PHYSICAL REVIEW B VOLUME 13, NUMBER 8 15 APRIL 1976

Effect of velocity-dependent screening on the form factors for transport properties

Mark Rasolt
Battelle Columbus Laboratories, 505 King Avenue, Columbus, Ohio 43201
and Department of Physics, The Ohio State University, Columbus, Ohio 43210

John F. Devlin
Battelle Columbus Laboratories, 505 King Avenue, Columbus, Ohio 43201

(Received 11 August 1975)

An investigation is made on the effect of velocity-dependent screening and the effect of rescattering off of a single ion on the Fermi-surface form factors. Application is made to the resistivity of liquid Na, K, Mg, and Al. Good results are obtained with these form factors. The effect of velocity dependence on thermoelectric power is also investigated and is shown to be very small.

I. INTRODUCTION

In calculations[1,2,3] of transport properties considerable effort has been made to include many-body effects on the scattering function (or so-called form factor) more and more accurately. Little attention has been paid to the following two aspects. First, the form factor is constructed from an equation which does not rigorously represent quasiparticle states. Thus, a form factor so derived cannot represent the scattering rigorously. Secondly, the scatterers are assumed to be very weak so that the Born approximation can be invoked, thereby neglecting rescattering effects. This work is an attempt to focus on these two aspects by discussing new ways for dealing with them consistantly.

This work is divided into a comparison of velocity-dependent and velocity-independent form factors. The first corresponds to the true scattering of quasiparticles while the latter is an approximation.[4] We find that the velocity-dependent form factors do not depend as strongly on exchange and correlation effects as the velocity-independent form factors used extensively in the past.

In Secs. II A and II B we propose a way to include rescattering, off a single ion to all orders in both the velocity-independent and velocity-dependent form factors. This essentially follows the work of Dagens, Rasolt, and Taylor.[5] In Sec. II C we generate an approximate form for the velocity-dependent form factors. In Sec. III A we apply the above to calculating the electrical resistivity of liquid Na, K, Mg, and Al. Finally, some of the effects of the velocity-dependent form factors on the thermoelectric power are discussed in Sec. III B. In particular, we find that the additional term coming directly from the velocity dependence cannot account for the relatively poor agreement between theory and experiment in the thermoelectric power.

This work is an attempt to suggest that new emphasis be put on constructing scattering functions from a more fundamental theory.

II. SCATTERING FUNCTION

A. Velocity-independent scattering function

We consider a single ion with a potential $V_{\text{ext}}(\vec{r})$ embedded in a jellium. In a local theory the quasiparticle states $\psi_{\vec{p}}$ are described by the equation

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}^2 + W(\vec{r})\right)\psi_{\vec{p}}(\vec{r}) = E_{\vec{p}}\,\psi_{\vec{p}}(\vec{r}) \ , \tag{1}$$

where

$$W(\vec{r}) = V_{\text{ext}}(\vec{r}) + V_H(\vec{r}) + V_{xc}(\vec{r}) \ . \tag{2}$$

Here $V_H(\vec{r})$ is the electrostatic potential of the electron gas and $V_{xc}(\vec{r})$ its exchange and correlation contribution. The induced density $n(\vec{r})$ is given by,

$$n(\vec{r}) = \sum_{\vec{p}} \psi^*_{\vec{p}}(\vec{r})\psi_{\vec{p}}(\vec{r}) \ . \tag{3}$$

For a small $V_{\text{ext}}(\vec{r})$, where linear response is applicable, the self-consistent solution of Eqs. (1)–(3) gives in Fourier space,

$$n(\vec{q}) = \frac{-V_{\text{ext}}(\vec{q})\Pi(\vec{q})}{1 + (4\pi e^2/q^2)\Pi(\vec{q})} \equiv \frac{-V_{\text{ext}}(\vec{q})\Pi(\vec{q})}{\epsilon(\vec{q})} \ , \tag{4a}$$

$$W(\vec{q}) = \frac{V_{\text{ext}}(\vec{q})}{1 + [4\pi e^2/q^2 - G(\vec{q})]\Pi_0(\vec{q})} \equiv \frac{V_{\text{ext}}(\vec{q})}{\tilde{\epsilon}(\vec{q})} \ , \tag{4b}$$

where $\Pi_0(\vec{q})$ is the screening function of the noninteracting electron gas (i.e., the Lindhard screening function), $\Pi(\vec{q})$ that of the *interacting* electron gas, and

$$G(\vec{q}) = 1/\Pi_0(\vec{q}) - 1/\Pi(\vec{q}) \ . \tag{5}$$

Finally, the transition probability $T_{\vec{p},\vec{p}'}$ of a quasiparticle state of momentum $\vec{p}$ to a state of momentum $\vec{p}'$ is proportional to $|W(\vec{q})|^2$, where $\vec{q}$ is the momentum transfer $\vec{q}=\vec{p}\,'-\vec{p}$.

For Na, K, Mg, and Al it was recently shown by Rasolt and Taylor[6] and by Dagens, Rasolt, and Taylor[5] (DRT) that nonlinear effects of $V_{\text{ext}}(\vec{r})$ are not negligible. We incorporate them following DRT by constructing an effective potential $V_{\text{eff}}(r)$, that reproduces in linear response the full charge-density induced by $V_{\text{ext}}(r)$ corresponding to the numerical solution of Eqs. (1)–(3) (see also Ref. 7). Such a $V_{\text{eff}}(r)$ used in the well-known Ziman[8] formula is an improvement over $V_{\text{ext}}(r)$ in that it includes rescattering off a single ion to all orders. It should be emphasized that in transcending the Born approximation we have ignored multicenter scattering. That this is justified is strongly suggested by the results of DRT. Finally, if we write the radial wave function in the form of the variable phase shift $\delta(\vec{r})$ (see Calogero[9]), then it is apparent that functions with the proper phase shifts will generate the correct density. The reverse is not true, i.e., the correct $n(\vec{r})$ does not ensure the proper phase shifts. However, since the adjustment from $V_{\text{ext}}(\vec{r})$ to $V_{\text{eff}}(\vec{r})$ is small (see DRT), we feel that $V_{\text{eff}}(\vec{r})$ (applied to *linear* order) generates the true phase shifts fairly accurately and thus reproduces the full cross section (or equivalently satisfies the optical theorem) to good accuracy.

B. Velocity-dependent scattering function

Most calculations of the transition probability $T_{\vec{p},\vec{p}\,'}$ assume Eq. (1) to be a fundamental starting point. See, e.g., Greenfield and Wiser[10] and Williams and Appapillai.[11] Consequently, great effort is made to improve upon the contribution of the many-body effects in $W(\vec{q})$, i.e., $\tilde{\epsilon}(\vec{q})$, through more sophisticated calculations of $G(\vec{q})$. Little attention is paid to the fact that Eq. (1) does not represent quasiparticle states[4,12,13] and hence cannot give the transition probability rigorously. For a weak $V_{\text{ext}}(\vec{r})$ the quasiparticles are scattered off the velocity-dependent potential given schematically in Fig. 1(a) by the dashed line ending at the cross. From a rigorous analysis of the response of an electron gas (to an external field) in the presence of $V_{\text{ext}}(\vec{r})$, it has been shown[14–16] that the approporiate form factor is given by

$$W(\vec{p},\vec{q},E)=Z(E)\,\tilde{\Lambda}(\vec{p},\vec{q},E)\,V_{\text{ext}}(\vec{q})/\epsilon(\vec{q})\ , \tag{6}$$

where $\tilde{\Lambda}(\vec{p},\vec{q},E)$ is the irreducible vertex function, $Z(E)$ is the quasiparticle renormalization constant, and E is the quasiparticle energy $[E=E(p)]$. (For simplicity we will hereafter omit the arguments of W, Z, and $\tilde{\Lambda}$.) We note in passing that if we define $W'=(1/\Omega_0)W$ (where Ω_0 is the volume per ion), then for electrons on the Fermi surface (FS) $p=p_f$ and $E=E(p_f)$; the limit as $q\to 0$ of W' is $-\frac{2}{3}(m/m^*)E_f$ (m^* is the effective mass of the interacting electron gas and $E_f=\hbar^2 p_{f2}/2m$).

As we did for the velocity-independent scattering function we next wish to incorporate in a simple way some of the nonlinearity associated with $V_{\text{ext}}(\vec{r})$. In Fig. 1(b) we present schematically some rescattering processes which enter the form factor W. The dashed lines ending at the cross represent the rescattering off $V_{\text{ext}}(\vec{r})$ (the so-called t matrix). We note that its full structure is extremely complex (some of the terms are shown in Fig. 9 of Ref. 14). In fact, the structure of Fig. 1(b) only corresponds to a subset of the full t matrix. We next note that the portion enclosed in the rectangle of Fig. 1(b) is the full density. Therefore, in constructing an effective interaction $V_{\text{eff}}(\vec{r})$ [the wiggly line in Fig. 1(c)], we again demand that it generate the full density. That is, $V_{\text{eff}}(\vec{r})$ is identical to the one constructed for the velocity-independent form factor. The form fac-

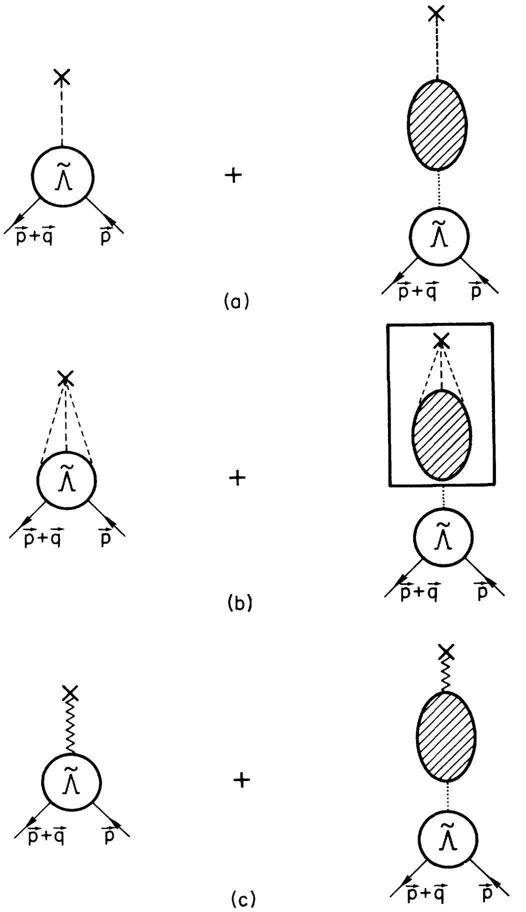

FIG. 1. Scattering function (or form factor) for the case of single and multiple scattering. Here × --- is the external potential, ⟶ is the Fermion propagator, ··· is the bare Coulomb interaction, and the shaded ellipsoid is the polarizability.

tor in Eq. (6) is now obtained by replacing $V_{\text{ext}}(\vec{q})$ by $V_{\text{eff}}(\vec{q})$.

C. Vertex function $\tilde{\Lambda}$

The main drawback of Eq. (6) and the reason it has been approximated by Eq. (4b) is the difficulty of evaluating $\tilde{\Lambda}$, which has not yet been calculated for general energy and momenta. The approximate form for $\tilde{\Lambda}$ suggested in this work is based on a FS-model calculation by Rasolt and Vosko.[12,13] In these works the mass operator $\Sigma(\vec{r}, \vec{r}', E)$ was approximated by

$$\Sigma(\vec{r}, \vec{r}', E) \approx V(\vec{r})\delta(\vec{r}-\vec{r}') + M_h[\vec{r}-\vec{r}'; E - V(\vec{r}) + \Delta(n(\vec{r})); n(\vec{r})] , \tag{7}$$

where

$$M_h(\vec{r}-\vec{r}'; E; n_0) \equiv \int \frac{d\vec{p}}{(2\pi)^3} M_h(\vec{p}, E, n_0)\, e^{i\vec{p}\cdot(\vec{r}-\vec{r}')} \tag{8}$$

and $M_h(\vec{p}, E, n_0)$ is the usual self-energy operator in momentum-energy space for a homogeneous electron gas with density n_0. Also in Eq. (7)

$$\begin{aligned} V(\vec{r}) &= V_{\text{ext}}(\vec{r}) + V_H(\vec{r}), \\ \Delta(n(\vec{r})) &= \mu_h(n(\vec{r})) + V(\vec{r}) - \mu , \end{aligned} \tag{9}$$

μ_h is the chemical potential for a uniform gas of density n, and μ is the chemical potential.

From Eq. (7), an expansion to linear order in $V_{\text{ext}}(\vec{r})$ and proper identification gives the following approximation for $\tilde{\Lambda}$:

$$\tilde{\Lambda} \approx 1 - \frac{\Pi(q)}{\Pi(0)} \left(\frac{\partial M_h(\vec{p}, E, n_0)}{\partial E} + \frac{\partial M_h(\vec{p}, E, n_0)}{\partial \mu_h} \right) . \tag{10}$$

Restricting electrons to the FS gives

$$\tilde{\Lambda} \approx 1 - [\Pi(q)/\Pi(0)](1 - Z^{-1} m K / m^* K_0) . \tag{11}$$

We note that Eqs. (10) and (11) satisfy the $q \to 0$ and $q \to \infty$ limits. Furthermore, as observed by Hedin and Lundqvist,[17] for intermediate $\vec{q}$ ($|q| \sim 2.28 p_f$ and $r_s = 4$ a.u.) Eq. (11) is in good agreement with the calculation of Watabe and Yasuhara.[18]

III. CALCULATIONS

A. Resistivity of Na, K, Mg, and Al

The resistivity of liquid metals can be obtained from the Ziman formula,[8]

$$\rho = \frac{3\pi (m^*)^2 \Omega_0}{4 e^2 \hbar^3 p_f^6} \int_0^{2p_f} |W'|^2 a(q)\, q^3\, dq , \tag{12}$$

where $a(q)$ is the structure factor of the liquid metal and W' is the screened form factor for FS scattering discussed in Sec. II. For Na and K we have used the accurate x-ray structure factors of Greenfield, Wellendorf, and Wiser[19] (GWW). For Mg and Al we used the hard-sphere structure factors (see Ashcroft and Lekner[20]) with a packing fraction of $\eta = 0.45$ assumed at the melting point.

For $V_{\text{eff}}(r)$ we chose a local non-energy-dependent form,

$$V_{\text{eff}}(\vec{r}) = -Ze^2/r - \Theta(R_M - r)(A - Ze^2/r) , \tag{13}$$

where Θ is the unit step function, A is the well depth, and R_M is the well radius. For Na, $A = 0.32$ Ry, $R_M = 1.94$ a.u.; for K, $A = 0.42$ Ry, $R_M = 2.98$ a.u.; for Mg, $A = 1.235$ Ry, $R_M = 1.72$ a.u.; and for Al, $A = 2.22$ Ry, $R_M = 1.40$ a.u. These coefficients are the ones that give good full charge densities, especially for the cases of Na and K. (See DRT for these densities.)

We have used five different $G(q)$ functions in this paper to study the effect of the two scattering functions (velocity dependent and velocity independent). These five functions are plotted in Fig. 2 and will henceforth be denoted as follows: HS refers to Hubbard and Sham,[21] SP refers to Shaw and Pynn,[22] TW refers to Toigo and Woodruff,[23] GT refers to Geldart and Taylor,[24] and VS refers to Vashishta and Singwi.[25]

The velocity-independent form of the potential of Eq. (13) is obtained from Eq. (4b) while the velocity-dependent form is obtained from Eq. (8). Incorporating Eq. (11) into Eq. (6) yields

$$W = [V_{\text{ext}}(q)/\epsilon(q)][Z + b_0 \Pi(q)/\Pi(0)] , \tag{14a}$$

where

$$b_0 = -Z + (m/m^*)(K/K_0) . \tag{14b}$$

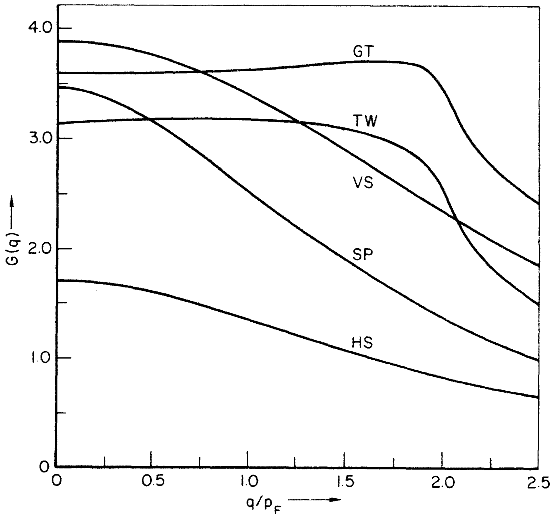

FIG. 2. $G(q)$ functions (in atomic units, $m = \hbar = e = 1$) used in this work. The notation is as follows: VS is Vashishta and Singwi (Ref. 25), GT is Geldart and Taylor (Ref. 24), TW is Toigo and Woodruff (Ref. 23), SP is Shaw and Pynn (Ref. 22), and HS is Hubbard and Sham (Ref. 21).

TABLE I. Resistivity results (in μΩ cm) for the velocity-independent and velocity-dependent form factors for liquid Na, K, Mg, and Al. The velocity-dependent results are in parentheses. The screening functions used are the same as those referred to in Fig. 2.

Screening functions	Na 100 °C	Na 200 °C	K 65 °C	K 135 °C	Mg 651 °C	Al 660 °C
Hartree	6.05	7.95	7.68	9.84	10.33	11.87
HS	7.15	9.40	9.03	11.58	12.02	13.83
	(7.14)	(9.37)	(8.80)	(11.27)	(11.97)	(14.39)
SP	8.30	10.92	10.89	13.98	13.05	14.71
	(9.79)	(12.90)	(13.41)	(17.26)	(13.92)	(15.64)
TW	10.01	13.21	13.38	17.23	15.14	16.59
	(8.91)	(11.73)	(11.76)	(15.13)	(13.37)	(15.13)
GT	11.28	14.91	15.56	20.09	16.54	17.67
	(9.78)	(12.91)	(13.34)	(17.20)	(14.11)	(15.69)
VS	9.81	12.94	13.41	17.27	14.45	15.82
	(10.39)	(13.71)	(14.35)	(18.50)	(14.51)	(16.07)
Experiment	9.6[a,b]	13.4[a]	13.1[a,b]	16.8[a,b]	27.4[a]	24.2[a]

[a] N. E. Cusack, Rep. Prog. Phys. 26, 361 (1963).
[b] J. Hennephof (private communication).

As we mentioned in Sec. II B, the compressibility sum rule is an integral part of the formulation of the velocity dependence. However, only one of the $G(q)$ functions that we have used satisfied this exactly, *viz.*, the GT function. *Therefore*, in order to use the other $G(q)$ functions in this theory, we have used the ratios of K/K_0 obtained from their $G(q=0)$ values. This automatically ensures that $W' \to -\frac{2}{3} E_f(m/m^*)$ as $q \to 0$. We have restricted ourselves to $m^* = m$ because of the uncertainties in calculating the quasiparticle mass and because the m^* only deviates slightly from m. (See Rice,[26] Hedin,[27] and Lundqvist.[28])

Figure 3 contains plots of the form factors of Na and Al for the Hartree, velocity-independent, and velocity-dependent cases. It is interesting to note that both the velocity-independent and velocity-dependent form factors show the same trends: they are larger than the Hartree and are close to one another though their structure originates from different formulations. The same trends were found for K and Mg.

Table I contains the results for the resistivity for velocity-independent and velocity-dependent scattering functions. We note that both are in much better agreement with experiment than the Hartree and the former is generally larger. Thus, we conclude that exchange and correlation effects are smaller for velocity-dependent form factors. For Na and K, the GT results with velocity dependence included are in very good agreement with experiment. This very good agreement of the Na and K results is partly a reflection of the quality of the GWW[19] experimental structure factors, in particular the temperature dependence. For Mg and Al we were not able to find structure factors of the quality of GWW, therefore, we used the hard-sphere model.[29] We have also used bare form factors for Na and K that did not include the rescattering effects and found that the velocity-dependent results were then much below experiment.

Finally, we emphasize here that besides attempting to produce good agreement between theory and experiment, we wish to more clearly discern the effect of the velocity-dependent screening formulation. Since great efforts have been put into constructing better $G(q)$ functions, this work suggests greater emphasis be put into constructing better

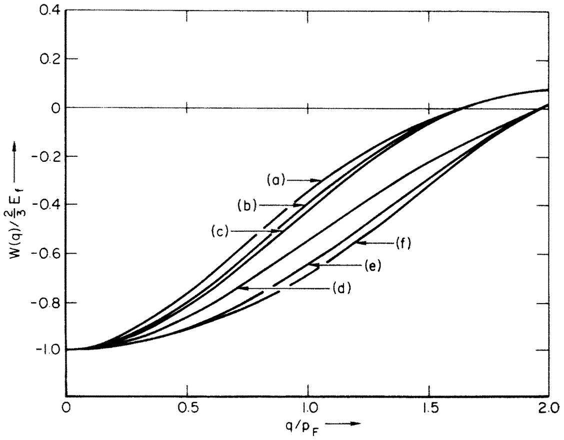

FIG. 3. Form factors for Al at 660 °C and Na at 100 °C using the GT screening function. (a) Hartree result for Al. (b) Velocity-dependent result for Al. (c) Velocity-independent result for Al. (d) Hartree result for Na. (e) Velocity-dependent result for Na. (f) Velocity-independent result for Na.

vertex functions [Eq. (10)].

B. Thermoelectric power

The thermoelectric power Q is given by[30]

$$Q=[(m^*/m)\pi^2k_B^2\,T/3\,eE_f](3-2s-\tfrac{1}{2}r)\ , \tag{15}$$

where

$$s=4p_f^4\,|W'(2p_f)|^2\,a(2p_f)\Big/\int_0^{2p_f}|W'|^2\,a(q)\,q^3\,dq \tag{16}$$

and

$$r=2p_f\int_0^{2p_f}\left(\frac{d}{dp}\,W'\right)W'\,a(q)\,q^3\,dq\Big/\int_0^{2p_f}|W'|^2\,a(q)\,q^3\,dq\ . \tag{17}$$

As we pointed out in Sec. II and as is apparent from Eqs. (15) and (17), the energy dependence of $V_{\text{ext}}(r)$ is crucial for calculating Q. It is, therefore, not possible to get meaningful results for Q using our energy independent $V_{\text{eff}}(r)$. There is, however, a contribution not dependent upon the energy dependence of $V_{\text{eff}}(r)$ which is of interest (see below).

Careful calculations by Devlin and van der Lugt[2] using the Shaw[31] nonlocal energy-dependent-model potential show that for the improved many-body contribution $[G(q)]$ the value of ρ improves while that of Q gets worse. This is perturbing since, as we saw, many-body contributions included in two different schemes showed similar trends from the Hartree results (see Fig. 3). In this section we wish to investigate the importance of the energy dependence in $Z\tilde{\Lambda}$ on Q. This contribution is absent in the velocity-independent structure factor and could be the source for the above discrepancy.

From Eqs. (6) and (11) it is apparent that this additional contribution is given by

$$r=\text{Re}\left[2p_f\int_0^{2p_f}\left(\frac{d}{dp}(\tilde{\Lambda}Z)\right)_{p=p_f}\frac{V_{\text{ext}}(q)}{\epsilon(q)}\,W'\,a(q)\,q^3\,dq\Big/\int_0^{2p_f}|W'|^2\,a(q)\,q^3\,dq\right]. \tag{18}$$

Our approximation for $\tilde{\Lambda}$ given by Eq. (10) allows us to estimate this contribution. With $Z^{-1}=1-\partial M_h(\vec{\text{p}},E,n_0)/\partial E$ and after some algebra and rearrangement of terms [it is convenient to change differentiation with respect to μ_h in Eq. (10) to that of p] we get

$$2p_f\left(\frac{d}{dp}\,(\tilde{\Lambda}Z)\right)_{p=p_f}=\frac{m}{m^*}\left[-2r_s\,\frac{\partial m^*}{\partial r_s}\,\frac{1}{m^*}\,\frac{K}{K_0}\,\frac{\Pi(q)}{\Pi(0)}+Z^2\left(1-\frac{\Pi(q)}{\Pi(0)}\right)\left(M_{\omega,\omega}+\frac{m^*}{m}\,M_{k,\omega}\right)\right], \tag{19}$$

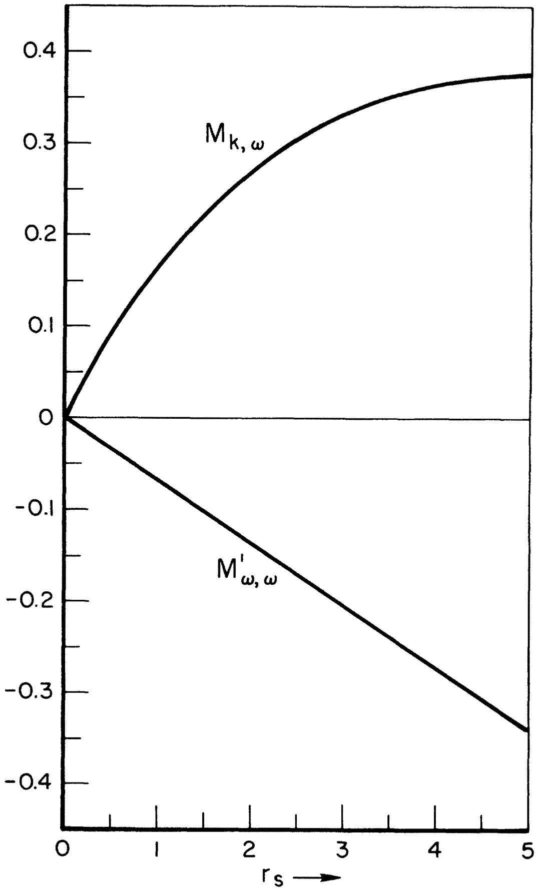

FIG. 4. $M^1_{\omega,\omega}$ and $M_{k,\omega}$ plotted as a function of r_s [see Eqs. (25) and (27) in the text].

where

$$M_{\omega,\omega}=\frac{\partial^2}{\partial\omega^2}\,M_h(k,\omega,n_0)\Big|_{\substack{\omega=0.25\\k=0.5}}\ , \tag{20}$$

$$M_{k,\omega}=\frac{\partial}{\partial k}\,\frac{\partial}{\partial\omega}\,M_h(k,\omega,n_0)\Big|_{\substack{\omega=0.25\\k=0.5}}\ ; \tag{21}$$

all energies have been changed to units of $\hbar^2(2p_f)^2/2m$ and momenta to $2p_f$. We again set $m^*=m$. Hence we get

$$2p_f\left(\frac{d}{dp}\,(\tilde{\Lambda}Z)\right)_{p=p_f}\approx Z^2\left(1-\frac{\Pi(q)}{\Pi(0)}\right)(M_{\omega,\omega}+M_{k,\omega})\ . \tag{22}$$

Our task is then to evaluate the last two terms of Eq. (22), and we do this in the random-phase approximation (RPA). In the RPA, $M_h(k,\omega,n_0)$ is given by

$$M_h(k,\omega,n_0)=\frac{-\alpha r_s}{2\pi^2}\int d^3q\int\frac{d\omega'}{2\pi i}\times\left(\frac{1-\Theta[(\vec{\text{k}}+\vec{\text{q}})^2-\frac{1}{4}]}{\omega+\omega'-(\vec{\text{k}}+\vec{\text{q}})^2-i\delta}+\frac{\Theta[(\vec{\text{k}}+\vec{\text{q}})^2-\frac{1}{4}]}{\omega+\omega'-(\vec{\text{k}}+\vec{\text{q}})^2+i\delta}\right)P_0(q,\omega')\ , \tag{23}$$

where $P_0(q, \omega')$ is the usual pair effective interaction. After differentiation with respect to ω and k and careful rotation to the imaginary axis we get for $M_{\omega,\omega}$

$$M_{\omega,\omega} = M^1_{\omega,\omega} + iM^2_{\omega,\omega} , \tag{24}$$

where

$$M^1_{\omega,\omega} = -\frac{\alpha r_s}{\pi^2}\int_0^\infty dq \int_0^\infty \frac{du}{q^2 + (\alpha r_s/4\pi)Q(q,u)} \times\left(\frac{1}{(1-q)^2+u^2} - \frac{2(1-q)^2}{[(1-q)^2+u^2]^2} - \frac{1}{(1+q)^2+u^2} + \frac{2(1+q)^2}{[(1+q)^2+u^2]^2}\right) , \tag{25}$$

and

$$M^2_{\omega,\omega} = \frac{-(\alpha r_s)^2}{2\pi}\int_0^1 \frac{dq}{q^4}\frac{1}{[\epsilon(q,0)]^2} . \tag{26}$$

For $M_{k,\omega}$ we get

$$M_{k,\omega} = -\frac{2\alpha r_s}{\pi}\int_0^1 \frac{dq}{q}\frac{1}{\epsilon(q,0)} + \frac{\alpha r_s}{\pi}\left(\frac{1}{\epsilon(1,0)} - 1\right) + \frac{2\alpha r_s}{\pi^2}\int_0^\infty dq \int_0^\infty \frac{du}{q^2 + (\alpha r_s/4\pi)Q(q,u)} \times\left(\frac{\frac{1}{2} - q^2}{(1-q)^2+u^2} - \frac{\frac{1}{2} - q^2}{(1+q)^2+u^2} - \frac{2(1-q)^2(\frac{1}{2} - q)}{[(1-q)^2+u^2]^2} + \frac{2(1+q)^2(\frac{1}{2} + q)}{[(1+q)^2+u^2]^2}\right) , \tag{27}$$

and $\alpha = (4/9\pi)^{1/3}$, $a_0 r_s = (3/4\pi n_0)^{1/3}$, $a_0 = \hbar^2/me^2$. In Eqs. (25)–(27),

$$\epsilon(q,0) = 1 + \frac{\alpha r_s}{\pi}\frac{1}{q^2}\left(\frac{1}{2} + \frac{1-q^2}{4q}\ln\left|\frac{1+q}{1-q}\right|\right) , \tag{28}$$

and

$$Q(q,u) = 2 + \frac{u^2+1-q^2}{2q}\ln\left(\frac{u^2+(q+1)^2}{u^2+(q-1)^2}\right) - 2u\left(\tan^{-1}\frac{(1-q)}{u} + \tan^{-1}\frac{(1+q)}{u}\right) . \tag{29}$$

[Note the q's in Eqs. (23)–(29) should not be confused with the previous momentum transfer $\vec{q}$.] After suitable transformations the integral in Eqs. (25) and (27) are evaluated numerically for a range of r_s. The results are plotted in Fig. 4. The imaginary part $M^2_{\omega,\omega}$ is neglected since it makes no contribution to r [see Eqs. (17) and (18)].

As can be seen, the terms $M^1_{\omega,\omega}$ and $M_{k,\omega}$ individually make for a sizable contribution, but of opposite sign. As in the case of calculating m^* (where large cancellation occurs between $\partial M/\partial\omega$ and $\partial M/\partial k$; see Rice[26]) they largely cancel out. The effect of the energy dependence of $\tilde{\Lambda}$ on the thermoelectric power [i.e., r of Eq. (18)] is calculated using Eqs. (17) and (22), Fig. 4, and the values of Z and K/K_0 given by Hedin[27] and Hedin and Lundqvist.[32] The GT results for Na, K, Mg, and Al are $r = 0.0076$, 0.0030, 0.0196, and 0.0156, respectively, and are seen to be very small. The other $G(q)$ functions yielded the same trend. We conclude that the aforementioned discrepancy in the thermoelectric-power calculations does not originate in the energy dependence of the vertex function, but in the lack of accuracy of the original pseudopotential.

ACKNOWLEDGMENT

We are pleased to acknowledge useful conversations with R. Taylor.

---

[1] W. Shyu, J. H. Wehling, M. R. Cordes, and G. D. Gasperi, Phys. Rev. B 4, 1802 (1971).

[2] J. F. Devlin and W. van der Lugt, Phys. Rev. B 6, 4462 (1972).

[3] P. V. S. Rao, Phys. Status Solidi B 52, 629 (1973).

[4] L. J. Sham and W. Kohn, Phys. Rev. 145, 561 (1966).

[5] L. Dagens, M. Rasolt, and R. Taylor, Phys. Rev. B 11, 2726 (1975).

[6] M. Rasolt and R. Taylor, Phys. Rev. B 11, 2717 (1975).

[7] *The Properties of Liquid Metals*, edited by S. Takeuchi (Taylor and Francis, London, 1973).

[8] J. M. Ziman, Philos. Mag. 6, 1013 (1961).

[9] F. Calogero, *Variable Phase Approach to Potential Scattering* (Academic, New York, 1967).

[10] A. J. Greenfield and N. Wiser, J. Phys. F 3, 1397 (1973).

[11] A. R. Williams and M. Appapillai, J. Phys. F 3, 772 (1973).

[12] M. Rasolt and S. H. Vosko, Phys. Rev. Lett. 32, 297 (1974).

[13] M. Rasolt and S. H. Vosko, Phys. Rev. B 10, 4195 (1974).

[14] J. S. Langer, Phys. Rev. 120, 714 (1960).

[15] J. S. Langer, Phys. Rev. 124, 997 (1961).

[16] J. S. Langer, Phys. Rev. 124, 1003 (1961).

[17] L. Hedin and B. I. Lundqvist, J. Phys. C 4, 2064 (1971).

[18] M. Watabe and H. Yasuhara, Phys. Lett. A 28, 329 (1968).

[19] A. J. Greenfield, J. Wellendorf, and N. Wiser, Phys. Rev. A 4, 1607 (1971).

[20] N. W. Ashcroft and J. Lekner, Phys. Rev. 145, 83 (1966).

[21] J. Hubbard, Proc. R. Soc. Lond. A 240, 539 (1957); 243, 336 (1958); L. J. Sham, *ibid.* 283, 33 (1965).

[22] R. W. Shaw, Jr. and R. Pynn, J. Phys. C 2, 2071

(1969).

[23] F. Toigo and T. O. Woodruff, Phys. Rev. B 2, 3958 (1970).

[24] D. J. W. Geldart and R. Taylor, Can. J. Phys. 48, 167 (1970).

[25] P. Vashishta and K. S. Singwi, Phys. Rev. B 6, 865 (1972).

[26] T. M. Rice, Ann. Phys. 31, 100 (1965).

[27] L. Hedin, Phys. Rev. 130, A796 (1965).

[28] B. I. Lundqvist, Phys. Konden. Mater. 6, 206 (1967).

[29] Preliminary results in Al, with a structure factor calculated using a pair potential corresponding to the above pseudopotential, indicate that the poor agreement for Al is due to the use of the hard-sphere structure factor.

[30] C. C. Bradley, T. E. Faber, E. G. Wilson, and J. M. Ziman, Philos. Mag. 7, 865 (1962).

[31] R. W. Shaw, Jr., Phys. Rev. 174, 769 (1968).

[32] L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich, (Academic, New York, 1969), p. 1.