] We use the boundary condition of outgoing waves at ∞, incoming (or ingoing) waves $\exp(-ikr)/r$ can equally well be used instead.

[15] Not to be confused with the function f of Sec. II.

[16] V. Bargmann, Rev. Mod. Phys. **21**, 488 (1949).

[17] See R. G. Newton, J. Math. Phys. **1**, 319 (1960).

[18] In the absence of resonances and zero-energy bound states, $\delta_m\propto k^{2m}$, $m\geq 1$ and the contribution to Δn from the origin vanishes in first approximation. A zero-energy resonance for $m=0$ is possible and $\delta_0\propto 1/\ln k_\rho$ and here again the contribution to Δn is negligible.

IV. DIELECTRIC THEORY

In the preceding sections a knowledge of the potential V was assumed and exact expressions for the density oscillations Δn were derived. In practice, however, one assumes a charge distribution such as a point charge, a line of charge, etc., as a source of the potential, and calculates approximately the screening of these charges by the electron gas, and the resulting screened potential. The most widely used approximate theory for dealing with this problem is the dielectric theory of Lindhard[19] which is equivalent to the treatment of Langer and Vosko,[7] and identical to the subsequent treatment of March and Murray.[20] In this section we shall discuss how the density oscillations as obtained by the dielectric theory are related to those of the exact theory.

We shall use spherical symmetry, and treat all dimensions ν, where $\nu=1, 2, 3$, simultaneously by using vectors in ν dimensions. Let $Q(X)$, where $X=|\mathbf{X}|$, be the density of the source charge, $\Delta n(X)$ the perturbation in the density of the electron gas, and $V(X)$ the resulting screened potential, then the dielectric theory[19] gives at zero temperature the following relations:

$$-q^2\langle\mathbf{q}|V\rangle=4\pi\epsilon^{-1}(\mathbf{q})\langle\mathbf{q}|Q\rangle, \tag{4.1}$$

$$\epsilon(\mathbf{q})=1+(4\pi/q^2)G(\mathbf{q}), \tag{4.2}$$

$$G(\mathbf{q})=\frac{k_f}{2\pi^2}\left[\frac{1}{2}+\frac{4k_f{}^2-q^2}{8qk_f}\ln\left|\frac{q+2k_f}{q-2k_f}\right|\right], \tag{4.3}$$

$$\langle\mathbf{q}|\Delta n\rangle=-\langle\mathbf{q}|V\rangle G(\mathbf{q}), \tag{4.4}$$

where $\epsilon(\mathbf{q})$ is the longitudinal static dielectric constant for the wave vector $\mathbf{q}$, and the angular brackets denote the Fourier transform, for example,

$$\langle\mathbf{q}|\Delta n\rangle\equiv\int\Delta n(\mathbf{X})\exp(-i\mathbf{q}\cdot\mathbf{X})d^\nu X.$$

We shall now discuss two methods for calculating $\Delta n(X)$ for large X. The first is an extension of the method used by Langer and Vosko,[7] namely, we invert Eq. (4.4) and we have, after expressing $\langle\mathbf{q}|V\rangle$ in terms of $\langle\mathbf{q}|Q\rangle$, that

$$\Delta n(X)=\frac{4\pi}{(2\pi)^\nu}\int\frac{\langle\mathbf{q}|Q\rangle G(q)}{q^2+4\pi G(q)}e^{i\mathbf{q}\cdot\mathbf{X}}d^\nu q. \tag{4.5}$$

The plane wave $\exp(i\mathbf{q}\cdot\mathbf{X})$ is now resolved into partial waves by using the Gegenbauer expansion,[21]

$$e^{i\mathbf{q}\cdot\mathbf{X}}=2^\alpha\Gamma(\alpha)\sum_{m=0}^{\infty}(\alpha+m)i^m\frac{J_{\alpha+m}(qX)}{(qX)^\alpha}C_m{}^\alpha(\cos\theta), \tag{4.6}$$

where $\alpha=\frac{1}{2}(\nu-2)$, J is the Bessel function, θ is the angle between $\mathbf{q}$ and $\mathbf{X}$, and $C_m{}^\alpha$ denotes the space harmonic. Due to spherical symmetry only the first term of the expansion (4.6) contributes to the integral (4.5). By inserting the asymptotic expression for Bessel's function and taking account of the logarithmic singularity of $G(q)$ at $q=2k_f$ we obtain by various methods the asymptotic formula,[22]

$$\Delta n(X)\sim-\mathfrak{A}(\nu)\langle 2\mathbf{k}_f|V\rangle X^{-(\nu+3)/2}\times\cos(2k_fX-(\pi/4)(\nu+1))[1+1/(4\pi k_f)]^{-1}, \tag{4.7}$$

$$\mathfrak{A}(\nu)\equiv k_f{}^{(\nu-1)/2}[8\pi^{(\nu+3)/2}]^{-1}, \tag{4.8}$$

which agrees with Langer and Vosko[7,22a] for $\nu=3$. Except for the last factor, Eq. (4.7) can be obtained from the corresponding expression of Secs. II and III by using the Born approximation to calculate the backward scattering amplitude at the Fermi energy. Thus, in the high-density limit for which $\pi k_f\gg1$, Eq. (4.7) becomes the Born approximation version of the exact scattering theory. For real metals with $k_f\sim\frac{1}{2}$ the last factor in (4.7) differs from unity by about 12%, and by twice as much if we included both directions of the electron spin.

We shall now derive Eq. (4.7) by working directly in X space. Equation (4.4) leads to the convolution,

$$\Delta n(X)=-\int V(X')K(\nu|\,|\mathbf{X}-\mathbf{X}'|)d^\nu X', \tag{4.9}$$

where the kernel $K(\nu|X)$ is defined by[23]

$$K(\nu|\mathbf{X})=\frac{1}{(2\pi)^\nu}\int G(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{X}}dq^\nu, \tag{4.10}$$

and has the asymptotic behavior

$$K(\nu|X)\sim\mathfrak{A}(\nu)X^{-(\nu+3)/2}\times\cos[2k_fX-(\gamma+1)(\pi/4)]. \tag{4.11}$$

For large X, there are two regions in X' space which contribute to the integral (4.9), namely, the regions $X\gg X'$, and $X\approx X'$ which contribute the densities $\Delta n^{(1)}$ and $\Delta n^{(2)}$, respectively. To calculate $\Delta n^{(1)}$ we substitute (4.11) in (4.9), and make the approximation $|\mathbf{X}-\mathbf{X}'|\sim X-\mathbf{X}'\cdot\hat{X}$, where the caret denotes a unit vector, and

[19] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **28**, No. 8 (1954).

[20] N. H. March and A. M. Murray, Proc. Roy. Soc. (London) **A261**, 119 (1961).

[21] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (The Macmillan Company, New York, 1945), p. 368.

[22] Because of spherical symmetry, the vector $2\mathbf{k}_f$ can point in any direction.

[22a] After this paper was submitted for publication, a paper by R. A. Brown [Phys. Rev. **141**, 568 (1966)] appeared. Brown's Eq. (3.11) is of the form given by our Eq. (4.7) for $\nu=2$.

[23] It is obvious that

$$K(2|\rho)=\int_{-\infty}^{\infty}K(3|r)dz,$$

and

$$K(1|x)=\int_{-\infty}^{\infty}K(2|\rho)dy,$$

and

$$K(3|r)=-\frac{1}{16\pi^3r^2}\frac{\partial}{\partial r}\left(\frac{1}{r}\sin2k_fr\right).$$

we obtain

$$\Delta n^{(1)}\sim -\mathcal{C}(\nu)X^{-(\nu+3)/2}\langle 2\mathbf{k}_f|V\rangle \times\cos[2k_fX-(\nu+1)(\pi/4)]. \quad (4.12)$$

Equation (4.12) *suggests* that

$$\Delta n\sim D\Delta n^{(1)}, \quad (4.13)$$

where D is a constant, which implies by Poisson's equation that

$$V\sim(\pi/k_f^2)\Delta n. \quad (4.14)$$

By substituting for V in (4.9) the tentative value (4.14), and writing $\mathbf{X}'=\mathbf{X}+\mathbf{S}$ and $X'\sim X+\hat{X}\cdot\mathbf{S}$, we recognize that the remaining integral is the Fourier transform of $K(\nu|X)$ for $q=2k_f$, namely, $G(2k_f)$ by Eq. (4.10). The consistency of Eqs. (4.12) to (4.14) is established, and we have

$$\Delta n^{(2)}\sim -\Delta n/(4\pi k_f). \quad (4.15)$$

By adding (4.12) and (4.14) we rederive Eq. (4.7). The contribution $\Delta n^{(1)}$ is obvious, and its computation is suggested by the way we calculate scattering amplitudes for short-range potentials. The contribution $\Delta n^{(2)}$ is due to the long-range oscillatory nature of the potential, and it is seen to become negligible in the high-density limit. In this limit Eq. (4.12), which is precisely the Born approximation version of the exact theory, becomes an accurate formula for the density oscillations.[24]

V. OSCILLATIONS AT FINITE TEMPERATURE

We shall now discuss the damping of the density oscillations in normal metals at temperatures for which $\beta\zeta\gg1$ and the Fermi surface is slightly diffuse. It is simple to start with the three-dimensional case. The Fermi-Dirac distribution function

$$F(k)=[1+\exp\tfrac{1}{2}\beta(k^2-k_f^2)]^{-1}$$

is inserted in the integrand of (3.3), and the limits of integration are now zero and infinity. The problem is then to perform the following integration:

$$J(\beta)\equiv\mathrm{Im}\int_0^\infty e^{2ikr}f(\pi,k)F(k)kdk, \quad (5.1)$$

for large r. If we assume that the scattering matrix is analytic in a small strip in the upper half k plane, we can as we discussed previously deform the contour of integration to a rectangle (with proper dents if necessary to avoid simple poles on the imaginary axis) whose vertices are $k=0$, ∞, $\infty+i\mu$, and $i\mu$. The integral is determined essentially by the residues of the simple poles of the distribution function $F(k)$ inside the rectangle. These poles are located at $k=k_n$, where $k_n^2=k_f^2+2\pi i(2n+1)/\beta$, $n=0, 1, 2\cdots$, and we have for all practical purposes that

$$J(\beta)\sim\frac{-2\pi}{\beta}\,\mathrm{Re}\sum_{n=0}^{\infty}e^{2ik_nr}f(\pi,k_n). \quad (5.2)$$

With $\beta k_f^2\gg1$ and $k_fr\gg1$, it is safe to make the approximation,

$$k_n\approx k_f+(2n+1)\pi i/(\beta k_f). \quad (5.3)$$

By approximating $f(\pi,k_n)$ with $f(\pi,k_f)$ we can sum the series to obtain:

$$J(\beta)\sim(-2\pi/\beta)\,\mathrm{Re}[f(\pi,k_f)e^{2ik_fr}][2\sinh\xi]^{-1}, \quad (5.4)$$

where, $\xi\equiv2\pi r/\beta k_f$. Obviously, $J(\beta)$ is related to its value at zero temperature, $J(\infty)$, by the equation

$$J(\beta)=J(\infty)(\xi/\sinh\xi), \quad (5.5)$$

which implies that the amplitude of the density oscillations is reduced from its value at 0°K by the factor $\xi/\sinh\xi$.

It is of interest to discuss the nature of these approximations. For large ξ the first term of the series (5.2) is dominant, and the oscillations decay exponentially with r as $r\exp(-2\pi r/\beta k_f)$, and our Eq. (5.5) is accurate. This supports the qualitative remark of Kohn and Vosko[6] but contradicts the empirical findings of March and Murray.[8] For small ξ the series (5.2) can be summed by the Euler Maclaurin[25] method and one finds that

$$J(\beta)\approx J(\infty)[1-\tfrac{1}{6}\xi^2+\cdots], \quad (5.6)$$

which agrees with (5.5) to second order. The same equation (5.6) also follows directly from (5.1) by applying the Sommerfeld method[26] for evaluating the Fermi-Dirac integrals, for small ξ implies that $\exp(2ikr)$ is a smooth function compared to $F(k)$ near $k=k_f$. This is not an accident, for in Appendix C we demonstrate that the Sommerfeld asymptotic method follows by summing the residues at the poles of the Fermi-Dirac function by the Euler Maclaurin method, and making a Taylor expansion at the Fermi energy. Thus Eq. (5.5) is good for small and large ξ, and should be reasonable for intermediate[27] ξ.

In one and two dimensions the results are the same, namely the amplitude of the oscillations is reduced from its zero-temperature value by the damping factor $\xi/\sinh\xi$, where $\xi=2\pi X/\beta k_f$. The details of the calculations are slightly different. In one dimension one integrates first over k_x and obtains a series of the type (5.2) in which k_f^2 is replaced by $k_f^2-k_\rho^2$; this series is

[24] The Fourier transform $\langle 2\mathbf{k}_f|V\rangle$ in (4.12) is expressed in terms of $\langle 2\mathbf{k}_f|Q\rangle$ by using Eq. (4.1) which is also accurate in the high-density limit.

[25] E. T. Whittaker and G. N. Watson, *A Course in Modern Analysis* (Cambridge University Press, New York, 1940), 4th ed., p. 125.

[26] See, for example, J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1950), Sec. 16g.

[27] For copper at room temperature $\beta k_f^2\sim560$ and ξ is of order 0.2 for r corresponding to the distance between an atom and its tenth nearest neighbor. This shows that in the nuclear-magnetic-resonance measurements of T. J. Rowland, Phys. Rev. **119**, 900 (1960), the thermal damping of the oscillations is completely negligible.

integrated term by term over k_y and k_z, and summed to give the final result. Most of the contribution to the integration over k_y and k_z comes from the vicinity of $k_y \approx k_z \approx 0$. In two dimensions, one again systematically integrates over k_ρ first and integrates the resulting series over k_z, and then sums it.

If the electron density is sufficiently low, or the temperature is sufficiently high, so that βk_f^2 is of order unity, we see that most of the contribution in (5.2) comes from $k=k_1$. We have from Eqs. (5.2) and (3.3) that

$$\Delta n(r,\beta) \sim -\frac{1}{\pi r^2 \beta} e^{-2r\,\mathrm{Im}k_1}\,\mathrm{Re}[e^{2ir\,\mathrm{Re}k_1} f(\pi,k_1)]. \quad (5.7)$$

Since $\mathrm{Re}k_1$ is now significantly different from k_f we see that, in addition to the severe damping of the oscillations, the periodicity of the oscillations is altered considerably and the memory of the Fermi surface is lost. In the extreme case, when Boltzmann statistics apply, the oscillations are completely lost and $\Delta n \propto \exp(-2r^2/\beta)$ for sufficiently large r.

It is of interest to remark that the dielectric theory gives the same damping factor as the exact theory. The details of the argument will become apparent in a future article dealing with a perturbation expansion of the density matrix.

Finally, this investigation suggests that the potential,

$$V(r) = Ar^{-3}\left(\frac{2\pi r}{\beta k_f}\right)\left(\sinh\frac{2\pi r}{\beta k_f}\right)^{-1}\cos(2k_f r+\theta),$$

might be suitable to represent the long-range interaction between ions in the liquid state of simple metals.

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APPENDIX A. ANALYTICITY OF S

Since $V(x)$ satisfies the conditions (2.12) and (2.13), it follows by the method of successive approximations of Bargmann[16] that the functions $f(q_x,x)$ and $g(q_x,x)$ which are defined for $x \geq 0$, are analytic functions of q_x for $\mathrm{Im}q_x \geq -\mu$, and $\mathrm{Im}q_x \leq \mu$, respectively. Therefore, S of (2.4) is analytic in the strip of interest, namely, $0 \leq \mathrm{Im}q_x \leq \mu$, and has no poles unless $f'(q_x)+ik_x f(q_x)=0$, and the problem is to show that such poles do not exist. For brevity we shall write q and k instead of q_x and k_x. Since f and g satisfy the equations

$$f''(q,x)+(q^2-2V)f(q,x)=0, \quad (A1)$$

$$g''(q^*,x)+(q^{*2}-2V)g(q^*,x)=0, \quad (A2)$$

we have

$$f(q,x)=g^*(q^*,x), \qquad f^*(q,x)=g(q^*,x). \quad (A3)$$

Multiply (A1) by g and (A2) by f, and subtract and integrate the result over x between the limits zero and x to obtain

$$[f'(q,x)g(q^*,x)-f(q,x)g'(q^*,x)] - [f'(q)g(q^*)-f(q)g'(q^*)] + (q^2-q^{*2})\int_0^x f(q,x')g(q^*,x')dx'=0. \quad (A4)$$

Assume now that

$$f'(q)+ikf(q)=0, \quad (A5)$$

and

$$g'(q^*)-ikg(q^*)=0, \quad (A6)$$

which follows from (A5) and (A3), and use these equations together with (A3) in (A4) to obtain for large x that

$$i(q+q^*)|e^{2iqx}|+2ik|f(q)|^2 + (q^2-q^{*2})\int_0^x |f(q,x')|^2dx'=0, \quad (A7)$$

which leads to

$$\mathrm{Im}k|f(q)|^2=0. \quad (A8)$$

From Eq. (A8) we have that either k is real, or $f(q)=0$. If $f(q)$ is zero then (A5) implies that $f'(q)=0$, and hence $f(q,x)=0$. If k is real, then q is either real, or pure imaginary. For $q=ip$, p real, f and g are real, and (A5) and (A6) cannot be met. If q is real, then from (A5) and (A6) we have that the Wronskian $f'g-fg'=2iq=-2ik|f(q)|^2$, or $|f(q)|^2$ is negative. All these absurd results show that Eqs. (A5) and (A6) cannot hold, and hence S has no poles in the domain, $|\mathrm{Im}q| \leq \mu$.

APPENDIX B. CONTINUUM LIMIT

In this Appendix the passage to the limits $L_1 \to \infty$, and $L_2 \to \infty$ is sketched. For simplicity, let $V(x)$ rise suddenly (step function) to a value higher than the Fermi level at the points $x=L_1$ and $x=L_2$. All the solutions $\phi(x)$ of Eq. (2.2) which are of interest correspond to bound states. For $k_x<\alpha$, $\phi(x)$ is essentially $(2L_2)^{-1/2}u(x)$, as L_1 and $L_2 \to \infty$, and the contribution of these states to the density remains as it is in Sec. II. For $k_x>\alpha$ we can write $\phi(x)=au(x)+bv(x)$, for $-L_2 \leq x \leq L_1$. For $x \geq L_1$, $\phi(x) \propto \exp-\lambda_1(x-L_1)$, and for $x \leq -L_2$, $\phi(x) \propto \exp\lambda_2(x+L_2)$, where λ_1 and λ_2 are attenuation constants determined by the height of the potential well, the case of rigid walls corresponds to $\lambda_1=\lambda_2=\infty$. The matching of ϕ and ϕ' at $x=L_1$ and $x=-L_2$ leads to

$$\frac{a}{b} = -\frac{v'(L_1)+\lambda_1 v(L_1)}{u'(L_1)+\lambda_1 u(L_1)} \equiv a_1, \quad (B1)$$

$$\frac{a}{b} = -\frac{v'(-L_2)-\lambda_2 v(-L_2)}{v'(-L_2)-\lambda_2 u(-L_2)} \equiv a_2, \quad (B2)$$

and

$$a^2/b^2=a_1a_2=\frac{[(\lambda_1-iq_x)e^{-iq_xL_1}+(\lambda_1+iq_x)S_{11}e^{iq_xL_1}](-ik_x-\lambda_2)S_{21}e^{ik_xL_2}}{(\lambda_1+iq_x)S_{12}e^{iq_xL_1}[(ik_x-\lambda_2)e^{-ik_xL_2}-(ik_x+\lambda_2)S_{22}e^{ik_xL_2}]}. \tag{B3}$$

In the denominator and numerator of (B3), we select only the term $\exp[i(q_xL_1+k_xL_2)]$ as having a definite value for the allowed states, as L_1 and L_2 independently $\to\infty$, neglect the other exponentials, and we have

$$|a^2|/|b^2|=|S_{11}S_{21}|/|S_{12}S_{22}|=q_x/k_x. \tag{B4}$$

From Eq. (B4) and the normalization condition, $\int_{-\infty}^{\infty}|\phi(x)|^2dx=1$, we obtain that

$$\begin{aligned}|a^2|&=\tfrac{1}{2}q_x(q_xL_2+k_xL_1)^{-1},\\ |b^2|&=\tfrac{1}{2}k_x(q_xL_2+k_xL_1)^{-1}.\end{aligned} \tag{B5}$$

From the Bohr quantization condition, $j\pi\sim q_xL_1+k_xL_2$, where j is an integer labelling the state, we have that the density $n(x)$ is given by

$$n(x)=\sum_j|\phi_j(x)|^2\sim\frac{1}{\pi}\int|\phi_j(x)|^2\left(L_1+L_2\frac{dk_x}{dq_x}\right)dq_x. \tag{B6}$$

By making the appropriate substitutions in (B6), and ignoring the cross terms, such as ab^*, we arrive at the same integrals of the text in terms of $|u|^2$ and $|v|^2$.

APPENDIX C. SOMMERFELD FORMULA

The problem is to evaluate the integral

$$\mathcal{I}=-\int_0^{\infty}\phi(E)(\partial F/\partial E)dE, \tag{C1}$$

where the function $\phi(E)$ is smooth over energy intervals of order KT near $E=\zeta$, and F is the Fermi-Dirac function. We shall assume first that $\phi(E)$ and its derivatives vanish at ∞. By a partial integration we have

$$\mathcal{I}=\phi(0)F(0)+\int_0^{\infty}\phi'(E)FdE, \tag{C2}$$

which, if we neglect terms of order $\exp(-\beta\zeta)$, can be written as

$$\mathcal{I}=\int_C\phi'(E)[1+e^{\beta(E-\zeta)}]^{-1}dE, \tag{C3}$$

where the path of integration C is taken along the imaginary axis from $i\infty$ to zero, along the real axis from zero to ∞, and along a line parallel to the imaginary axis at ∞. On the imaginary axis $F\approx1$, and this path contributes in first order $\phi(0)$ which equals $\phi(0)F(0)$ to within terms of order $\exp(-\beta\zeta)$. Since $\phi(E)$ vanishes at ∞, the contour in (C3) can be closed by the line $\mathrm{Im}E=2\pi iN\beta$, where N is a large positive integer; on this line $F\leq1$, and the contribution to the integral is zero. Thus $\mathcal{I}$ is determined by the residues at the simple poles of the distribution function F in the first quadrant of the complex E plane, namely,

$$\begin{aligned}\mathcal{I}&=-\omega\sum_{n=0}^{\infty}\phi'(\zeta+\tfrac{1}{2}\omega+n\omega),\\ \omega&\equiv2\pi i/\beta.\end{aligned} \tag{C4}$$

By applying the Euler Maclaurin summation formula,[25] and observing the vanishing of ϕ and its derivatives at ∞, Eq. (C4) yields

$$\mathcal{I}=\phi(\zeta+\tfrac{1}{2}\omega)-\tfrac{1}{2}\omega\phi'(\zeta+\tfrac{1}{2}\omega)-\sum_{m=1}(-1)^m\frac{B_m}{(2m)!}\omega^{2m}\phi^{2m}(\zeta+\tfrac{1}{2}\omega), \tag{C5}$$

where the first few Bernoullian numbers B_m are: $B_1=\frac{1}{6}$, $B_2=B_4=1/30$, $B_3=1/42$. The function $\phi(\zeta+\frac{1}{2}\omega)$ and its derivatives ϕ^{2m} are now expanded at ζ in a Taylor series, and we have

$$\mathcal{I}=\phi(\zeta)+\sum_m C_m(\tfrac{1}{2}\omega)^m\phi^m(\zeta), \tag{C6}$$

$$c_{2n+1}=\frac{1}{(2n+1)!}-\frac{1}{(2n)!}-\sum_{m=1}^{n}(-1)^m\frac{2^{2m}}{(2m)!}\frac{B_m}{(2n+1-2m)!}, \tag{C7}$$

$$c_{2n}=\frac{1}{(2n)!}-\frac{1}{(2n-1)!}-\sum_{m=1}^{n}(-1)^m\frac{2^{2m}}{(2m)!}\frac{B_m}{(2n-2m)!}. \tag{C8}$$

By performing the simple computations, we find that $c_1=c_3=c_5=c_7=0$, as we expect from the fact that $\mathcal{I}$ is real, and $c_2=-\frac{1}{6}$, $c_4=7/360$, $c_6=-31/(6!)(21)$, $c_8=127/(15)8!$, and

$$\mathcal{I}=\phi(\zeta)+\tfrac{1}{6}(\pi KT)^2\phi''(\zeta)+\frac{7}{360}(\pi KT)^4\phi^4(\zeta)+\frac{31}{(21)6!}(\pi KT)^6\phi^6(\zeta)+\frac{127}{(15)8!}(\pi KT)^8\phi^8(\zeta)+\cdots, \tag{C9}$$

which is the Sommerfeld formula.

Finally, the case when $\phi(E)$ does not vanish at ∞, can be handled by multiplying ϕ by a convergence factor such $\exp(i\lambda E)$, with λ positive and real. The above method now goes through, and by setting $\lambda=0$ at the end of the calculation we obtain (C9).