Pseudopotential theory of effective interaction in simple metal

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Abstract. The second order pseudopotential theory suggests the possibility of a break-up of the total energy of simple metals into a purely volume-dependent part and an effective central pairwise interaction between ions. In the present paper finite contributions for these two parts of the energy have been extracted in a form convenient for calculation. Using the local Heine-Abarenkov model potential, a reliable effective ion-ion interaction is generated and the volume-dependent energy is calculated for Al. The relative contributions of the effective interaction and the volume-dependent energy term to various metallic properties are also calculated. The importance of volume dependence on the effective interaction is also discussed.

The interatomic force constants upto eighth neighbour are derived from the effective interaction and it is found that the force constants beyond the third neighbour are negligibly small. This result is also confirmed by the calculation of dispersion curves with force constants obtained from the effective interaction upto the third neighbour which is found to reproduce the results of the full pseudopotential calculations. The force constants obtained are also used to study some finite temperature properties of Al in the quasi-harmonic approximation and the limitations of the theory are pointed out.

Keywords. Effective interaction; pseudopotential, lattice mechanics; unified study; simple metal.

1. Introduction

The problem of constructing a reliable and useful effective inter-ionic potential for metals is of considerable interest especially in the studies of defect properties of solids and some thermodynamic properties of solids and liquids. The second-order pseudopotential theory, however, suggests, the possibility of a break-up of the total energy of simple metals into a purely volume-dependent part and an effective central pairwise interaction between ions. It was Cohen (1962) who first pointed out that the band structure energy may be thought of as giving rise to an indirect interaction between the ions. In order to extract the effective inter-ionic potential it is essential to develop this description of the band structure energy. Nonetheless, the problem of extraction of the effective interaction between the ions consistent with the basic energy expression of the pseudopotential theory is very intricate and the different studies (Cochran 1963; Harrison 1963; Shyu and Gaspari 1967, 1968; Rasolt and Taylor 1975; Dagens *et al* 1975; Soma and Satoh 1980) made so far are incomplete in this regard.

A meaningful break-up of the total energy into a purely volume-dependent part and a·part derivable from an effective interaction $V_{eff}(r)$ demands finite contributions from the two parts to various properties of the system. This point is not properly

clarified in the previous attempts made to isolate the effective pair interaction from the pseudopotential studies. We therefore insist that the correct $V_{\text{eff}}(r)$ must not only reproduce the force constants of the pseudopotential theory but also make a finite contribution to the perfect lattice energy/ion which together with the volume-dependent terms will correctly give the pseudopotential energy/ion. Such a formulation will provide an opportunity of a unified study with the effective interaction and such possibilities are explored in the present paper. In the framework of the usual second-order pseudopotential theory the total crystal energy per atom E of metallic solid is composed of the electron gas energy E_g, electrostatic energy E_{es} (Ewald-Fuchs) and first (non-Coulomb) and the second-order energy E^1 and E^2 respectively, *i.e.*

$$E = E_g + E_{\text{es}} + E^1 + E^2. \tag{1}$$

The second and the fourth terms are of special importance and are given by

$$E_{\text{es}} = (Z^2 e^2/2) \left[{\sum_j}' \{Erfc\,(\eta R_j)/R_j\} + (4\pi/\Omega) {\sum_G}' \{\exp\,(- G^2/4\eta^2)/G^2\} \right.$$

$$\left. - \pi/\eta^2\Omega - 2\eta/\sqrt{\pi} \right] \tag{1a}$$

where $\mathbf{R}_j$ is a direct lattice vector, $\mathbf{G}$, a reciprocal lattice vector and η is the Ewald convergence factor ($R_j = |\mathbf{R}_j|$, $G = |\mathbf{G}|$)

and $$E^2 = {\sum_G}' F_G, \tag{1b}$$

F_G being the well-known energy-wavenumber characteristic function and is given by

$$F_G = (\Omega G^2/8\pi e^2) |\omega_G^0|^2 (1 - \epsilon_G)/\epsilon_G,$$

where ω_G^0 is the bare-ion pseudopotential form-factor, ϵ_G is the static dielectric function.

All the individual terms in (1) are finite and are reducible to function of volume per atom (Ω). Thus in this expression for the total energy the identity of the purely structure-dependent terms gets lost. The extrication of a reliable effective interaction, consistent with both the energy expression and the force constants, therefore, requires careful analysis of the various terms in the basic pseudopotential energy expression.

In the next section we discuss the difficulties with the usual effective interaction expression as such for simple metals and develop an alternative expression consistent with the above idea.

2. Formulation of the effective interaction of simple metals

The various discussions on effective interaction of metals made so far assume an

expression for the two-body potential proposed by Cochran (1963) and Harrison (1963) from their pseudopotential studies which reads

$$V_{\text{eff}} (r) = (2\pi)^{-3} \int \phi_{bs} (q) \exp (iq \cdot r) \, dq + Z^2 e^2/r$$

$$= (2\pi)^{-3} \int [\phi_{bs} (q) + 4\pi Z^2 e^2/q^2] \exp (iq \cdot r) \, dq \qquad (2)$$

where $\qquad \phi_{bs} (q) = 2\Omega \, F_q.$

No expression for purely volume-dependent energy terms is generally given along with this expression for the effective two-body interaction. Unless both the expressions are given one cannot verify whether the two expressions together reproduce the energy per ion for a perfect lattice. One can, however, try to calculate the contributions to energy per ion in a perfect lattice from (2) and find out the expression for the purely volume-dependent energy so that the correct pseudopotential energy is reproduced. But this programme can be worked out only if (2) leads to a definite and finite expression for the energy per ion in a perfect lattice.

But the trouble with this expression as such is that when one calculates the contribution to the perfect lattice and writes the corresponding sum over reciprocal lattice vector G, the first term makes finite contribution together with the $G = 0$ term of the second, but the remaining part of the second term still produces two divergent terms making the expression indeterminate. Explicitly the perfect lattice energy/ion given by (2) is

$$\tfrac{1}{2} \sum_j{}' V_{\text{eff}} (R_j) = \tfrac{1}{2} \left(\sum_j V_{\text{eff}} (R_j) - V_{\text{eff}} (R = 0) \right),$$

$$= (\tfrac{1}{2}\Omega) \left[\sum_G{}' (\phi_{bs} (G) + 4\pi Z^2 e^2/G^2) \right] - (2\pi)^{-3}/2 \int (\phi_{bs} (q),$$

$$+ 4\pi Z^2 e^2/q^2) \, dq$$

$$= (\tfrac{1}{2}\Omega) \sum_G{}' \phi_{bs} (G) + (\Omega^2/2) \, d^2 \, E_g/d\Omega^2 + E^1 - 1/(4\pi^2)$$

$$\int (q^2 \, \phi_{bs} (q)) \, dq + 1/(2\Omega) \sum_G{}' 4\pi Z^2 e^2/G^2 - (Z^2 e^2/\pi) \int dq. \qquad (3)$$

The last two terms of (3) are evidently divergent, making (3) indeterminate. Also, these two terms which actually represent electrostatic interaction, cannot be compared with the Ewald-Fuchs expression in any limit. Thus it is difficult to obtain a finite contribution to E from (2) for $V_{\text{eff}} (r)$ in a straightforward manner. Moreover the expression for the second-order elastic constants in the long-wave theory obtained from the effective interaction (2) cannot be compared with those obtained in the

homogeneous deformation theory. Instead we express the effective pair-wise interaction in the following form:

$$V_{\text{eff}}(r) = (Z^2 e^2/r) \, Erfc \, (\eta r) + (2\pi)^{-3} \, [\int \{(4\pi \, Z^2 \, e^2/q^2) \exp \, (-q^2/4\eta^2)$$

$$+ \, \phi_{bs}(q)\} \exp \, (i \, \mathbf{q} \cdot \mathbf{r}) \, d\mathbf{q}]. \tag{4}$$

The purely-volume dependent term is proposed to be

$$U(\Omega) = E_g - (\Omega/2) \, d^2 \, E_g/d \, \Omega^2 + \{\tfrac{1}{2}/(2\pi)^3\} \int \phi_{bs}(q) \, dq \tag{5}$$

The two expressions (2) and (4) are apparently different but their equivalence may be realised by noting that (see appendix)

$$Erf \, (\eta r)/r = (\tfrac{1}{2}\pi^2) \int \{\exp \, (- \, q^2/4\eta^2)/q^2\} \exp \, (i \, \mathbf{q} \cdot \mathbf{r}) \, d\mathbf{q},$$

so $$Z^2 e^2/r = (Z^2 e^2/r) \, Erfc \, (\eta r) + (2\pi)^{-3} \int (4\pi \, Z^2 e^2/q^2) \exp \, (- \, q^2/4\eta^2)$$

$$\exp \, (i \, \mathbf{q} \cdot \mathbf{r}) \, d\mathbf{q}.$$

Now let us see how (4) for $V_{\text{eff}}(r)$ helps us in getting a finite contribution to E and together with (5) reproduce the total perfect lattice energy per ion given by (1). The finiteness of (5) is apparent and the contribution from (4) to the perfect lattice energy per ion may be obtained in the identical fashion adopted earlier for (2). The contribution of the first term of (4) is straightforward and gives the first term of E_{es} in (1a) and altogether we get

$$\tfrac{1}{2} \sum_j{}' V_{\text{eff}}(R_j) = (Z^2 e^2/2) \left[\sum_j{}' Erfc \, (\eta R_j)/R_j + (4\pi/\Omega)\right.$$

$$\sum_G{}' \exp \, (- \, G^2/4\eta^2)/G^2 - 2\eta/\sqrt{\pi} - \pi/(\Omega\eta^2)\Big] + (\tfrac{1}{2}\Omega) \sum_G{}' \phi_{bs}(G)$$

$$- (2\pi)^{-3}/2 \int \phi_{bs}(q) \, dq + (\Omega^2/2) \, d^2 \, E_g/d \, \Omega^2 + E^1. \tag{6}$$

We notice that the pair interaction (4) makes a finite contribution and together with (5) gives the pseudopotential energy correctly. Finnis (1975) and Taole and Glyde (1979) discussed the problem in a different way. Though they have obtained the expression for purely volume-dependent energy correctly, their analysis is very complicated and suffers from very questionable mathematical steps like (see p. 1873 of Taole and Glyde 1979)

$$1/r = \sum_q (4\pi/q^2) \exp \, (i \, \mathbf{q} \cdot \mathbf{r}),$$

where the q-sum includes the $q = 0$ term. For $r \neq 0$, the left side remains finite while the right side diverges because of the $q = 0$ term.

We discuss in the following section some interesting numerical results which follow from a study in the effective interaction in Al. It may be pointed out that the effective volume-dependent energy in (5) is very different from what one expects from the pseudopotential expression. The problems we would like to discuss are the relative importance of the purely volume-dependent part and the effective ion-ion interaction to different properties of the solid, the range of the ion-ion interaction the nature of volume dependence of the ion-ion interaction and its relative significance in the Cauchy relation breakdown for second-order elastic constants etc. It may be pointed out that these studies are possible only if a correct break-up of the pseudopotential energy into a purely volume-dependent part and an effective pair interaction has been made. Apart from the Cauchy breakdown, it is possible to isolate the importance of the volume dependence in the effective interaction in different elastic constants.

The force constants obtained from (4) are identical with those considered by Wallace (1969) in pseudopotential longwave theory. The radial (K_r) and tangential (K_t) force constants from (4) are given by

$$K_r = \mathrm{d}^2 V_{\text{eff}}(r)/\mathrm{d}r^2 = (2 Z^2 e^2/r^3) [Erfc(\eta r) + 2 \eta r$$

$$(1 + \eta^2 r^2) \exp(-\eta^2 r^2)/\sqrt{\pi}] + 1/(2\pi^2 r) \int [4\pi Z^2 e^2 \exp(-q^2/4\eta^2)$$

$$+ q^2 \phi_{b_s}(q)] (2 \sin qr/(qr^2) - 2 \cos qr/r - q \sin qr) \mathrm{d}q,$$

and
$$K_t = (1/r) \mathrm{d} V_{\text{eff}}(r)/\mathrm{d}r = -(Z^2 e^2/r^3) [Erfc(\eta r) + 2\eta r \exp(-\eta^2 r^2)/\sqrt{\pi}]$$

$$+ (\tfrac{1}{2} \pi^2 r^2) \int [4\pi Z^2 e^2 \exp(-q^2/4\eta^2) + q^2 \phi_{bs}(q)] \cos qr - \sin qr/qr) \mathrm{d}q$$

From K_r and K_t we get the interatomic force constants $K_{\alpha\beta}$ defined as the tensor

$$K_{\alpha\beta} = (\mathrm{d}^2 V_{\text{eff}}(r)/\mathrm{d}r_\alpha \, \mathrm{d}r_\beta) = (\delta_{\alpha\beta} - r_\alpha r_\beta/r^2) K_t + (r_\alpha r_\beta/r^2) K_r \qquad (7)$$

The calculated force constants give important information regarding the range of the pair-interaction. When force constants up to the third neighbour are taken for Al, they reproduce the phonon frequency obtained from the full pseudopotential calculation fairly accurately, showing that for Al, the range of effective interaction does not go much beyond the third neighbour.

In the usual second-order pseudopotential theory the Helmholtz free energy F per atom in metallic crystal is given by

$$F = E + F_{qh}(\Omega, T), \qquad (8)$$

where E is the static crystal energy upto the second-order (given by (1)) calculated *via* the static density of electrons under constant Fermi energy *i.e.* at $T = 0$.

In the Einstein approximation, the quasi-harmonic lattice vibrational energy is given by

$$F_{qh}(\Omega, T) = \frac{3 KT}{2} \ln(\hbar^2 \langle \omega^2 \rangle / K^2 T^2), \qquad (9)$$

where the average Einstein frequency $\langle \omega^2 \rangle^{1/2}$ is given by

$$\langle \omega^2 \rangle = \tfrac{1}{3} \sum_{j\,a}{}' K_{aa}(R_j),$$

the thermal equilibrium condition is given by

$$(\partial F/\partial \Omega)_{\Omega_0,\,T} = -p = 0,$$

from which the value of the equilibrium lattice constant a_0 at any temperature T for which $\hbar \langle \omega^2 \rangle^{1/2} \ll KT$ may be obtained. The coefficient of thermal expansion can be calculated by numerical methods from certain a_0 values around a particular temperature T. The equation of state may also be obtained from the equation

$$p(\Omega) = -(\partial F/\partial \Omega)_T = -(\mathrm{d}E/\mathrm{d}\Omega) + (3\,KT/\Omega)\,\gamma(\Omega),$$

at a finite temperature T; the Grüneisen coefficient $\gamma(\Omega)$ is given by

$$\gamma(\Omega) = -(\mathrm{d}\ln\langle\omega\rangle/\mathrm{d}\ln\Omega).$$

3. Results and discussions

Using the local Heine-Abarenkov model, the pseudopotential with parameters determined from earlier unified studies (Sen 1982), the effective ion-ion interaction and the volume-dependent energy is calculated for Al.

In figure 1 the effective two-body potential for Al is shown and our curve is compared with the curves obtained by Dagens *et al* (1975) and Harrison (1966). The first two curves are very similar, but the result of Harrison (1966) is entirely different from the present calculation due to the difference in the pseudopotential used in the two cases. In fact the effective interaction strongly depends on the pseudopotential. Dagens *et al* have generated the interatomic potential by adjusting the parameters of a non-local pseudopotential to fit the self-consistent charge density which is still considered as the most reliable one. The agreement of the present effective interaction curve with the curve obtained by Dagens *et al* reflects the strength of unified study which determines the pseudopotential in the present study. The present theory is simpler and provides a clearer understanding of the physics.

The effective potential for Al shows a strong repulsive contribution for the nearest neighbours. The first minimum of the interionic potential lies between the second and the third nearest neighbours. It is very interesting that almost the entire crystal energy of Al is given by (5) and only 1% is given by the effective two-body interaction. The contribution of the volume part and the effective interaction part to the crystal energy of Al are $-4\cdot3117$ Ryd and $0\cdot0430$ Ryd respectively. Despite very small contribution to the total energy, the effective pair-interaction contributes significantly to the properties which involve derivatives of energy, *e.g.* pressure and elastic constants and are shown in table 1. Moreover, the volume dependence of the effective interaction is equally important as the purely volume-dependent energy in the Cauchy breakdown of elastic constants.
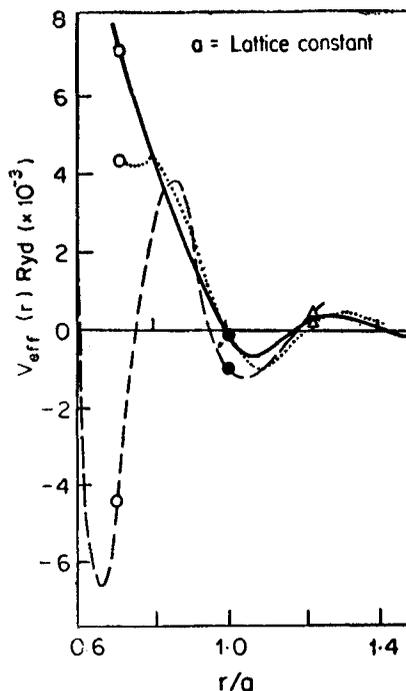
Figure 1. The effective ion-ion potential $V_{eff}(r)$ for Al ———— present calculation, ... Dagens *et al* (1975), ——— Harrison (1966). The first three neighbour positions are shown in the figure.

Table 1. Different types of contributions to some static properties of Al.

Type of contribution	P	C_{11}	C_{12}	C_{44}	$(C_{12} - C_{44})$
			(in 10^{12} dyn / cm^2)		
(a)	-0.2018	-0.3798	0.0238	-0.2018	0.2256
(b)	0.1345	1.2594	0.5336	0.5336	0.0000
(c)	0.0673	0.0876	-0.0471	0.0673	-0.1144
Total	0.0000	0.9672	0.5103	0.3991	0.1112

(a) Contributions of purely volume-dependent part
(b) Contributions of effective interaction (neglecting the volume dependence)
(c) Contributions due to volume dependence of the effective interaction.

Table 2. Radial (K_r) and tangential (K_t) interatomic force constants for first eight neighbours for Al.

							(in dyn cm^{-1})	
Neighbour	1st	2nd	3rd	4th	5th	6th	7th	8th
K_r	22055	2635	-884	238	204	-320	91	163
K_t	-1258	-168	49	-32	16	1	-9	3

The numerical results obtained for the interatomic force constants for the first eight neighbours are listed in table 2. They are found to converge monotonically as the neighbour separation increases.

In table 3 phonon frequencies obtained for certain q-values with force constants upto third neighbours for Al are compared with the results of full pseudopotential

calculation (Sen 1982). Obviously the discrepancy is larger in the low q region. Even then, the maximum error is less than 7% at 200.

Calculated values of the equilibrium lattice constant a_0 obtained at various temperatures compare favourably with the experimental data and are shown in table 4. An estimate of the thermal expansion coefficient at $T = 400K$ is also shown and the discrepancy with the observed value will be discussed presently.

The theoretical values of Grüneisen coefficient as a function of the atomic volume are displayed in table 5 and are in excellent agreement with the quoted empirical values (Kormer *et al* 1962). Gerasimov (1978) has also obtained similar agreement in his study with HA pseudopotential. The thermal expansion coefficient as obtained in the present study is somewhat high (15%) compared to the experimental data. Since it is related to the macroscopic Grüneisen coefficient together with the bulk modulus and specific heat, this discrepancy concerns bulk modulus and specific heat. In fact the present pseudopotential model underestimates the bulk modulus by 20% (Sen 1982) and this discrepancy is common to most of the model pseudopotential calculations.

The equation of state at T=300K is shown and compared with experimental data in figure 2. In the above calculation also, the summation over the force constant (in the vibrational energy part) is extended to 5th neighbour only and is found to be fairly rapidly converging.

The discrepancy between the calculated and the experimental equation of state is about 15%. It is apparent here that the agreement in the Grüneisen coefficient does not guarantee the agreement in the equation of state results because the empirical data

Table 3. Some phonon frequencies in 10^{12} Hz for Al from force constants upto third neighbour.

| Symmetry directions	1OOL	1OOT	0·5.5.5L	0·5.5.5T	·2OOL	·2OOT
ν from force constants (equation (7))	9·6	5·93	9·99	4·33	3·01	1·7
ν from full pseudopotential calculation[a]	9·64	5·84	9·85	4·16	2·95	1·6

[a]Sen D (1982).

Table 4. Equilibrium lattice constants of Al at different temperatures.

Temp. in K	Equil. lattice constant a_0 in a.u. (calculated)	Equil. lattice constant a_0 in a.u. from density data[a]	Linear thermal expansion coefficients (calculated)	Linear thermal expansion coefficients (expt.)[b]
293	7·6510	7·6556		
313	7·6555	7·6593		
333	7·6600	7·6638	$2·90 \times 10^{-5}$ per degree at 400K	$2·49 \times 10^{-5}$ per degree at 400K
353	7·6645	7·6670		
373	7·6700	7·6702		
413	7·6775	2·6777		
493	7·6978	7·6938		

[a]Simmons (1971); [b]AIP Handbook (1972).

Table 5. Calculated Grüneisen coefficient γ for Al.

Ω in a.u.^{3}	$\gamma(\Omega)$	Ω in a.u.^{3}	$\gamma(\Omega)$
112	2·19	102	1·87
110	2·13	100	1·83
108	2·05	98	1·79
106	1·96	96	1·75
104	1·91	94	1·72
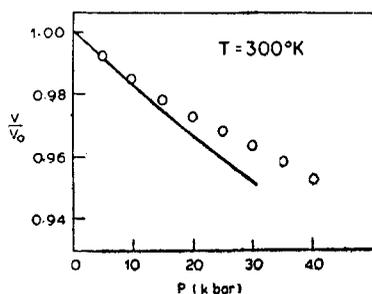
Figure 2. Equation of state for Al at $T = 300K$. Experimental points are taken from Vaidya and Kennedy (1970).

for the Grüneisen coefficient are extracted from experimental results with similar approximations used in the theoretical calculation (Zeldovich and Raizer 1967). The equation of state has so far received little attention in the pseudopotential studies. Specially for Al, the only earlier calculation we have come across is due to Hafner (1975) who has calculated the equation of state at $T=0K$. The calculated results are in large discrepancies with the experimental data.

The present pseudopotential model which works so well in describing the crystal energy, equilibrium, phonon spectra, Grüneisen coefficient, electrical resistivity and thermoelectric power of Al (Sen 1982), (Sen *et al* 1981) fails to explain the elastic constants equation of state and the thermal expansion coefficient of Al. This perhaps reflects, some limitations of the local second-order theory. Another possible source of error in the calculation of the thermal properties is the Einstein approximation which is expectedly valid for temperatures much higher than the Debye temperature. For Al Θ_D is 394K and this approximation in the present study is not beyond question. Moreover, the usual quasiharmonic theory of metals assumes a constant Fermi surface approximation even at $T \neq 0$ and uses $T=0$ Fermi distribution for electrons even when the metal is at a higher temperature. Zeldovich and Raizer (1967) have observed that the contribution (P_e) of electron excitations to the total pressure at ambient pressure and temperature is insignificant. Notwithstanding, the thermal excitation changes the screening function of the electron gas (Takanaka and Hara 1973) and consequently gives rise to a temperature dependent inter-ionic potential (Takanaka and Yamamoto 1977). The effect of this temperature dependence and the error involved in Einstein approximation is at present under investigation.

Appendix

It is easily seen that the two forms of the effective interaction given in (2) and (4) become equivalent if the following relation holds good,

$$(2/r\sqrt{\pi})\int_0^{\eta r}\exp(-x^2)\,dx=(\tfrac{1}{2}\pi^2)\int\{\exp(-q^2/4\eta^2)$$

$$\exp(i\,\mathbf{q}\cdot\mathbf{r})/q^2\}\,d\mathbf{q} \qquad\qquad (A1)$$

If we perform the integration with respect to θ, Φ in the right side expression and and make a change of variables then the above relation reduces to (we put $\eta r = y$ and $qr = p$)

$$(2/\sqrt{\pi})\int_0^y\exp(-x^2)\,dx=(2/\pi)\int_0^\infty\{\exp(-p^2/4y^2)\sin p/p\}\,dp. \qquad (A2)$$

To prove the equality we note that the left side is really $Erf(y)$ and has the well-known power series expansion

$$Erf(y)=(2/\sqrt{\pi})\sum_1^\infty(-1)^n\,y^{2n-1}/\{(n-1)!\,(2n-1)\}.$$

The right side expression can be written as

$$(2/\pi)\int_0^\infty\exp(-p^2/4y^2)\,(1-p^2/3!+p^4/5!-\ldots)\,dp.$$

The infinite series in the integrals is a continuous function of q and converges uniformly. Hence a term-by-term integration can be performed. Using the result

$$\int_0^\infty\{\exp(-p^2/4y^2)\,p^{2n-2}/(2n-1)!\}\,dp=\sqrt{\pi}\,y^{2n-1}/\{(n-1)!\,(2n-1)\}$$

The relation (A1) follows immediately. It is interesting to note that (A2) gives a general form of Ewald Θ-transformation. If $\mathbf{r}$ is interpreted as a lattice vector and both sides are summed over all lattice vectors, we get immediately the usual Θ-transformation relation.

References

American Institute of Physics Handbook 1972 3rd edition (New York: McGraw-Hill)
Cochran W 1963 *Proc. R. Soc. (London)* A276 308
Cohen M H 1962 *Metallic solid solutions* (eds) J Friedel and A Guinier (New York: Benjamin)

Dagens L, Rasolt M and Taylor R 1975 *Phys. Rev.* **B11** 8 2726
Finnis M W 1975 *J. Phys.* **F5** 2227
Gerasimov V M 1978 *Sov. Phys. Solid State* **20** 1486
Hafner J 1975 *Z. Phys.* **B22** 351
Harrison W A 1963 *Phys. Rev.* **129** 2503, 2512
Harrison W A 1966 *Pseudopotentials in the theory of metals* (New York: Benjamin) p. 45
Kormer C B, Funtikov A I, Urlin V D and Kolesnikova A N 1962 *Sov. Phys. JETP* **15** 477
Rasolt M and Taylor R 1975 *Phys. Rev.* **B11** 8 2717
Sen D 1982 *United study and effective interaction in metals* Ph.D. Thesis (University of Calcutta).
Sen D, Sarkar S K, Roy D and Sengupta S 1981 *Phys. Rev.* **B24** 876
Shyu W M and Gaspari G D 1967 *Phys. Rev.* **163** 667
Shyu W M and Gaspari G D 1968 *Phys. Rev.* **170** 687
Simmons G and Wang H 1971 *Single crystal elastic constants and calculated aggregate properties* (Cambridge: MIT Press)
Soma T and Satoh T 1980 *J. Phys.* **F10** 1081
Takanaka K and Hara H 1973 *Prog. Theor. Phys.* **50** 1132
Takanaka K and Yamamoto R 1977 *Phys. Status Solidi* **B84** 813
Taole S H and Glyde H R 1979 *Can. J. Phys.* **57** 1870
Vaidya S N and Kennidy G C 1970 *J. Phys. Chem. Solids* **31** 2329
Wallace D C 1969 *Phys. Rev.* **182** 778
Zeldovich Ya B and Raizer Yu 1967 *Physics of shock waves and high temperature hydrodynamic phenomena* (New York: Academic Press) Vol. 2