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Temperature Dependence of the Elastic Constants

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The following two equations are proposed for the temperature dependence of the elastic stiffness constants: $c_{ij} = c_{ij}^0 - s/(e^{t/T} - 1)$ and $c_{ij} = a - bT^2/(T+c)$, where c_{ij}^0 , s , t , a , b , and c are constants. The applicability of these two equations and that of Wachtman's equation is examined for 57 elastic constants of 22 substances. The first equation has a theoretical justification and gives the best over-all results. Neither of the three equations give the theoretically expected T^4 dependence at low temperatures, and therefore they are not expected to give very accurate results at very low temperatures ($\lesssim \Theta_D/50$). A new melting criterion is also examined.

I. INTRODUCTION

The theory of the temperature dependence of the elastic constants was first developed by Born and co-workers.¹ In this theory, the temperature dependence of the elastic constants arises from the variation of the lattice potential energy due to anharmonicity. In the limiting cases, the theory^{1,2} shows that the lattice contribution to $c_{ij}(T) - c_{ij}(0)$ should vary as T^4 at very low temperatures and as T at high temperatures. Here c_{ij} represents an elastic stiffness constant.

During the last two decades the variation of the elastic constants with temperature has been measured for a large number of substances. On the experimental side, in Fig. 1, we show a typical set of data. The general pattern conforms to theoretical expectation. However, the T^4 dependence at low temperatures has not yet been unambiguously established; the scanty evidence which is available

appears to indicate that its range of validity is rather small. Further, some metallic substances have been found³⁻⁵ to show a T^2 dependence at low temperatures. Bernstein⁶ has shown that such a dependence can arise from the temperature dependence of the electron energy due to the Fermi-Dirac distribution of electrons.

We may note here that there are many substances whose one or more elastic stiffness constants do not show the type of behavior shown in Fig. 1 (e.g., see figures in Hearmon⁷). In the present paper we shall not consider such elastic constants, but confine ourselves to those that show the regular behavior typified in Fig. 1.

Attempts have been made to represent the temperature dependence of elastic constants by empirical equations. We quote here three of these.

Sutton⁸ was able to represent the variation of c_{44} of aluminum over the range 63-773 °K with an accuracy better than $\frac{1}{2}\%$ by the following equation:

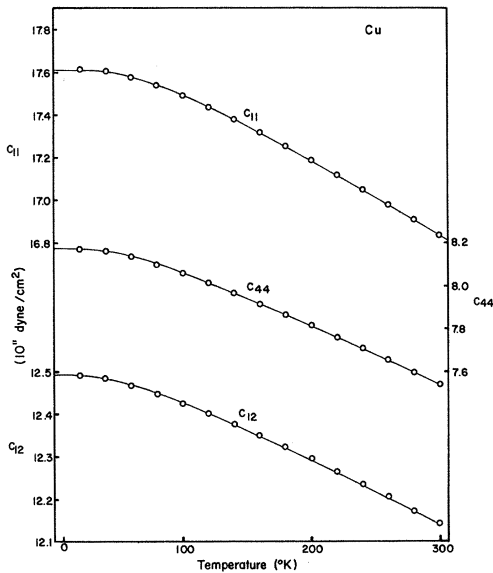


FIG. 1. Experimental and calculated adiabatic elastic stiffness constants of copper. The curves shown were obtained from Eq. (4). Smoothed experimental data points are from Overton and Gaffney (Ref. 9).

$$c_{44} = Ae^{-B\beta T} R^{-2}, \quad (1)$$

where β is the volume expansion coefficient and R is the ratio of volume at temperature T to that at some fixed temperature.

Overton and Gaffney⁹ found that a similar relation

$$c_{44}/c_{44}(0^\circ\text{K}) = e^{-B\alpha T}/(1 + \int_0^T \alpha dT)^9, \quad (2)$$

where α is the linear expansion coefficient, represents c_{44} of copper within 0.2% from 0 to 300 °K.

Wachtman *et al.*¹⁰ suggested the following equation for Young's modulus:

$$E = E_0 - BT \exp(-T_0/T). \quad (3)$$

The equation was shown to give very good results for Al_2O_3 , MgO , and ThO_2 over the temperature range 77–850 °K. Later this equation was shown to hold very well¹¹ for ThO_2 over a temperature range of 1300 °K. Anderson¹² has attempted to give a theoretical justification to Wachtman's equation. In the present paper we would apply Eq. (3) to elastic stiffness constants and in this context E would represent an elastic stiffness constant.

Some workers^{13,14} have employed polynomials in T .

The purpose of the present paper is to suggest two equations for the variation of elastic stiffness constants with temperature and to examine their applicability and that of Wachtman's equation (3) to 22 substances. The proposed equations are

$$c_{ij} = c_{ij}^0 - s/(e^{t/T} - 1) \quad (4)$$

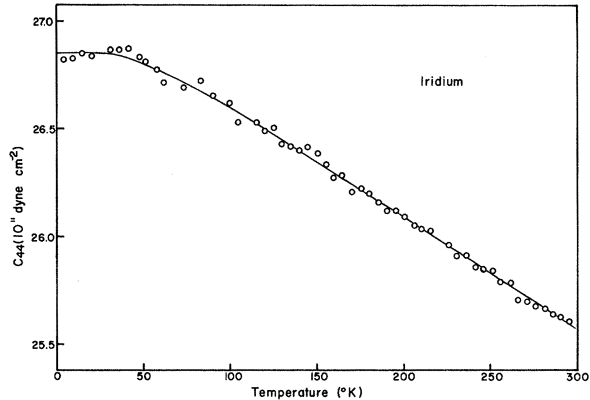


FIG. 2. Experimental and calculated c_{44} for iridium. The curve shown was obtained from Eq. (4); the experimental points are from MacFarlane *et al.* (Ref. d, Table I).

and

$$c_{ij} = a - bT^2/(T+c). \quad (5)$$

Here c_{ij}^0 , s , t , a , b , and c are constants. c_{ij}^0 and a represent the values of the elastic constant at 0 °K according to the two equations. A theoretical justification for Eq. (4) is offered in the discussion.

II. RESULTS

In order to examine the applicability of these equations, adiabatic elastic-constant data of 22 substances of different types were chosen. To obtain the parameters, the following procedure was adopted which we illustrate with Eq. (4). t was given a

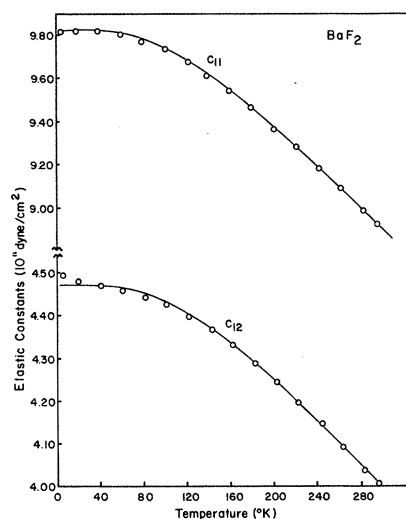


FIG. 3. Experimental and calculated c_{11} and c_{12} for BaF_2 . The curves shown were obtained from Eq. (4); the experimental points are from Gerlich (Ref. m, Table I).

TABLE I. Values of parameters in Eqs. (4), (5), and (3). A greater number of significant figures has been retained than is warranted by the accuracy of the data to ensure that the calculated values from these parameters give the least average percentage difference from the experimental ones.

Substance	Source of data	c_{ij}	c_{ij}^0	s	t	a	b	c	E_0	B	T_0
		$(10^{11} \text{ dyn/cm}^2)$	$(10^{11} \text{ dyn/cm}^2)$	$(10^{11} \text{ dyn/cm}^2)$	(°K)	$(10^{11} \text{ dyn/cm}^2)$	(10^8 dyn/cm^2)	(°K)	$(10^{11} \text{ dyn/cm}^2)$	(10^8 dyn/cm^2)	(°K)
Aluminum	a	c_{11}	11.42160	1.011141	258.4	11.44279	6.16193	420.4	11.42512	4.14083	153.2
		c_{12}	6.19493	0.205109	293.6	6.19963	1.05999	445.0	6.19562	0.74319	175.2
		c_{44}	3.16054	0.256479	168.0	3.17067	1.68226	130.0	3.16201	1.57075	94.6
		c_{11}	17.60940	0.760041	206.4	17.63202	4.59823	219.8	17.61319	3.83126	118.8
Copper	b	c_{12}	12.48920	0.238363	158.4	12.49588	1.78424	154.4	12.49031	1.55267	90.2
		c_{44}	8.17063	0.452830	163.4	8.18513	3.22506	149.8	8.17355	2.84804	91.6
		c_{11}	20.16417	0.324932	89.6	20.17807	3.73613	54.6	20.16611	3.66870	48.4
		c_{12}	16.96747	0.290603	109.8	16.97910	2.75801	70.8	16.96865	2.69399	60.8
Iridium	d	c_{44}	4.54398	0.062821	49.6	4.54716	1.28164	26.8	4.54438	1.27357	26.2
	c_{44}	26.85003	0.711340	132.2	26.87719	5.91307	102.8	26.85088	5.55755	76.6	
Iron	e	c_{11}	24.31652	0.388752	97.2	24.34539	4.01393	47.0	24.33093	3.95073	43.2
	c_{44}	12.18518	0.405473	211.2	12.19421	2.62812	275.2	12.18689	2.00422	122.6	
Lead	f	c_{11}	5.56030	0.094859	43.5	5.56643	2.19582	21.7	5.56229	2.18422	21.5
		c_{12}	4.54199	0.077379	66.2	4.54627	1.19124	37.0	4.54203	1.18210	36.5
		c_{44}	1.94370	0.038874	24.6	1.94702	1.58026	10.5	1.94434	1.58167	12.2
		c_{11}	6.33683	0.377516	200.5	6.34552	2.48786	245.0	6.33829	1.96420	116.5
Magnesium	g	c_{33}	6.64007	0.432300	191.5	6.65142	2.81604	207.0	6.64052	2.37656	114.5
		c_{44}	1.83686	0.230590	233.0	1.84214	1.42414	328.5	1.83777	1.03919	136.5
		c_{66}	1.87219	0.163720	191	1.87630	1.08078	212	1.87329	0.88184	107
		c_{12}	2.59236	0.096157	423	2.59246	2.59246	275	2.59246	0.26111	275
Molybdenum	h	c_{13}	2.16868	0.106632	509.5	2.16868	2.16868	275.2	2.16868	0.23997	329.0
	c_{11}	47.33368	1.688087	276.5	47.44370	6.31211	162.5	47.34983	6.17770	148.5	
Silicon	i	c_{44}	11.09852	0.273832	255.5	11.11203	1.11832	165.5	11.10283	1.08057	138.0
		c_{11}	16.75018	0.532972	407	16.76601	3.42607	1232.4	16.75241	1.44137	251
		c_{12}	6.50079	0.231036	334.8	6.50986	1.08879	502.8	6.50277	0.72854	193.8
		c_{44}	8.00735	0.224966	497.4	8.00790	3.12089	67.2	8.00790	0.51791	319.6
Silver	c	c_{11}	13.14898	0.315748	105.2	13.16171	3.12089	67.2	13.14968	3.06059	59.0
	c_{12}	9.73543	0.221625	141.0	9.74216	1.71854	110.2	9.73763	1.58538	74.4	
Tantalum	j	c_{44}	5.10897	0.139351	74.0	5.11582	1.91721	41.6	5.10974	1.90121	39.8
	c_{11}	26.64638	1.854980	433.0	26.64776	2.28139	64.0	26.64776	4.92228	288.0	
Thorium	k	c_{44}	8.73376	0.208622	96.0	8.74249	2.28139	64.0	8.73592	2.19624	51.0
		c_{11}	7.78493	0.333704	252.0	7.80688	1.49873	190.0	7.78884	1.37298	141.0
		c_{12}	4.82199	-0.467814	612	4.82131	2.61099	328.5	4.82131	-0.91491	408
		c_{44}	5.12123	0.678869	329.5	5.15640	3.48977	853	5.12617	2.18834	193.5
Tungsten	j	c_{11}	53.25499	6.462494	616	16.32619	3.48977	853	53.25687	13.43547	431
	c_{44}	16.31577	0.568995	346	16.32619	3.48977	853	16.31748	1.76633	209	
Mg-Ag	l	c_{11}	8.61985	2.949684	890.4	8.62205	4.02328	602.4	8.62205	4.02328	602.4
	c_{12}	5.76069	5.811370	1265.4	5.76237	6.23894	909.6	5.76237	6.23894	909.6	

TABLE I. (continued)

Substance	Source of data	c_{ij}^0 (10^{11} dyn/cm 2)	s (10^{11} dyn/cm 2)	t (°K)	a (10^{11} dyn/cm 2)	b (10^8 dyn/cm 2)	c (°K)	E_0 (10^{11} dyn/cm 2)	B (10^8 dyn/cm 2)	T_0 (°K)
MgAg		5.19024	1.079610	428.6	5.23019	3.47561	531.0	5.19920	2.62183	243.6
MgCu $_2$	l	12.47302	2.986063	796.0				12.47929	4.22934	505.6
		7.16662	1.411804	735.6				7.17057	2.11263	456.0
		4.21997	0.831033	651.6				4.22251	1.39808	402.0
BaF $_2$	m	9.81800	1.700638	316.6	9.84390	14.74914	1098.4	9.82000	5.92110	199.0
		4.46896	0.997402	342.0				4.47059	3.21967	214.4
KF	n	7.58496	0.249776	60.0	7.60669	4.16961	26.8	7.58918	4.17821	30.4
		1.29271	0.080453	325.6	1.29391	0.75618	1285.0	1.29300	0.26339	194.4
LiBr	o	4.72427	0.454125	131.4	4.75561	3.44099	64.0	4.72876	3.50586	70.6
		2.05292	0.193328	226.8	2.05802	1.11235	265.0	2.05385	0.88824	130.8
LiCl	p	5.87116	0.268565	68.2	5.88793	4.00185	36.6	5.87806	3.93707	33.0
		2.67122	0.202014	204.8	2.67825	1.13968	181.0	2.67213	1.02837	118.4
RbCl	p	4.50119	0.176814	56.8	4.51260	3.13842	28.6	4.50389	3.12290	28.8
		0.49706	0.002090	31.2	0.49721	0.06716	14.4	0.49711	0.06697	14.8
TiBr	q	4.46895	0.213729	75.8	4.47820	2.90607	46.6	4.46913	2.85701	42.0
		1.88147	0.022585	16.8	1.88558	1.33589	4.65	1.88260	1.33935	7.45
Benzene	r	1.00700	0.127209	118.0	1.01224	1.14298	81.2	1.00699	1.10736	68.0
		0.92521	1.399136	426	0.99635	5.20004	600	0.93995	3.51573	248
		1.01282	5.677769	707				1.02454	10.05501	480

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TABLE II. Values of parameters in Eq. (5'). A greater number of significant figures has been retained than is warranted by the accuracy of the data to ensure that the calculated values from these parameters give the least average percentage difference from the experimental ones.

Substance	Elastic Constant	a (10^{11} dyn/cm 2)	b' (10^5 dyn/cm 2 deg 2)
Magnesium	c_{12}	2.593 68	0.362 614
	c_{13}	2.170 12	0.276 100
Silicon	c_{44}	8.012 37	0.643 163
Tantalum	c_{11}	26.670 58	6.490 597
Thorium	c_{12}	4.811 82	-0.881 567
Tungsten	c_{11}	53.325 08	10.698 119
MgAg	c_{11}	8.668 42	2.539 548
	c_{12}	5.819 32	2.083 236
MgCu $_2$	c_{11}	12.524 93	3.248 429
	c_{12}	7.190 96	1.789 699
	c_{44}	4.233 49	1.319 261
BaF $_2$	c_{12}	4.478 47	5.491 108
Benzene	c_{22}	1.158 31	7.974 149

series of values at large intervals; for each of these values, c_{ij}^0 and s were obtained by the method of least squares. Using these parameters, average percentage differences between observed and calculated c_{ij} 's were obtained. It was anticipated and found that the average percentage difference showed a minimum for a certain value of t . This minimum was located more accurately by varying t in smaller steps. Similar procedures were used for Eqs. (3) and (5). In Eq. (5), it was found in several cases that the average percentage differences did not show a minimum but rather tended to an asymptotic value. In these cases, the following asymptotic form of Eq. (5) was adopted:

$$c_{ij} = a - b'T^2. \quad (5')$$

a and b' were calculated by the method of least squares. The parameters thus obtained for Eqs. (4), (5), and (3) are listed in Table I, and those for Eq. (5') in Table II. The temperature range for most of the substances listed in Table I is 0–300 °K except Mo (73–973 °K), Si (78–300 °K), Th (80–340 °K), MgAg (80–500 °K), MgCu $_2$ (80–500 °K), and benzene (170–973 °K). The sources for the experimental data are given in Table I. In some papers the workers have tabulated the actual experimental values, while in many others smoothed data have been recorded. In three cases (Ir, Si, and BaF $_2$), the experimental data were given in graphs only. In Figs. 1–4 we compare the calculated values by Eq. (4) with the observed ones for four typical cases.

III. DISCUSSION

A theoretical justification of Eq. (4) can be given as follows. Leibfried and Ludwig 2 have shown that the temperature dependence of adiabatic elastic

constants can be represented as follows:

$$c_{ij} = c_0(1 - D\bar{\epsilon}), \quad (6)$$

where D is a parameter which depends on the type of the crystal or model used and $\bar{\epsilon}$ is the mean energy per oscillator. If we assume an Einstein model for the solid,

$$\bar{\epsilon} = \frac{1}{2}h\nu + \frac{h\nu}{e^{h\nu/kT} - 1}. \quad (7)$$

Substitution of (6) and (7) yields Eq. (4). But beyond this, of course, we depart from theory in that we leave the parameters free and determine them from the experimental data.

It may be noted here that Eq. (6) gives only the lattice contribution to the temperature dependence, while Eq. (4) represents the total temperature dependence, i. e., it includes the electronic contribution. Consequently, a close correspondence between the parameter t and the Einstein frequency ν is not expected.

At low temperatures, the temperature-dependent part of Eq. (4) behaves like $e^{-h\nu/kT}$ rather than T^4 . This, however, is not very important, at least for practical purposes. The range of validity of T^3 law for specific heats is usually considered to be up to $\sim \Theta_D/50$ (Blackman 15); it would be reasonable to assume that this would also be the limit for the T^4 law for the elastic constants. The change in the elastic constants between 0 and $\sim 6^\circ\text{K}$ is extremely small, and at least for many practical purposes, the precise temperature dependence does not affect the magnitude of the elastic constant one way or the other. In addition, for metallic substances there is the T^2 dependence of the electronic contribution. It is not clear which term (lattice or electronic) would be the dominant one at such low temperatures.

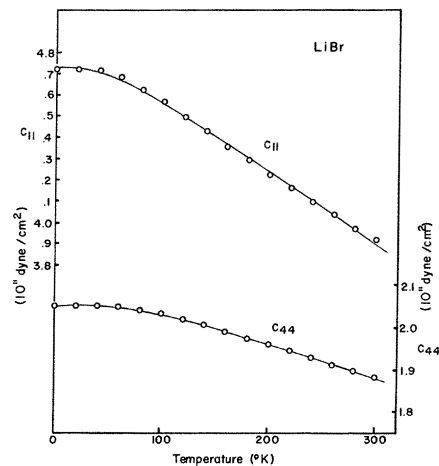


FIG. 4. Experimental and calculated c_{11} and c_{12} of lithium bromide. The curves shown were obtained from Eq. (4); the experimental points are from Marshall and Cleavelin (Ref. 6, Table I).

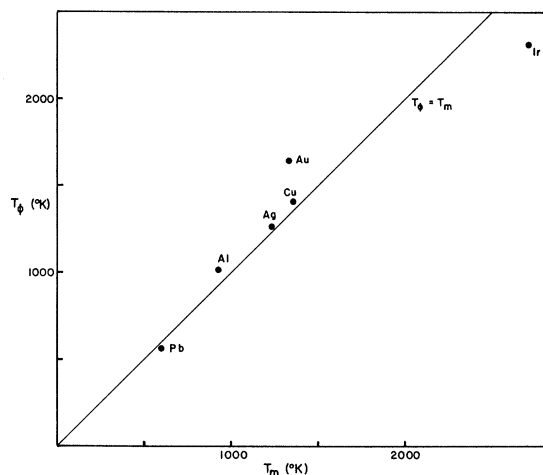


FIG. 5. T_ϕ , the temperature at which $c_{44} = 0.55c_{44}(0^\circ\text{K})$, plotted versus the melting point T_m .

The justification of Eq. (5), at least for metals, lies in the fact that at low temperatures, the second term varies as T^2 , which would be the case theoretically if the electronic term were dominant, and at high temperatures it varies as T , which is in agreement with theory and experiment.

Next we turn our attention to consider the degree of success achieved by the three equations in representing the experimental data. It will be noticed in Figs. 1–4 that Eq. (4) gives very good agreement with the experimental values.

The performance of the three equations can be conveniently discussed in terms of “average percentage differences.” It will be convenient to explain this quantity by an example. For the elastic constant c_{11} of aluminum, we have 16 data in the temperature range 0–300 °K. By “average percentage difference” we mean the average of the *absolute* values of the percentage differences between the experimental and the calculated values at these 16 temperatures. As a typical case, we give here a summary of the results obtained from Eq. (4). The average percentage differences for various categories are approximately as follows: elements, ~0.04%; intermetallic compounds, ~0.2%; ionic compounds, ~0.1%; and benzene, ~0.2%. These may be compared with the absolute accuracy of the experimental values, which is usually of the order of 1%. We may note here that the relative variations (with the temperature) of the elastic constants

are measured to a greater accuracy than the absolute values, but no estimates of relative accuracy are available. Among the three equations, Eq. (4) gives the least percentage differences in 30 cases; Eqs. (5) and (5') together, in 13 cases; and Eq. (3), in 8 cases. However, we may note that the differences between the results of the three equations are not too great.

It may be noted here that in many cases the recorded experimental values are those obtained by smoothing the measured values. This smoothing, in many cases, appears to have been done by a hand-drawn curve. The results obtained here show that one of the three equations (the one that gives the least errors in that particular case) can be conveniently employed for smoothing and representing the experimental data, at least above $\Theta_D/50$.

The elastic constant c_{12} for some materials shows an increase with temperature. If the increase is regular and linear in T at high temperatures, the three equations discussed above can be employed. We have included here one such typical case: c_{12} of thorium.

These equations can be used for interpolation and to a certain extent for extrapolation. Some thirty years ago, Born¹⁶ derived the general conditions for the stability of a crystal lattice and suggested that at the melting point the rigidity modulus should vanish, $c_{44} = 0$. Subsequent investigations have shown that this is not correct. Here we examine an alternative possibility; somewhat in the spirit of the Lindemann melting equation, we assume that melting takes place when c_{44} is reduced to a value given by $c_{44} = fc_{44}(0^\circ\text{K})$, where f is a certain factor which would depend on the crystal structure and the nature of the binding. In similar substances it should be the same. In our list we have six fcc metals; for these we have calculated the temperature T_ϕ corresponding to $f = 0.55$, using Eq. (4). The results are plotted versus the melting point T_m in Fig. 5. The fact that the points are close to the line $T_\phi = T_m$ appears to indicate that the suggestion has some merit.

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PHYSICAL REVIEW B

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Calculation of the Dielectric Function for a Degenerate Electron Gas with Interactions.

I. Static Limit*

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A new procedure for calculating the frequency- and wave-vector-dependent dielectric response function is described. It is based on decoupling and solving the equations of motion for the Green's functions of the charge-density operators by a moment-conserving method which is discussed. By use of this method an expression for the dielectric function in the static limit ($\omega \rightarrow 0$) is obtained; it depends on a function $G(k)$, for which numerical values are calculated and tabulated. Evidence that the procedure described here leads to reliable values of $G(k)$ for small, intermediate, and large values of k is presented.

I. INTRODUCTION

It has proved possible to relate many of the important properties of metals to a model in which the ions are replaced by a uniform distribution of positive charge and the conduction electrons are treated as a Fermi gas (which for metals under normal conditions is highly degenerate). Much has been learned by ignoring the Coulomb interactions between the electrons, but in recent years efforts have been made to include these interactions in the theory. Many such efforts have been focused on calculating the frequency- and wave-vector-dependent dielectric response (or screening) function $\epsilon(\vec{k}, \omega)$, because this function is the key to understanding many of the properties of metals - including those related to transport phenomena.

It is well known that the expression for $\epsilon(\vec{k}, \omega)$ first given by Lindhard,¹ which can be obtained by making the random-phase approximation^{2,3} (RPA), leads to some unphysical features of the pair distribution function in the range of metallic densities ($2 \leq r_s \leq 5$). In a classic paper⁴ Hubbard proposed to replace the Lindhard expression

$$1 - 1/\epsilon(\vec{k}, \omega) = Q_0(\vec{k}, \omega) / [1 + Q_0(\vec{k}, \omega)] \quad (1.1)$$

by the more general (and hopefully more accurate) expression

$$1 - \frac{1}{\epsilon(\vec{k}, \omega)} = \frac{Q_0(\vec{k}, \omega)}{1 + [1 - G(\vec{k})] Q_0(\vec{k}, \omega)}, \quad (1.2)$$

where

$$Q_0(\vec{k}, \omega) = 4\lambda^2 F_0(\vec{k}, \omega) / k^2, \quad (1.3)$$

with

$$\lambda^2 = (\pi a_0 k_f)^{-1} = \alpha r_s / \pi;$$

$$\alpha = (4/9\pi)^{1/3}, \quad F_0(\vec{k}, \omega)$$

is the polarizability of the free-electron gas. The function $G(\vec{k})$ appearing in (1.2) takes into account exchange and correlation effects; Hubbard proposed for it the form

$$G(\vec{k}) = \frac{1}{2} [k^2 / (k^2 + k_f^2)], \quad (1.4)$$

with k_f the Fermi momentum. Many other forms of $G(\vec{k})$ have since been proposed (for a review see Geldart and Vosko⁵ and Shaw⁶), but we shall refer particularly to one suggested by Singwi, Tosi, Land, and Sjölander⁷⁻⁹ (STLS). STLS arrived at an expression formally equivalent to (1.2) by an equation-of-motion method which relates $G(\vec{k})$, $S(\vec{k})$ (the static form factor), and $\epsilon(\vec{k}, \omega)$ self-consistently.

In a recent paper Shaw⁶ has emphasized that calculations of metallic properties depend strongly