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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: $c_{ij}=c^0_{ij}-s/(e^{t/T}-1)$ and $c_{ij}=a-bT^2/(T+c)$, where c^0_{ij}, 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 found[3-5] to show a T^2 dependence at low temperatures. Bernstein[6] 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 Hearmon[7]). 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.

Sutton[8] 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:

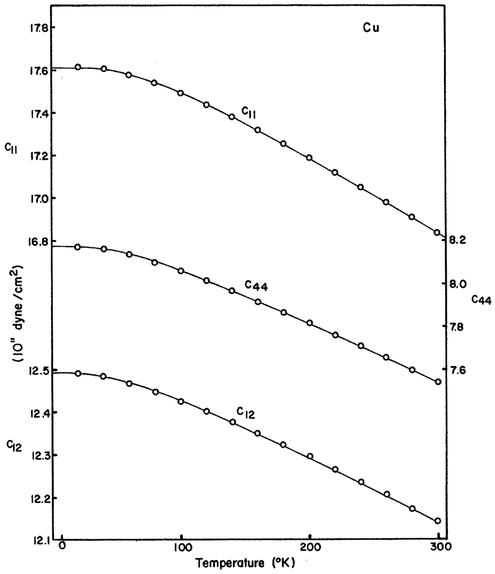

FIG. 1. Experimental and calculated adiabatic elastic stiffness constants of copper. The curves shown were obtained from Eq. (4). Smoothed experimental data points are from Overton and Gaffney (Ref. 9).

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

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 Gaffney[9] found that a similar relation

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

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:

$$E=E_0-BT\exp(-T_0/T). \tag{3}$$

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 well[11] for ThO_2 over a temperature range of 1300 °K. Anderson[12] 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

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

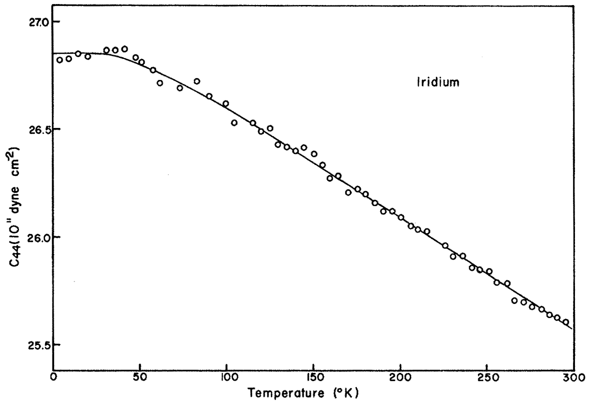

FIG. 2. Experimental and calculated c_{44} for iridium. The curve shown was obtained from Eq. (4); the experimental points are from MacFarlane *et al.* (Ref. d, Table I).

and

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

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

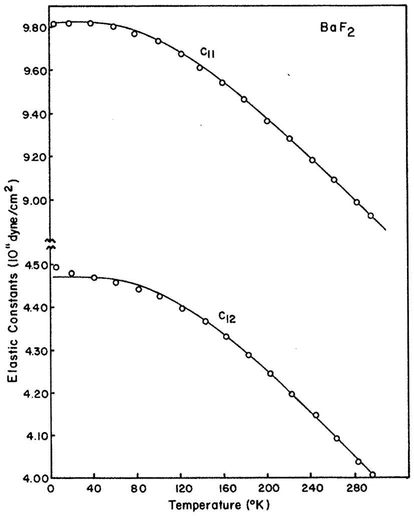

FIG. 3. Experimental and calculated c_{11} and c_{12} for BaF_2. The curves shown were obtained from Eq. (4); the experimental points are from Gerlich (Ref. m, Table I).

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 (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)
Aluminum	a	c_{11}	11.421 60	1.011 141	258.4	11.442 79	6.161 93	420.4	11.425 12	4.140 83	153.2
		c_{12}	6.194 93	0.205 109	293.6	6.199 63	1.059 99	445.0	6.195 62	0.743 19	175.2
		c_{44}	3.160 54	0.256 479	168.0	3.170 67	1.682 26	130.0	3.162 01	1.570 75	94.6
Copper	b	c_{11}	17.609 40	0.760 041	206.4	17.632 02	4.599 23	219.8	17.613 19	3.831 26	118.8
		c_{12}	12.489 20	0.238 363	158.4	12.495 88	1.784 24	154.4	12.490 31	1.552 67	90.2
		c_{44}	8.170 63	0.452 830	163.4	8.185 13	3.225 06	149.8	8.173 55	2.848 04	91.6
Gold	c	c_{11}	20.164 17	0.324 932	89.6	20.178 07	3.736 13	54.6	20.166 11	3.668 70	48.4
		c_{12}	16.967 47	0.290 603	109.8	16.979 10	2.758 01	70.8	16.968 65	2.693 99	60.8
		c_{44}	4.543 98	0.062 821	49.6	4.547 16	1.281 64	26.8	4.544 38	1.273 57	26.2
Iridium	d	c_{44}	26.850 03	0.711 340	132.2	26.877 19	5.913 07	102.8	26.850 88	5.557 55	76.6
Iron	e	c_{11}	24.316 52	0.388 752	97.2	24.345 39	4.013 93	47.0	24.330 93	3.950 73	43.2
		c_{44}	12.185 18	0.405 473	211.2	12.194 21	2.628 12	275.2	12.186 89	2.004 22	122.6
Lead	f	c_{11}	5.560 30	0.094 859	43.5	5.566 43	2.195 82	21.7	5.562 29	2.184 22	21.5
		c_{12}	4.541 99	0.077 379	66.2	4.546 27	1.191 24	37.0	4.542 03	1.182 10	36.5
		c_{44}	1.943 70	0.038 874	24.6	1.947 02	1.580 26	10.5	1.944 34	1.581 67	12.2
Magnesium	g	c_{11}	6.336 83	0.377 516	200.5	6.34552	2.487 86	245.0	6.338 29	1.964 20	116.5
		c_{33}	6.640 07	0.432 300	191.5	6.651 42	2.816 04	207.0	6.640 52	2.376 56	114.5
		c_{44}	1.836 86	0.230 590	233.0	1.842 00	1.424 14	328.5	1.837 77	1.039 19	136.5
		c_{66}	1.872 19	0.163 720	191	1.876 30	1.080 78	212	1.873 29	0.881 84	107
		c_{12}	2.592 36	0.096 157	423				2.592 46	0.261 11	275
		c_{13}	2.168 68	0.106 632	509.5				2.168 83	0.239 97	329.0
Molybdenum	h	c_{11}	47.333 68	1.688 087	276.5	47.443 70	6.312 11	162.5	47.349 83	6.177 70	148.5
		c_{44}	11.098 52	0.273 832	255.5	11.112 03	1.118 32	165.5	11.102 83	1.080 57	133.0
Silicon	i	c_{11}	16.750 18	0.532 972	407	16.766 01	3.426 07	1232.4	16.752 41	1.441 37	251
		c_{12}	6.500 79	0.231 036	334.8	6.509 86	1.088 79	502.8	6.502 77	0.728 54	193.8
		c_{44}	8.007 35	0.224 966	497.4				8.007 90	0.517 91	319.6
Silver	c	c_{11}	13.148 98	0.315 748	105.2	13.161 71	3.120 89	67.2	13.149 68	3.060 59	59.0
		c_{12}	9.735 43	0.221 625	141.0	9.742 16	1.718 54	110.2	9.737 63	1.585 38	74.4
		c_{44}	5.108 97	0.139 351	74.0	5.115 82	1.917 21	41.6	5.109 74	1.901 21	39.8
Tantalum	j	c_{11}	26.646 38	1.854 980	438.0				26.647 76	4.922 28	288.0
		c_{44}	8.733 76	0.208 622	96.0	8.742 49	2.281 39	64.0	8.735 92	2.196 24	51.0
Thorium	k	c_{11}	7.784 93	0.333 704	252.0	7.806 88	1.498 73	190.0	7.788 84	1.372 98	141.0
		c_{12}	4.821 99	−0.467 814	612				4.821 31	−0.914 91	408
		c_{44}	5.121 23	0.678 869	329.5	5.156 40	2.610 99	328.5	5.126 17	2.188 34	193.5
Tungsten	j	c_{11}	53.254 99	6.462 494	616				53.256 87	13.435 47	431
		c_{44}	16.315 77	0.568 995	346	16.326 19	3.489 77	853	16.317 48	1.766 33	209
MgAg	l	c_{11}	8.619 85	2.949 684	890.4				8.622 05	4.023 28	602.4
		c_{12}	5.760 69	5.811 370	1265.4				5.762 37	6.238 94	909.6

TABLE I. *(continued)*

Substance	Source of data	c_{ij}	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		c_{44}	5.190 24	1.079 610	428.6	5.230 19	3.475 61	531.0	5.199 20	2.621 83	243.6
$MgCu_2$	l	c_{11}	12.473 02	2.986 063	796.0				12.479 29	4.229 34	505.6
		c_{12}	7.166 62	1.411 804	735.6				7.170 57	2.112 63	456.0
		c_{44}	4.219 97	0.831 033	651.6				4.222 51	1.398 08	402.0
BaF_2	m	c_{11}	9.818 00	1.700 638	316.6	9.843 90	14.749 14	1098.4	9.820 00	5.921 10	199.0
		c_{12}	4.468 96	0.997 402	342.0				4.470 59	3.219 67	214.4
KF	n	c_{11}	7.584 96	0.249 776	60.0	7.606 69	4.169 61	26.8	7.589 18	4.178 21	30.4
		c_{44}	1.292 71	0.080 453	325.6	1.293 91	0.756 18	1285.0	1.293 00	0.263 39	194.4
LiBr	o	c_{11}	4.724 27	0.454 125	131.4	4.755 61	3.440 99	64.0	4.728 76	3.505 86	70.6
		c_{44}	2.052 92	0.193 328	226.8	2.058 02	1.112 35	265.0	2.053 85	0.888 24	130.8
LiCl	p	c_{11}	5.871 16	0.268 565	68.2	5.887 93	4.001 85	36.6	5.878 06	3.937 07	33.0
		c_{44}	2.671 22	0.202 014	204.8	2.678 25	1.139 68	181.0	2.672 13	1.028 37	118.4
RbCl	p	c_{11}	4.501 19	0.176 814	56.8	4.512 60	3.138 42	28.6	4.503 89	3.122 90	28.8
		c_{44}	0.497 06	0.002 090	31.2	0.497 21	0.067 16	14.4	0.497 11	0.066 97	14.8
TlBr	q	c_{11}	4.468 95	0.213 729	75.8	4.478 20	2.906 07	46.6	4.469 13	2.857 01	42.0
		c_{12}	1.881 47	0.022 585	16.8	1.885 58	1.335 89	4.65	1.882 60	1.339 35	7.45
		c_{44}	1.007 00	0.127 209	118.0	1.012 24	1.142 98	81.2	1.006 99	1.107 36	68.0
Benzene	r	c_{11}	0.925 21	1.399 136	426	0.996 35	5.200 04	600	0.939 95	3.515 73	248
		c_{22}	1.012 82	5.677 769	707				1.024 54	10.055 01	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}	4.23349	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:

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

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 smoothened 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:

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

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,

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

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 ~ $\Theta_D/50$ (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 ~ 6 °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.

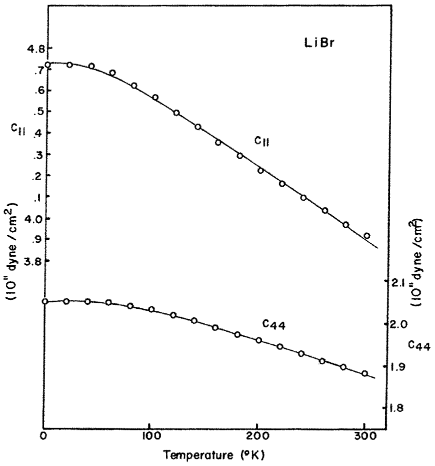

FIG. 4. Experimental and calculated c_{11} and c_{12} of lithium bromide. The curves shown were obtained from Eq. (4); the experimental points are from Marshall and Cleavelin (Ref. o, Table I).

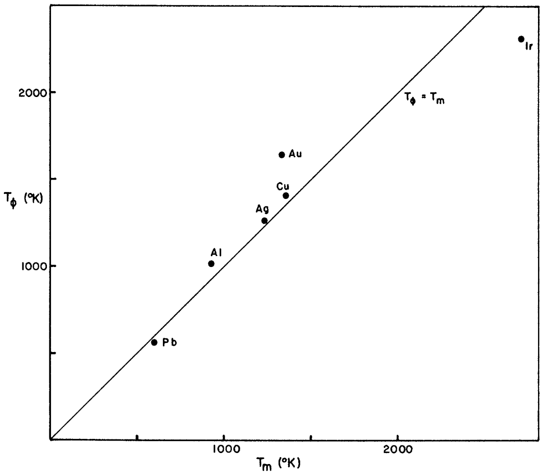

FIG. 5. T_ϕ, the temperature at which $c_{44} = 0.55 c_{44}$ (0 °K), plotted versus the melting point T_m.

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, Born[16] 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 $c_{44} = f c_{44}$ (0 °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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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 paper[4] Hubbard proposed to replace the Lindhard expression

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

by the more general (and hopefully more accurate) expression

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

where

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

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

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

with k_f the Fermi momentum. Many other forms of $G(\vec{k})$ have since been proposed (for a review see Geldart and Vosko[5] and Shaw[6]), but we shall refer particularly to one suggested by Singwi, Tosi, Land, and Sjölander[7-9] (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 Shaw[6] has emphasized that calculations of metallic properties depend strongly