$=10.72-\ln E$, where E is in electron volts. For the $\langle 110\rangle$ chains $S=d$ and Eq. (3) becomes $\Lambda=(13I_0/\gamma)-1$. The upper solid curve in Fig. 2 follows from this relation with I_0 computed from Eq. (9) with $n=0$. The dashed curve shows the trend of Λ with energy as revealed by the calculations of Gibson *et al.* (see their Fig. 27). The agreement is satisfactory, the slightly greater focusing found in the three-dimensional model probably resulting from the effect of neighboring chains of atoms. The lower curve in Fig. 2 corresponds to $I_0=1$, that is, to the commonly used equivalent hard-sphere approximation.

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Anharmonic Contribution to the Energy of a Dilute Electron Gas—Interpolation for the Correlation Energy

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The first anharmonic contribution to the ground-state energy of a body-centered cubic lattice of electrons, oscillating in a uniform background positive charge, has been calculated. The result is $-0.73r_s^{-2}$ rydbergs, with r_s the radius, in Bohr units, of the sphere equivalent in volume to that occupied per electron. Combining this term with previous results gives for the ground-state energy of a dilute electron gas the expression $E=E_{\text{exp}}-1.792r_s^{-1}+2.65r_s^{-\frac{3}{2}}-0.73r_s^{-2}+O(r_s^{-\frac{5}{2}})$, where E_{exp} comes from the overlapping of electronic wave functions and falls off exponentially with $r_s^{\frac{1}{2}}$; while the r_s^{-1} and $r_s^{-\frac{3}{2}}$ terms are, respectively, the Coulomb energy of a bcc lattice and the zero-point energy of the electrons.

The "correlation" energy corresponding to the above expression, as well as the kinetic and potential parts, has been plotted and an interpolation has been made between the low-density curve and the high-density expression of Gell-Mann and Brueckner. The interpolated curves give strong evidence that the next term in the above low-density expansion for E is approximately $-0.8r_s^{-\frac{5}{2}}$. If the high-density expression is rapidly converging near $r_s=1$, it also is predicted that the r_s term in the high-density expansion will be approximately $-0.02r_s$.

WIGNER[1] originally pointed out that the ground-state energy of an electron gas (electrons moving in a uniform background of positive charge) approaches the energy for a body-centered cubic lattice of electrons as the density approaches zero. This energy, as calculated by Fuchs,[2] is $-1.792r_s^{-1}$ rydbergs per electron, where r_s is, in Bohr units, the radius of a sphere equal in volume to the volume per electron of the gas. The next approximation to the energy of the dilute gas is obtained from the zero-point motion of the electrons about their lattice points, which becomes a problem of evaluating the normal modes of the oscillations. Recently, two accurate calculations for the zero-point motion have been made independently,[3,4] the results agreeing within one percent. We shall take the average of these two results, $2.65r_s^{-\frac{3}{2}}$, which may be compared with the values $3r_s^{-\frac{3}{2}}$ and $2.7r_s^{-\frac{3}{2}}$ obtained by Wigner[1] from two different estimates.

A complete solution of the lattice dynamics which is encountered in the dilute electron gas problem is obtained by expanding the Coulomb potential in powers of displacements of the electrons about their respective lattice points. The energy then is an infinite series in powers of $r_s^{-\frac{1}{2}}$, the terms beyond the $r_s^{-\frac{3}{2}}$ term being the anharmonic corrections, which may be calculated from perturbation theory. The first anharmonic correction, the r_s^{-2} term, comes from the sum of a second-order energy perturbation due to cubic terms in the displacements, and the first-order perturbation due to the quartic terms in displacements.

From Appendix II of reference 4, the cubic and quartic terms lead, respectively, to the energy expressions (in rydbergs), per electron:

$$\epsilon_3=-\left(\frac{3}{\pi}\right)^{8/3}\frac{r_s^{-8}}{24}N^{-2}\sum_{\mathbf{f}\mathbf{f}'ss's''}|B(\mathbf{f},\mathbf{f}',s,s',s'')|^2 \times[\omega(\mathbf{f},s)\omega(\mathbf{f}',s')\omega(\mathbf{f}+\mathbf{f}',s'')]^{-1} \times[\omega(\mathbf{f},s)+\omega(\mathbf{f}',s')+\omega(\mathbf{f}+\mathbf{f}',s'')]^{-1}, \quad (1)$$

and

$$\epsilon_4=\left(\frac{3}{\pi}\right)^{5/3}\frac{r_s^{-5}}{8}N^{-2}\sum_{\mathbf{n}\neq0}\left[\sum_{\mathbf{f},s}\frac{D_{\mathbf{n}}(\mathbf{f},s)}{\omega(\mathbf{f},s)}\right]^2\frac{1}{n}, \quad (2)$$

where

$$B=\sum_{\mathbf{n}\neq0}[\sin\mathbf{f}\cdot\mathbf{n}+\sin\mathbf{f}'\cdot\mathbf{n}-\sin(\mathbf{f}+\mathbf{f}')\cdot\mathbf{n}][\mathbf{v}(\mathbf{f},s)\cdot\nabla_n] \times[\mathbf{v}(\mathbf{f}',s')\cdot\nabla_n][\mathbf{v}(\mathbf{f}-\mathbf{f}',s'')\cdot\nabla_n]\frac{1}{n}, \quad (3)$$

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[1] E. P. Wigner, Phys. Rev. **46**, 1002 (1934); Trans. Faraday Soc. **34**, 678 (1938).
[2] K. Fuchs, Proc. Roy. Soc. (London) **A151**, 585 (1935).
[3] Rosemary Coldwell-Horsfall and A. A. Maradudin, J. Math. Phys. **1**, 395 (1960).
[4] W. J. Carr, Jr., Phys. Rev. **122**, 1437 (1961).

and

$$D_n(\mathbf{f},s)=(1-\cos\mathbf{f}\cdot\mathbf{n})[\mathbf{v}(\mathbf{f},s)\cdot\nabla_n]^2. \qquad (4)$$

The $\mathbf{v}$'s are the polarization vectors for the normal modes, the ω's are essentially the frequencies ($\omega=\frac{1}{2}h\nu$ in rydbergs, with ν the frequency), the $\mathbf{f}$'s are the wave vectors, $s=1$, 2, 3 denotes the three polarizations, N is the number of electrons, ∇ is the gradient operator, and $\mathbf{n}$ is a lattice vector in real space having components that are all even or all odd integers. Since values of $\mathbf{v}$ and ω have been tabulated in reference 4 for 512 points in $\mathbf{f}$ space, these points being the centers of space-filling polyhedra having 1/512 times the volume of the unit cell in $\mathbf{f}$ space, we use the approximation whereby each sum over $\mathbf{f}$ is replaced by $N/512$ times the sum over the 512 points. The resulting expression for ϵ_3 was programmed for machine computation, as indicated in the Appendix, and evaluated on an IBM 704 electronic data processing system. The result is

$$\epsilon_3=-1.14r_s^{-2}. \qquad (5)$$

A check on the accuracy of the calculation was obtained by simultaneously running the program for the case where all the ω's are set equal to unity, a case which can be evaluated analytically. In this special case, which corresponds to the Einstein independent oscillator model, exact values of the sum for all points in $\mathbf{f}$ space were obtained by summing over $\mathbf{f}'$, s, s', and s''. From a comparison with these points it was concluded that the approximate method of summation was accurate within 2 to 3%. It is to be noted that all terms in (1) are positive or zero so that the error in the sum is no greater than that of the individual terms.

An interesting feature of the calculation was the fact that the function of $\mathbf{f}$ obtained after summing the right-hand side of (1) over $\mathbf{f}'$, s, s', and s'' rarely deviates by more than 25% from its average value, except near $\mathbf{f}=0$, where the expression goes to zero. Another point to be noted is that the value of (1) is about four times as large as the value obtained from an Einstein approximation, indicating that the independent oscillator model can be used only as an order of magnitude estimate for the anharmonicity of lattice vibrations.

The contribution of the quartic term to the energy was obtained with the aid of a desk computor, the result being

$$\epsilon_4=0.409r_s^{-2}. \qquad (6)$$

The sum of (5) and (6) gives $-0.73r_s^{-2}$ ry, with an estimated accuracy of 3%, for the first anharmonic correction to the energy. Thus the ground-state energy of a dynamic bcc lattice of electrons in a uniform background of positive charge is

$$E_l=-1.792r_s^{-1}+2.65r_s^{-\frac{3}{2}}-0.73r_s^{-2}+O(r_s^{-\frac{5}{2}}). \qquad (7)$$

However, Eq. (7) gives the energy of an electron gas only in so far as the electrons may be treated as distinguishable. When the electronic wave functions begin to overlap appreciably, additional terms proportional to $\exp(-\text{const}\times r_s^{\frac{1}{2}})$ enter into the expression, as first pointed out by Wigner.[1] These exponential terms arise principally from exchange, as shown in reference 4. Although, formally, exchange effects easily may be included, actual calculation is difficult and the following approximation has been used:

$$E_{\text{exp}}=(21r_s^{-1}-4.8r_s^{-3/4}-1.16r_s^{-5/4})\exp(-2.06r_s^{1/2})$$
$$-(2.06r_s^{-5/4}-0.66r_s^{-7/4})\exp(-1.55r_s^{1/2}), \qquad (8)$$

the expression corresponding to the exponential terms which arise from an antisymmetric wave function describing an antiferromagnetic arrangement of independent oscillators centered about the lattice points. Although (8) is not exact, it is satisfactory for determining at what r_s the exponential terms become important, and for making small corrections to the total energy E. Thus for sufficiently large r_s

$$E=E_{\text{exp}}-1.792r_s^{-1}+2.65r_s^{-\frac{3}{2}}-0.73r_s^{-2}. \qquad (9)$$

It is found that E_{exp} is small compared with E_l for r_s greater than 5 or 6, and therefore between this value and ∞, Eq. (9) is a good approximation to the energy providing (a) the series (7) continues to converge rapidly, and (b) there are no other states which in this range of r_s "cross over" and lie appreciably lower in energy.

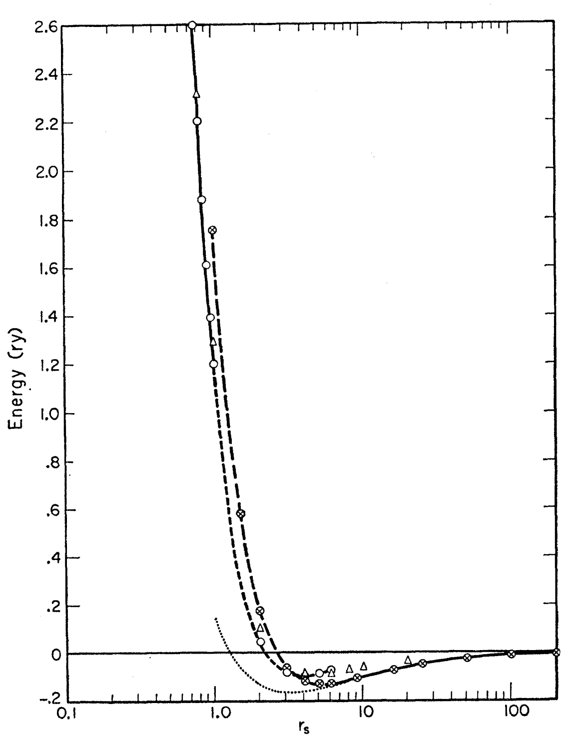

FIG. 1. Energy of the electron gas plotted against r_s. ○, from Eq. (10); ⊗, from Eq. (9); △, points for $2.21r_s^{-2}-0.916r_s^{-1}$; $\cdots$, from the first three terms of Eq. (7).

The equations are plotted in Fig. 1 where the dotted line shows E_l alone as given by the first three terms in (7), and the solid and dashed curve shows a plot of E as obtained from (9). The dashed part of the curve is included to show that (9) has the correct qualitative features even for smaller values of r_s. Because of the anharmonic correction this curve is appreciably lower in energy near the intermediate densities than a similar curve plotted in reference 4.

The other solid and dashed curve in Fig. 1 is a plot of the leading terms in the Gell-Mann and Brueckner[5] expression for the high-density region:

$$E=2.21r_s^{-2}-0.916r_s^{-1}+0.0622\ln r_s-0.096. \quad (10)$$

With DuBois'[6] value for the third-order terms, the expression for this region becomes

$$E=2.21r_s^{-2}-0.916r_s^{-1}+0.0622\ln r_s-0.096 +r_s(0.0049\ln r_s+C). \quad (11)$$

However, the constant C has not yet been evaluated and we have used (10) in plotting Fig. 1. Again, the dashed extension shows the behavior of the expression (10) outside the range of quantitative validity.

The correct values for the ground-state energy must lie below the points given by the triangles in Fig. 1 since these points are for $2.21r_s^{-2}-0.916r_s^{-1}$, which is the expectation value of the Hamiltonian for a determinant of plane waves. In the intermediate range of $2<r_s<6$, which is of greatest interest, both the high-density and low-density expressions show qualitatively reasonable behavior. Whether the inclusion of higher order terms in the expansions (7) and (10) would make them converge toward or diverge away from the correct energy in this region is a question which cannot be answered definitely, but the evidence is discussed in the next section, where an interpolation is made between the high- and low-density expressions.

CORRELATION ENERGY

The expression

$$E_C=E-2.21r_s^{-2}+0.916r_s^{-1},$$

called the correlation energy, is of considerable interest in connection with the binding energy of solids, since it is widely used as a correction term in the Wigner-Seitz calculation. Since E_C has only a logarithmic singularity at $r_s=0$, it is somewhat better for interpolation purposes than E, assuming that if E is a smoothly varying function E_C is likewise. Inasmuch as E_C is the difference between two functions which have minima at different points, it is not entirely obvious that E_C should be free of "bumps" at intermediate densities even if the energy E happened to be; nevertheless, in the following the assumption of "smoothness" will be made.

[5] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).
[6] D. F. DuBois, Ann. Phys. **7**, 174 (1959).

As Mott[7] has pointed out, the high-density electron gas is analogous to a metal, and the low-density case to a nonmetal. Therefore, in going from low to high density, it is reasonable to expect one or more transitions corresponding to the change from nonmetallic to metallic properties; i.e., the level which is the ground state at low density will be crossed by the lowest metallic band of energy levels. At the crossing there will, in effect, be a discontinuity in the slope of the energy-versus-density curve. Our assumption of "smoothness" implies that the discontinuity is small. In this regard, we follow the tacit assumption of Wigner and others who have attempted to evaluate the correlation energy by interpolation procedures. Within our present knowledge, this is the best assumption that we can make.

For interpolating between high- and low-density results it is helpful to consider the kinetic and potential energy curves in addition to that for the total energy, as March[8] has pointed out. If T is the expectation value for the kinetic energy and V that for the potential energy, the virial theorem can be used to derive the expressions

$$T=-\partial r_s E/\partial r_s, \quad (12)$$

$$V=\partial r_s^2 E/r_s\partial r_s. \quad (13)$$

It is to be noted from (13) that the first anharmonic term in (7) is entirely kinetic energy, whereas the zero-point energy is half kinetic and half potential. Also it is to be noted that (12) places a useful limit on some of the energy expressions; the minimum value of T for electrons is the Fermi energy, and therefore

$$(-\partial r_s E/\partial r_s)-(2.21/r_s^2)\geqslant 0. \quad (14)$$

If the expression (10) is used for the energy, one obtains

$$0.0338-0.0622\ln r_s\geqslant 0. \quad (15)$$

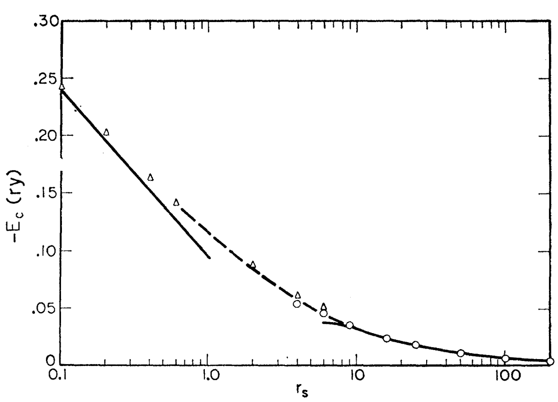

FIG. 2. Correlation energy versus r_s. Upper and lower solid curves obtained from Eqs. (10) and (9). Dashed curve is the interpolated curve. ○, points obtained by adding the term $-0.8r_s^{-3/2}$ to (9). △, points obtained from Eq. (11) with $C=-0.02$.

[7] N. F. Mott, Phil. Mag. **6**, 287 (1961).
[8] N. H. March, Phys. Rev. **110**, 604 (1958).

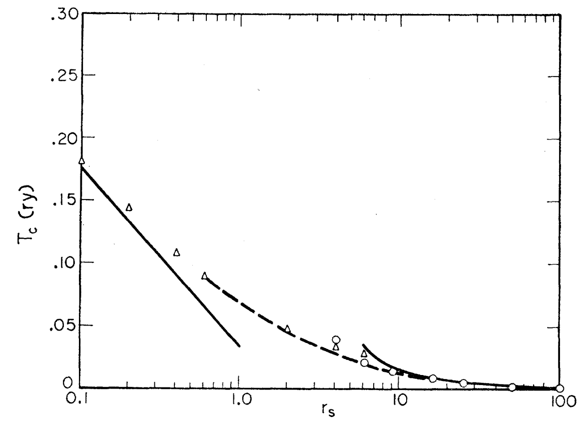

FIG. 3. Kinetic part of the correlation energy versus r_s. Upper and lower solid curves obtained from Eqs. (10) and (9). Dashed curve is the interpolated curve. ○, points obtained by adding the term $-0.8r_s^{-\frac{5}{4}}$ to (9). △, points obtained from Eq. (11) with $C=-0.02$.

Because the inequality breaks down for $r_s>1.73$ the energy expression (10), in the neighborhood of $r_s=1.73$ and beyond, cannot be a close approximation to the correct energy. Ferrell[9] has given a more restrictive condition by showing it is necessary that $(\partial r_s V/\partial r_s)\leqslant 0$, which for (10) is violated for $r_s>1.05$.

Following March we define the correlation kinetic and potential energies by

$$T_C=T-2.21r_s^{-2}, \tag{16}$$

and

$$V_C=V+0.916r_s^{-1}. \tag{17}$$

In Figs. 2, 3, and 4 the solid curves are obtained from Eqs. (9) and (10) and the dashed curves are our conception of the best interpolation between these two expressions. Although some freedom exists in making the interpolation, this freedom is restricted by the necessity of fitting three rather than one curve, and the requirement that $E_C=T_C+V_C$. Further, all reasonable smooth interpolations have the feature, in the low-density range, that the interpolated curve falls above the solid line for E_C, and below it for T_C and V_C. This is just the type of discrepancy which could be corrected by higher order terms in (7). If ar_s^n is a term in the energy, the corresponding term in T is $-(n+1)ar^n$ and in V, $(n+2)ar^n$. For $n<-2$ the correction to E has the same sign as that for T and the opposite sign as that for V, which is the desired qualitative behavior. Since the next term in (7) is $ar_s^{-\frac{5}{4}}$ it is of interest to see if this term alone can explain the discrepancies in the low-density range of Figs. 2, 3, and 4. Such a term gives the ratios $\Delta T/\Delta E=\frac{3}{2}$, $\Delta V/\Delta E=-\frac{1}{2}$, and by the choice $a=-0.8$ the three calculated curves of Figs. 2, 3, and 4 can be made essentially to coincide (as shown by the circles) with the interpolated curves between $r_s=6$ and infinity. Thus strong evidence exists that the next term in (7) is $-0.8r_s^{-\frac{5}{4}}$. Also, agreement could be extended up to $r_s=4$ by choosing an $r_s^{-7/2}$ term; however, if the analysis were to be carried this far it would be desirable to have a more accurate evaluation of E_{exp}.

[9] R. A. Ferrell, Phys. Rev. Letters 1, 443 (1958).

TABLE I. Comparison of the correlation energy E_c, obtained here, with previous estimates. The energies are in rydberg units.

	r_s 2	3	4	5	6
Present	−0.085	−0.068	−0.058	−0.051	−0.046
Wigner (corrected)[10]	−0.090	−0.081	−0.075	−0.069	−0.064
Hubbard[11]	−0.099	−0.086	−0.074	−0.067	
Nozières and Pines[12]	−0.094	−0.081	−0.072	−0.065	

In regard to the high-density region, our interpolated curves may be used to estimate the constant C in Eq. (11). If the value -0.02 is taken, the equation gives the points indicated by triangles in Figs. 2, 3, and 4. We predict, therefore, that, if the high-density expansion is rapidly converging near $r_s=1$, and if DuBois' value for the $r_s \ln r_s$ term is correct, a calculation of the constant C in (11) will give the result $C\approx-0.02$.

It will be noted from Fig. 2 that the magnitude of the correlation energy we obtain in the intermediate region is 15 to 30% lower than previous estimates.[1,10–12] A comparison is given in Table I. The error in our results due to the use of a smooth interpolation is difficult to estimate.

APPENDIX

Herein we give some details of the calculation of the cubic anharmonic contribution to the ground-state energy.

The gradient operations in the expression for $B(\mathbf{f},\mathbf{f}',\mathbf{f}'',s,s',s'')$ are carried out and Eq. (3) becomes

$$B=3\sum_{t=1}^{3}\{(\mathbf{v}_2\cdot\mathbf{v}_3)(\mathbf{v}_1\cdot\mathbf{M}(\mathbf{f}_t)+(\mathbf{v}_3\cdot\mathbf{v}_1)(\mathbf{v}_2\cdot\mathbf{M}(\mathbf{f}_t)) +(\mathbf{v}_1\cdot\mathbf{v}_2)\mathbf{v}_3\cdot\mathbf{M}(\mathbf{f}_t))-D_{ijk}v_{1i}v_{2j}v_{3k}\}, \tag{A.1}$$

where

$$\mathbf{M}(\mathbf{f})=-\nabla_f\sum_{\mathbf{n}\neq0}\frac{e^{-i(\mathbf{f}\cdot\mathbf{n})}}{n^5}, \tag{A.2}$$

$$D_{ijk}(\mathbf{f})=5(\nabla_f)_i\left[(\nabla_f)_j\left[(\nabla_f)_k\sum_{\mathbf{n}\neq0}\frac{e^{-i(\mathbf{f}\cdot\mathbf{n})}}{n^7}\right]\right]. \tag{A.3}$$

For convenience we have written $\mathbf{v}_1$, $\mathbf{v}_2$, and $\mathbf{v}_3$ instead of $\mathbf{v}(\mathbf{f},s)$, $\mathbf{v}(\mathbf{f}',s')$, and $\mathbf{v}(\mathbf{f}'',s'')$, respectively. $\mathbf{f}_t$ takes the values $\mathbf{f}$, $\mathbf{f}'$, and $\mathbf{f}''$, where $\mathbf{f}''=-\mathbf{f}-\mathbf{f}'+$a reciprocal

[10] D. Pines, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1955), Vol. 1, p. 367.
[11] J. Hubbard, Proc. Roy. Soc. (London) A243, 336 (1958).
[12] P. Nozières and D. Pines, Phys. Rev. 111, 442 (1958).

lattice vector. We now use the relation

$$\frac{1}{n^l}=\frac{1}{\Gamma(l/2)}\int_0^\infty \exp(-n^2u)u^{(l/2-1)}du, \tag{A.4}$$

and the Ewald transformation formula,

$$\sum_{\mathbf{n}} \exp(-i\mathbf{f}\cdot\mathbf{n}-n^2u) = V_b\left(\frac{\pi}{u}\right)^{\frac{3}{2}} \sum_{\mathbf{b}} \exp\left[-\frac{\pi^2}{u}\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)^2\right], \tag{A.5}$$

to obtain the following expression for the sums in Eqs. (A.2) and (A.3):

$$\sum_{\mathbf{n}\neq 0}\frac{e^{-i\mathbf{f}\cdot\mathbf{n}}}{n^l}=\frac{\tau^{l/2}}{\Gamma(l/2)}\left[V_b\left(\frac{\pi}{\tau}\right)^{\frac{3}{2}}\sum_{\mathbf{b}}\phi_{-\frac{1}{2}l+\frac{1}{2}}(x) -\frac{2}{l}+\sum_{\mathbf{n}\neq 0} e^{-i\mathbf{f}\cdot\mathbf{n}}\phi_{\frac{1}{2}l-1}(x')\right], \tag{A.6}$$

where

$$\phi_m(y)=\int_1^\infty \beta^m e^{-\beta y}d\beta, \quad x=\frac{\pi^2}{\tau}\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)^2, \quad x'=n^2\tau,$$

V_b is the volume of the unit cell in the space reciprocal to $\mathbf{n}$, the $\mathbf{b}$ are the reciprocal lattice vectors, and τ is a convergence parameter.

When Eq. (A.6) is substituted into Eqs. (A.2) and (A.3), and the gradient operations are performed, the following expressions are obtained:

$$\mathbf{M}(\mathbf{f})=-\frac{\tau^{\frac{5}{2}}}{\Gamma(\frac{5}{2})}\left[V_b\left(\frac{\pi}{\tau}\right)^{\frac{5}{2}}\sum_{\mathbf{b}}\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)\phi_{-1}(x) -\sum_{\mathbf{n}\neq 0}\mathbf{n}\sin(\mathbf{f}\cdot\mathbf{n})\phi_{\frac{3}{2}}(x')\right], \tag{A.7}$$

and

$$D_{ijk}(\mathbf{f})=\frac{5\tau^{\frac{7}{2}}}{\Gamma(\frac{7}{2})}\left[V_b\left(\frac{\pi}{\tau}\right)^{\frac{5}{2}}\sum_{\mathbf{b}}\left\{\frac{\pi^2}{\tau^2}\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_i\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_j \times\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_k\phi_0(x)-\frac{1}{2\tau}\sum_i\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_i\delta_{kj}\phi_{-1}(x)\right\} +\sum_{\mathbf{n}\neq 0}n_in_jn_k\sin(\mathbf{f}\cdot\mathbf{n})\phi_{\frac{5}{2}}(x')\right]. \tag{A.8}$$

Further simplification is obtained by use of the recurrence relations for the ϕ_m's,

$$\phi_m(y)=\phi_0(y)+\frac{m}{y}\phi_{m-1}(y),$$

and the value of τ is chosen to give rapid convergence of both the direct and reciprocal lattice sums. With the value $\tau=\pi^2/16$ it was necessary to use only the first six vectors $\mathbf{n}$ in the bcc lattice sum and the first two vectors $\mathbf{b}$ in the fcc lattice sum. The final expressions for the $\mathbf{M}$'s and the D's are then given by

$$\mathbf{M}(\mathbf{f})=-\left(\frac{\pi}{4}\right)^5\frac{1}{\Gamma(\frac{5}{2})}\left\{\frac{4^4}{\pi^{\frac{5}{2}}}\sum_{\mathbf{b}=[000]}^{[110]}\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)\phi_{-1}(x) -\sum_{\mathbf{n}=[111]}^{[400]}\mathbf{n}\sin(\mathbf{f}\cdot\mathbf{n})\left[\phi_0(x')\left(1+\frac{3}{2x'}\right) +\frac{3}{(2x')^2}\phi_{-\frac{1}{2}}(x')\right]\right\}, \tag{A.9}$$

$$D_{ijk}(\mathbf{f})=\left(\frac{\pi}{4}\right)^7\frac{5}{\Gamma(\frac{7}{2})}\left\{\left[\frac{4^8}{\pi^{9/2}}\sum_{\mathbf{b}=[000]}^{[110]}\left\{\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_i\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_j \times\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_k\phi_0(x)-\frac{1}{32}\left[\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_i\delta_{jk} +\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_j\delta_{ki}+\left(\mathbf{b}-\frac{\mathbf{f}}{2\pi}\right)_k\delta_{ij}\right]\phi_{-1}(x)\right\} +\sum_{\mathbf{n}=[111]}^{[400]}n_in_jn_k\sin(\mathbf{f}\cdot\mathbf{n})\left\{\phi_0(x')\left(1+\frac{5}{2x'} +\frac{5\cdot 3}{(2x')^2}\right)+\frac{5\cdot 3}{(2x')^3}\phi_{-\frac{1}{2}}(x')\right\}\right]\right\}, \tag{A.10}$$

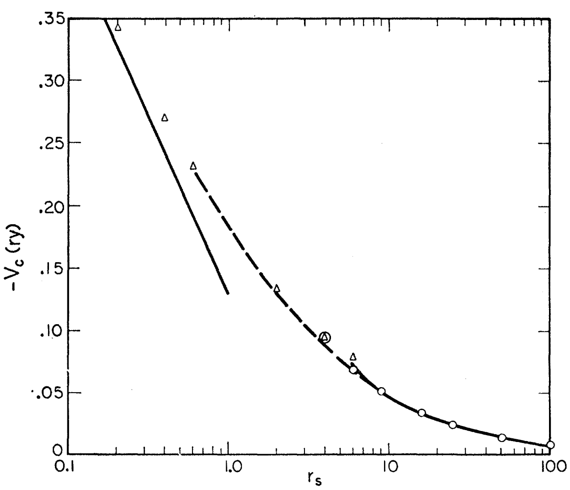

FIG. 4. Potential part of the correlation energy versus r_s. Upper and lower solid curves obtained from Eqs. (10) and (9). Dashed curve is the interpolated curve. ○, points obtained by adding the term $-0.8r_s^{-\frac{3}{2}}$ to (9). △, points obtained from Eq. (11) with $C=-0.02$.

TABLE II. Table of the lattice sums defined by Eqs. (A.2) and (A.3) in the Appendix.

f	M_x	M_y	M_z	D_{xxx}	D_{yyy}	D_{zzz}	D_{xyy}	D_{xzz}	D_{yxx}	D_{yzz}	D_{zxx}	D_{zyy}	D_{xyz}
[110]	0.484	0.484	0	1.404	1.404	0	0.415	0.601	0.415	0.601	0	0	0
[200]	0.705	0	0	1.616	0	0	0.954	0.954	0	0	0	0	0
[211]	0.548	0.268	0.268	1.426	0.907	0.907	0.656	0.656	0.142	0.293	0.142	0.293	−0.170
[220]	0.437	0.437	0	1.242	1.242	0	0.338	0.603	0.338	0.603	0	0	0
[222]	0.298	0.298	0.298	0.968	0.968	0.968	0.260	0.260	0.260	0.260	0.260	0.260	−0.389
[310]	0.565	0.170	0	1.119	0.660	0	0.820	0.887	−0.015	0.203	0	0	0
[321]	0.384	0.235	0.122	0.899	0.846	0.526	0.456	0.566	0.060	0.271	0.008	0.076	−0.258
[330]	0.244	0.244	0	0.684	0.684	0	0.173	0.362	0.173	0.362	0	0	0
[332]	0.176	0.176	0.127	0.563	0.563	0.593	0.128	0.191	0.128	0.191	0.020	0.020	−0.532
[400]	0.481	0	0	0.617	0	0	0.894	0.894	0	0	0	0	0
[411]	0.400	0.070	0.070	0.545	0.411	0.411	0.728	0.728	−0.093	0.032	−0.093	0.032	−0.138
[420]	0.326	0.102	0	0.462	0.580	0	0.550	0.617	−0.135	0.064	0	0	0
[422]	0.222	0.084	0.084	0.337	0.518	0.518	0.388	0.388	−0.094	−0.003	−0.094	−0.003	−0.434
[431]	0.157	0.067	0.052	0.239	0.385	0.341	0.251	0.295	−0.080	0.030	−0.050	−0.032	−0.304
[433]	0.062	0.051	0.051	0.101	0.331	0.331	0.105	0.105	−0.047	−0.030	−0.047	−0.030	−0.697
[440]	0	0	0	0	0	0	0	0	0	0	0	0	0
[442]	0	0	0.068	0	0	0.458	0	0	0	0	−0.059	−0.059	−0.584
[444]	0	0	0	0	0	0	0	0	0	0	0	0	−0.800
[510]	0.297	0.003	0	0.126	0.273	0	0.679	0.681	−0.171	−0.085	0	0	0
[521]	0.191	0.016	0.013	0.009	0.348	0.274	0.479	0.470	−0.261	−0.168	−0.122	−0.085	−0.210
[530]	0.085	−0.085	0	−0.147	0.147	0	0.314	0.258	−0.314	−0.258	0	0	0
[532]	0.048	−0.048	0.030	−0.182	0.182	0.397	0.224	0.197	−0.224	−0.197	−0.123	−0.123	−0.497
[600]	0.194	0	0	−0.096	0	0	0.533	0.533	0	0	0	0	0
[611]	0.155	−0.040	−0.040	−0.141	0.188	0.188	0.458	0.458	−0.208	−0.181	−0.208	−0.181	−0.085
[620]	0.115	−0.115	0	−0.198	0.198	0	0.408	0.363	−0.408	−0.363	0	0	0
[622]	0.062	−0.062	−0.062	−0.261	0.261	0.261	0.285	0.285	−0.285	−0.285	−0.285	−0.285	−0.289
[710]	0.077	−0.077	0	−0.135	0.135	0	0.265	0.256	−0.265	−0.256	0	0	0
[800]	0	0	0	0	0	0	0	0	0	0	0	0	0

where

$$\phi_0(y)=e^{-y}/y,\quad \phi_{-1}(y)=-\mathrm{Ei}(-y),$$
$$\phi_{-\frac{1}{2}}(y)=\left(\frac{\pi}{y}\right)^{\frac{1}{2}}[1-\Phi(y^{\frac{1}{2}})], \tag{A.11}$$
$$\Phi(y^{\frac{1}{2}})\equiv\frac{2}{\sqrt{\pi}}\int_0^y \exp(-\alpha^2)d\alpha,$$

$\mathrm{Ei}(-y)$ being the exponential integral. The values obtained for $\mathbf{M}(\mathbf{f})$ and $D(\mathbf{f})$ are given in Table II.

The program was further simplified by writing Eq. (A.1) in the form

$$\begin{aligned}\tfrac{1}{3}B=\{&v_{2x}v_{3x}[\mathbf{v}_1\cdot\mathbf{M}(1)+2v_{1x}M_x(1)-v_{1x}D_{xxx}-v_{1y}D_{xxy}\\&-v_{1z}D_{xxz}]+v_{2y}v_{3y}[\mathbf{v}_1\cdot\mathbf{M}(1)+2v_{1y}M_y(1)-v_{1x}D_{xyy}\\&-v_{1y}D_{yyy}-v_{1z}D_{yyz}]+v_{2z}v_{3z}[\mathbf{v}_1\cdot\mathbf{M}(1)+2v_{1z}M_z(1)\\&-v_{1x}D_{xzz}-v_{1y}D_{yzz}-v_{1z}D_{zzz}]+(v_{2x}v_{3y}+v_{3x}v_{2y})(v_{1x}M_y\\&+v_{1y}M_x-v_{1x}D_{xxy}-v_{1y}D_{xyy}-v_{1z}D_{xyz})+(v_{2y}v_{3z}\\&+v_{3y}v_{2z})(v_{1y}M_z+v_{1z}M_y-V_{1x}D_{xyz}-v_{1y}D_{yyz}\\&-v_{1z}D_{yzz})+(v_{2z}v_{3x}+v_{3z}v_{2x})(v_{1z}M_x+v_{1x}M_z\\&-v_{1x}D_{xxz}-v_{1y}D_{xyz}-v_{1z}D_{xzz})\}+\text{cyclic permutation}\\&\text{of the indices 1, 2, and 3.}\end{aligned}\tag{A.12}$$

Thus it was necessary to state only one of these permutations, say {231}, explicitly.