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A new method for the evaluation of slowly convergent series

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A new method is presented which sums certain slowly convergent series. It is based on the use of the Hankel integral transform and Schlömilch series. This method is applied with great success to the computation of lattice sums in ionic crystals. In particular, the Madelung constant is calculated with great accuracy through rather simple calculations: The final results only involve elementary functions so that the numerical evaluation is quite easy.

I. INTRODUCTION

It is commonly admitted that the interaction potential in an ionic crystal follows the law $qq'/r - A/r^s$. q and q' are the charges of the ions and r is the distance between them. The total interaction for an ion is therefore described by the following lattice sums:

$$\alpha = \sum\sum\sum{}' (\pm) r^{-1} \quad (= \text{Madelung constant of the crystal}), \tag{1}$$

$$M_s = \sum\sum\sum{}' r^{-s} \quad (s > 3). \tag{2}$$

The symbol (±) indicates that the signs of the ions are taken into account (and also the modulus of the charges if they are not equal for the various ions). The prime means that the summation is extended to all the ions in the crystal except that for which $r = 0$.

Many solutions have been proposed for evaluating these sums. The natural method of counting (increasing r) is not interesting since the convergence is bad. Evjen[1] has modified the way of counting to improve the convergence. In spite of its success it must be recognized that the convergence remains poor. The method is almost interesting when one deals with very complicated multiple sums, for which no analytic method can be used. Madelung[2] calculated α by means of Fourier series. The convergence of the method is quite good. However it is not very elegant and Evjen[1] pointed out that the treatment lacked rigor in some places. The most powerful method with regard to the available accuracy is due to Ewald[3]. Unfortunately the method is far from simple. Born and Huang[4,5] have based another method on the properties of Jacobi's theta functions but the method loses its initial elegance when applied to numerical computations. Very recently[6] Glasser showed how it was possible to sum (1) and (2) when the lattice is even-dimensional but pointed that no extension seems to exist to the important three-dimensional case. Now one could ask: why a new method? Our answer lies in the two following points:

In spite of the existence of numerous summation methods there is some need for a simple method leading to very accurate values through accessible intermediate calculations.

Such a simple method exists and provides an interesting application of the so-called "Schlömilch series" in mathematical physics.

II. MATHEMATICAL PRELIMINARIES

A. A useful Laplace transform

Let us first recall a formula which shall play an important role:

$$(a^2+b^2)^{-s} = [2^{1-2s}\pi^{1/2}/\Gamma(s)]\int_0^\infty x^{2s-1}\exp(-ax) \times [J_{s-1/2}(bx)/(bx/2)^{s-1/2}]\,dx. \tag{3}$$

If we have to sum on both a and b, it might be very tempting to sum first with respect to a since the integrand is simply the general term of a geometric series. However there is a better method: it is possible to sum with respect to b. One obtains a Schlömilch series with very useful properties.

B. Some theorems about Schlömich series

These series were first investigated by Schlömilch[7] in the last century. Now this subject is classic and it is developed in advanced books dealing with the theory of Bessel functions.[8] We present some classical results about Schlömilch series which are interesting for our purpose. Schlömilch has investigated the problem of expanding an arbitrary function into a Schlömilch series:

$$f(x) = [a_0/2\Gamma(s+1)] + \sum_{m=1}^{\infty}[a_m J_s(mx) + b_m H_s(mx)]/(mx/2)^s$$

where J_s and H_s are Bessel and Struve functions, respectively.[8] Nielsen[9] has found the following results (all the functions below are even):

$$\begin{aligned} f_s(x) &= [1/2\Gamma(s+1)] + \sum_{m=1}^{\infty}(-1)^m J_s(mx)/(mx/2)^s \\ &= (1/2)\sum_{-\infty}^{+\infty}(-1)^m J_s(mx)/(mx/2)^s = 0 \quad \text{if } 0<x<\pi \\ &= [2\pi^{1/2}/x\Gamma(s+1/2)]\sum_{n=1}^{q}[1-(2n-1)^2\pi^2/x^2]^{s-1/2} \\ &\qquad \text{if } (2q-1)\pi < x < (2q+1)\pi. \end{aligned} \tag{4}$$

It is also possible to establish that:

$$\begin{aligned} g_s(x) &= [1/2\Gamma(s+1)] + \sum_{m=1}^{\infty} J_s(mx)/(mx/2)^s \\ &= (1/2)\sum_{-\infty}^{+\infty} J_s(mx)/(mx/2)^s \\ &= [\pi^{1/2}/x\Gamma(s+1/2)] \quad \text{if } 0<x<2\pi \\ &= [\pi^{1/2}/x\Gamma(s+1/2)] + [2\pi^{1/2}/x\Gamma(s+1/2)] \\ &\quad \times \sum_{n=1}^{q}[1-(2n\pi/x)^2]^{s-1/2} \quad \text{if } 2q\pi < x < 2(q+1)\pi. \end{aligned} \tag{5}$$

From these two fundamental formulas we deduce other simple expressions:

$$[1/\Gamma(s+1)] + 2\sum_{m=1}^{\infty} J_s(2mx)/(mx)^s = \sum_{-\infty}^{+\infty} J_s(2mx)/(mx)^s = f_s(x) + g_s(x), \quad (6)$$

$$\sum_{m=1}^{\infty} J_s[(2m-1)x]/[(2m-1)x/2]^s = \sum_{-\infty}^{+\infty} J_s[(4p+1)x]/[(4p+1)x/2]^s = \sum_{-\infty}^{+\infty} J_s[(4p+3)x]/[(4p+3)x/2]^s = \frac{1}{2}\sum_{-\infty}^{+\infty} J_s[(2p+1)x]/[(2p+1)x/2]^s = \tfrac{1}{2}[g_s(x) - f_s(x)]. \quad (7)$$

C. Hobson integral and its consequences

The modified Bessel function of the third kind K_s admits the following integral representation due to Hobson:

$$\int_a^{\infty} \exp(-bx)(x^2-a^2)^{s-1/2}\,dx = (2a/b)^s \pi^{-1/2}\Gamma(s+1/2)K_s(ab). \quad (8)$$

This formula enables us to calculate the following expressions:

$$P_s(b) = \int_0^{\infty} \exp(-bx)x^{2s} f_s(x)\,dx \quad (s \geq 0) \quad (9)$$

and

$$Q_s(b) = \int_0^{\infty} \exp(-bx)x^{2s} g_s(x)\,dx \quad (s > 0). \quad (10)$$

One finds without difficulty through (4), (5), and (8) that

$$P_s(b) = 2(2\pi/b)^s[K_s(\pi b) + 3^s K_s(3\pi b) + 5^s K_s(5\pi b) + \cdots], \quad (11)$$

$$Q_s(b) = 2^{2s-1}b^{-2s}\Gamma(s) + 2(2\pi/b)^s[2^s K_s(2\pi b) + 4^s K_s(4\pi b) + \cdots]. \quad (12)$$

These expansions are very rapidly convergent. For example if in (11) we set $s=0$ and $b=1$, the first term in the brackets is $K_0(\pi) \sim 3.10^{-2}$ while the third term is $K_0(5\pi) \sim 5.10^{-8}$; the third term brings a relative correction less than 2.10^{-6}. The quick convergence is the consequence of the asymptotic behaviour of $K_s(z) \sim (\pi/2z)^{1/2}\exp(-z)$.

III. EVALUATION OF LATTICE SUMS

We shall apply the new method to the evaluation of α and M_s in the three fundamental cubic lattices: the NaCl structure, the CsCl structure and the ZnS structure. The method extends without difficulties to the noncubic systems.

A. The NaCl structure

The coordinates of the ions are integers m, n and p. The charge of each ion is $(-1)^{m+n+p+1}$.

1. The Madelung constant α (NaCl)

$$\alpha(\text{NaCl}) = \sum\sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+p+1}(m^2+n^2+p^2)^{-1/2}$$
$$= \sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+1}\int_0^{\infty}\exp[-x(m^2+n^2)^{1/2}] \times\left[\sum_{-\infty}^{+\infty}(-1)^p J_0(px)\right]dx + \sum_{-\infty}^{+\infty}{}'(-1)^{p+1}\int_0^{\infty}J_0(px)\,dx,$$

where use has been made of (3). The Schlömilch series in the first term equals $2f_0(x)$. Therefore one has, with the aid of (9),

$$\alpha(\text{NaCl}) = 2\ln 2 + 4\sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+1}\{K_0[\pi(m^2+n^2)^{1/2}] + K_0[3\pi(m^2+n^2)^{1/2}] + \cdots\}$$
$$= 2\ln 2 + 16[K_0(\pi) - K_0(\pi\sqrt{2}) - K_0(2\pi) + 2K_0(\pi\sqrt{5}) - K_0(\pi\sqrt{8}) + 2K_0(3\pi) - 2K_0(\pi\sqrt{10}) + 2K_0(\pi\sqrt{13}) - K_0(4\pi) + \cdots].$$

If four terms in the brackets are retained, one finds $\alpha = 1.7479$. The relative error δ equals 2.10^{-4}. Nine terms give $1.747\,56$ ($\delta < 2.10^{-6}$). This simple example shows how neat the method is. The same result might be obtained by using Poisson's simple summation formula but it almost appears as an accident.[13]

2. Calculation of M_{2s} (NaCl)

$$M_{2s}(\text{NaCl}) = \sum\sum_{-\infty}^{+\infty}\sum{}'(m^2+n^2+p^2)^{-s}$$
$$= [2^{1-2s}\pi^{1/2}/\Gamma(s)]\sum_{-\infty}^{+\infty}\sum{}'\int_0^{\infty}\exp[-x(m^2+n^2)^{1/2}]x^{2s-1} \times \sum_{-\infty}^{+\infty}J_{s-1/2}(px)/(px/2)^{s-1/2}\,dx + 2\sum_1^{\infty}[\pi^{1/2}/\Gamma(s)]\int_0^{\infty}(x/2p)^{s-1/2}J_{s-1/2}(px)\,dx$$
$$= 2\sum_1^{\infty}p^{-2s} + [2^{2-2s}\pi^{1/2}/\Gamma(s)] \times \sum_{-\infty}^{+\infty}\sum{}' Q_{s-1/2}[(m^2+n^2)^{1/2}].$$

The first term reduces to the Riemann zeta function; the second term splits into two parts in agreement with (12); the first part is written as

$$[2^{2-2s}\pi\Gamma(2s-1)/[\Gamma(s)]^2]\sum_{-\infty}^{+\infty}\sum{}'(m^2+n^2)^{1/2-s}.$$

The double series has been calculated by Glasser[6] who found that

$$\sum_{-\infty}^{+\infty}\sum{}'(m^2+n^2)^{-s} = 4\zeta(s)\beta(s).$$

The final result is now immediate:

$$M_{2s}(\text{NaCl}) = 2\zeta(2s) + [2^{4-2s}\pi\Gamma(2s-1)/[\Gamma(s)]^2]\,\zeta(s-1/2)\,\beta(s-1/2) + [2^{5/2-s}\pi^s/\Gamma(s)]\sum_{-\infty}^{+\infty}\sum{}'(m^2+n^2)^{(1-2s)/4} \times\{2^{s-1/2}K_{s-1/2}[2\pi(m^2+n^2)^{1/2}] + 4^{s-1/2}K_{s-1/2}[4\pi(m^2+n^2)^{1/2}] + \cdots\}.$$

Numerical examples:

$$M_{10} = 2\zeta(10) + (35\pi/32)\zeta(9/2)\beta(9/2) + (\pi^5/96\sqrt{2})\{4.\,2^{9/2}K_{9/2}(2\pi) + 4.\,4^{9/2}K_{9/2}(4\pi) + 4.\,2^{9/4}K_{9/2}(2\pi\sqrt{2}) + 4.\,6^{9/2}K_{9/2}(6\pi)$$

$$+4.4^{9/2}2^{-9/4}K_{9/2}(4\pi\sqrt{2})+8.4^{9/2}5^{-9/4}K_{9/2}(2\pi\sqrt{5})+\cdots\}$$

The series in the brackets converges quickly: three terms in the series give M_{10} with three significant figures; six terms give M_{10} with seven figures. One finds

$$M_{10}(\text{NaCl})=6.426\,104.$$

B. The CsCl structure

The coordinates of the ions are $(m+1/2,\ n+1/2,\ p+1/2)$ = positive ions and (m,n,p) = negative ions.

1. The Madelung constant α (CsCl)

$$\alpha(\text{CsCl})=\sum\sum_{-\infty}^{+\infty}\sum{}'\{[(m+1/2)^2+(n+1/2)^2+(p+1/2)^2]^{-1/2}-(m^2+n^2+p^2)^{-1/2}\}$$

$$=2\sum\sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+p+1}(m^2+n^2+p^2)^{-1/2}+6\sum\sum_{-\infty}^{+\infty}\sum\{[4m^2+(2n+1)^2+(2p+1)^2]^{-1/2}-[4m^2+(2n+1)^2+4p^2]^{-1/2}\}.$$

Under that form the expression is well prepared for the introduction of a Schlömilch series; using (3), (6), and (7) one finds

$$\alpha(\text{CsCl})=2\alpha(\text{NaCl})+6\sum_{-\infty}^{+\infty}\sum\int_0^\infty\exp\{-x[4m^2+(2n+1)^2]^{1/2}\}\sum_{-\infty}^{+\infty}\{J_0[(2p+1)x]-J_0(2px)\}\,dx,$$

$$\alpha(\text{CsCl})=2\alpha(\text{NaCl})-12\sum_{-\infty}^{+\infty}\sum P_0\{[4m^2+(2n+1)^2]^{1/2}\}$$

$$=2\alpha(\text{NaCl})-24\sum_{-\infty}^{+\infty}\sum\{K_0(\pi[4m^2+(2n+1)^2]^{1/2})+K_0(3\pi[4m^2+(2n+1)^2]^{1/2})+\cdots\}$$

$$=2\alpha(\text{NaCl})-48[K_0(\pi)+2K_0(\pi\sqrt{5})+2K_0(3\pi)+2K_0(\pi\sqrt{13})+2K_0(\pi\sqrt{17})+4K_0(5\pi)+2K_0(\pi\sqrt{29})+\cdots]$$

$$=2.035\,35.$$

2. Calculation of M_{2s}(CsCl)

$$M_{2s}(\text{CsCl})=\sum\sum_{-\infty}^{+\infty}\sum{}'\{[(m+1/2)^2+(n+1/2)^2+(p+1/2)^2]^{-s}+(m^2+n^2+p^2)^{-s}\}=M_{2s}(\text{NaCl})+2^{2s}\sum\sum_{-\infty}^{+\infty}\sum[(2m+1)^2+(2n+1)^2+(2p+1)^2]^{-s}.$$

The triple series is easily calculated by using the method which is now familiar to the reader; one finds

$$[2^{1-2s}\pi^{1/2}/\Gamma(s)]\sum\sum_{-\infty}^{+\infty}(Q_{s-1/2}\{[(2m+1)^2+(2n+1)^2]^{1/2}\}-P_{s-1/2}\{[(2m+1)^2+(2n+1)^2]^{1/2}\}).$$

Using (11) and (12) one finds a first contribution of the type $\sum_{-\infty}^{+\infty}\sum[(2m+1)^2+(2n+1)^2]^{-s}$. Its value is given by Glasser[6]: $2^{2-s}(1-2^{-s})\zeta(s)\beta(s)$. Finally one finds

$$M_{2s}(\text{CsCl})=M_{2s}(\text{NaCl})+2^{s+3/2}\pi^{1/2}[\Gamma(s-1/2)/\Gamma(s)]\times(1-2^{1/2-s})\zeta(s-1/2)\beta(s-1/2)-[2^{s+7/2}\pi^s/\Gamma(s)]\sum_0^\infty\sum[(2m+1)^2+(2n+1)^2]^{(1-2s)/4}(K_{s-1/2}(\pi[(2m+1)^2+(2n+1)^2]^{1/2})-2^{s-1/2}K_{s-1/2}\{2\pi[(2m+1)^2+(2n+1)^2]^{1/2}\}+3^{s-1/2}\cdots).$$

Numerical examples:

$$M_{10}(\text{CsCl})=M_{10}(\text{NaCl})+(105\pi/96)(16\sqrt{2}-1)\zeta(\tfrac{9}{2})\beta(\tfrac{9}{2})-(32\pi^5\sqrt{2}/3)[2^{-9/4}K_{9/2}(\pi\sqrt{2})-2^{9/4}K_{9/2}(2\pi\sqrt{2})+2^{-9/4}3^{9/2}K_{9/2}(3\pi\sqrt{2})-2^{27/4}K_{9/2}(4\pi\sqrt{2})+2.10^{-9/4}K_{9/2}(\pi\sqrt{10})+\cdots]$$

$$=40.3043.$$

C. The ZnS structure

The negative ions lie at the sites $(m/2,\ n/2,\ p/2)$ with $m+n+p$ even. The positive ions lie at the sites $(m/2+1/4,\ n/2+1/4,\ p/2+1/4)$ with the same condition.

1. The Madelung constant α (ZnS)

$$\alpha(\text{ZnS})=\sum\sum_{-\infty}^{+\infty}\sum{}'\{12[(4m+1)^2+(4n+3)^2+(4p+3)^2]^{-1/2}+4[(4m+1)^2+(4n+1)^2+(4p+1)^2]^{-1/2}-(m^2+n^2+p^2)^{-1/2}-6[4m^2+(2n+1)^2+(2p+1)^2]^{-1/2}\}.$$

The two first terms can be transformed together into $\sum\sum_0^\infty\sum16[(2m+1)^2+(2n+1)^2+(2p+1)^2]^{-1/2}=2\sum\sum_{-\infty}^{+\infty}\sum[(2m+1)^2+(2n+1)^2+(2p+1)^2]^{-1/2}$ through simple arithmetical devices. We find that

$$\alpha(\text{ZnS})=\alpha(\text{CsCl})-6\sum\sum_{-\infty}^{+\infty}\sum[4m^2+(2n+1)^2+(2p+1)^2]^{-1/2}.$$

The triple series will be evaluated in Sec. III.C2 for a general exponent s. Here we take the limit when s tends to 1/2. We find:

$$\alpha(\text{ZnS})=\alpha(\text{CsCl})+3\ln2-48[K_0(\pi\sqrt{2})+K_0(2\pi\sqrt{2})+2K_0(\pi\sqrt{10})+2K_0(\pi\sqrt{18})+2K_0(\pi\sqrt{26})+\cdots]$$

$$=3.782\,926.$$

This simple formula gives α with seven significant figures!

2. Calculation of M_{2s} (ZnS)

Using the arithmetical devices used in Sec. III C.1, M_{2s} is easily brought into the form

$$M_{2s}(\text{ZnS})=\sum\sum_{-\infty}^{+\infty}\sum{}'\{2^{4s-1}[(2m+1)^2+(2n+1)^2+(2p+1)^2]^{-s}+(m^2+n^2+p^2)^{-s}+3.2^{2s}[4m^2+(2n+1)^2+(2p+1)^2]^{-s}\}$$

$$= 2^{2s-1}M_{2s}(\mathrm{CsCl}) - (2^{2s-1} - 1)M_{2s}(\mathrm{NaCl}) + 3.\,2^{2s}\sum\sum_{-\infty}^{+\infty}\sum[4m^2 + (2n+1)^2 + (2p+1)^2]^{-s}.$$

The triple series can be evaluated as above. One finds

$$[2^{1-2s}\pi^{1/2}/\Gamma(s)]\sum_{-\infty}^{+\infty}\sum (Q_{s-1/2}\{(2n+1)^2 + (2p+1)^2]^{1/2}\} + P_{s-1/2}\{[(2n+1)^2 + (2p+1)^2]^{1/2}\}).$$

Finally, one has

$$M_{2s}(\mathrm{ZnS}) = 2^{2s-1}M_{2s}(\mathrm{CsCl}) - (2^{2s-1} - 1)M_{2s}(\mathrm{NaCl}) + 3\pi^{1/2}2^{s+3/2}(1 - 2^{1/2-s}) [\Gamma(s-1/2)/\Gamma(s)]\zeta(s-1/2)\beta(s-1/2) + 3[2^{s+7/2}\pi^s/\Gamma(s)]\sum_0^\infty\sum[(2n+1)^2 + (2p+1)^2]^{(1-2s)/4}(K_{s-1/2}\{\pi[(2n+1)^2 + (2p+1)^2]^{1/2}\} + 2^{s-1/2}K_{s-1/2}\{2\pi[(2n+1)^2 + (2p+1)^2]^{1/2}\} + \cdots).$$

Numerical example:

$$M_{10}(\mathrm{ZnS}) = 512M_{10}(\mathrm{CsCl}) - 511M_{10}(\mathrm{NaCl}) + (105\pi/32)(16\sqrt{2} - 1)\zeta(9/2)\beta(9/2) + 32\pi^5\sqrt{2}[2^{-9/4}K_{9/2}(\pi\sqrt{2}) + 2^{9/4}K_{9/2}(2\pi\sqrt{2}) + 2^{-9/4}3^{9/2}K_{9/2}(3\pi\sqrt{2}) + 2^{27/4}K_{9/2}(4\pi\sqrt{2}) + 2.\,10^{-9/4}K_{9/2}(\pi\sqrt{10}) + \cdots] = 17\,740.$$

D. Refinement of the above results

The evaluation of M_{2s} and α has been performed in a satisfactory way: the calculations are neat and the final results are expressed in the form of very quickly convergent series. However tables of the K_s functions are needed. When $s = n + \frac{1}{2}$ (n integer), the tabulation is easily performed since $K_{n+1/2}$ is an elementary function (product of an exponential by a polynomial). When $s = n$ (integer), the problem is less simple. If a relative accuracy of about 10^{-6} is judged sufficient, one can use Watson's table[8] (with seven figures). In practice, this accuracy is quite sufficient. However it is possible to refine the results by expressing α and M_{2s} in terms of elementary functions only. This statement is obvious in the case of M_{2s} provided $s = n$ is an integer. If $s = n + \frac{1}{2}$ we shall see that this is also true. Now we present the refined method and we apply it to the evaluation of α. If $s \neq n$ or $n + \frac{1}{2}$, the problem is not soluble in terms of elementary functions; since K_s is not tabulated in these cases the evaluation of M_{2s} would require further investigation. Fortunately the two possibilites $s = n$ or $s = n + \frac{1}{2}$ are in practice quite sufficient. So we try to refine the previous result:

$$\alpha(\mathrm{NaCl}) = 2\ln 2 + 4\sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+1}\{K_0[\pi(m^2+n^2)^{1/2}] + K_0[3\pi(m^2+n^2)^{1/2}] + \cdots\}.$$

First, we calculate:

$$S(z) = \sum_{-\infty}^{+\infty}\sum{}'(-1)^{m+n+1}K_0[z(m^2+n^2)^{1/2}]. \tag{13}$$

We show that the use of Schlömilch series allows us to transform (13). We have

$$S(z) = \sum_{-\infty}^{+\infty}\sum{}' = S_1 + S_2 = 2\sum_{m=1}^{\infty}\sum_{n=-\infty}^{+\infty} + 2\sum_{n=1}^{\infty} \quad (m=0).$$

To calculate S_1, we start with the formula

$$K_0[z(m^2+n^2)^{1/2}] = m\int_0^\infty (t^2+z^2)^{-1/2}J_0(nt)K_1[m(t^2+z^2)^{1/2}]t\,dt.$$

which is introduced in the definition of S_1: a Schlömilch series immediately appears which is summed accordingly to (4):

$$S_1 = 2\sum_{m=1}^{\infty}(-1)^{m+1}\,2m\int_0^\infty f_0(t)(t^2+z^2)^{-1/2}K_1[m(t^2+z^2)^{1/2}]t\,dt.$$

Using Eq. (4), we find a development with integrals of the type:

$$\int_0^\infty (u^2+z^2)^{-1/2}K_1[m(u^2+z^2)^{1/2}]\,du = (\pi/2mz)\exp(-mz).$$

We get:

$$\sum_{n=-\infty}^{+\infty}(-1)^nK_0[z(m^2+n^2)^{1/2}] = 2\pi\{(z^2+\pi^2)^{-1/2} \times\exp[-m(z^2+\pi^2)^{1/2}] + (z^2+9\pi^2)^{-1/2}\exp[-m(z^2+9\pi^2)^{1/2}] + \cdots\}$$

and finally

$$S_1(z) = 4\pi\sum_{k=0}^{\infty}[z^2+(2k+1)^2\pi^2]^{-1/2}\{\exp[z^2+(2k+1)^2\pi^2]^{1/2} + 1\}^{-1}.$$

$S_2(z)$ is evaluated by means of a similar technique (see Appendix A). The final result expresses $\alpha(\mathrm{NaCl})$ in terms of elementary functions [except for the use of $\zeta(1/2)$ and $\beta(1/2)$ which are tabulated]:

$$\alpha(\mathrm{NaCl}) = 4(1-2^{1/2})\zeta(1/2)\beta(1/2) + 16\sum_{k,l=0}^{\infty}\sum[(2l+1)^2+(2k+1)^2]^{-1/2} \{\exp[(2l+1)^2+(2k+1)^2]^{1/2}\pi + 1\}^{-1}. \tag{14}$$

This expansion exhibits remarkable convergence; eight terms give α with twelve figures!:

$$\alpha(\mathrm{NaCl}) = 1.747\,564\,594\,63.$$

Note that one term gives α correct with four figures:

$$\alpha(\mathrm{NaCl}) \approx 4(1-2^{1/2})\zeta(1/2)\beta(1/2) + 16.\,2^{-1/2}[\exp(\pi 2^{1/2}) + 1]^{-1} = 1.747.$$

Of course the same procedure gives the values of $\alpha(\mathrm{CsCl})$ and $\alpha(\mathrm{ZnS})$ (see Appendix B for more details):

$$\alpha(\mathrm{CsCl}) = 2\alpha(\mathrm{NaCl}) - 12\sum_{l=1}^{\infty}(2l-1)^{-1}\operatorname{csch}(2l-1)\pi - 24\sum_{k,l=1}^{\infty}\sum[2l-1)^2+k^2]^{-1/2}\operatorname{csch}\pi[(2l-1)^2+k^2]^{1/2} = 2.035\,361\,509\,45, \tag{15}$$

$$\alpha(\text{ZnS}) = \alpha(\text{CsCl}) + 3\ln 2 - 6\sum_{l=1}^{\infty} l^{-1}\,\text{csch}(l\pi)$$
$$+ 12\sum_{k,l=1}^{\infty}\sum(-1)^{k+1}(k^2+l^2)^{-1/2}\,\text{csch}[\pi(k^2+l^2)^{1/2}]$$
$$= 3.782\,926\,104\,08.$$

In the special case of the NaCl structure, the refined result might be derived from Poisson's double summation formula.[13]

E. The exp(−ar)/r potential

The same method applies when more complicated lattice sums must be evaluated. Let us examine the important case where the interaction is of the type $\exp(-ar)/r$. We must calculate ($a > 0$):

$$S = \sum\sum_{-\infty}^{+\infty}\sum{}' r^{-1}\exp(-ar).$$

We calculate this sum in the NaCl structure. We start with the formula

$$\int_0^\infty t(t^2+a^2)^{-1/2}J_0(xt)\exp[-y(t^2+a^2)^{1/2}]\,dt$$
$$= (x^2+y^2)^{-1/2}\exp[-a(x^2+y^2)^{1/2}].$$

We set $x = p$ and $y = (m^2+n^2)^{1/2}$ (with the notation of Sec. III.A.1). We obtain

$$S = \sum\sum_{-\infty}^{+\infty}\sum{}'\int_0^\infty t(t^2+a^2)^{-1/2}J_0(pt)\exp[-(m^2+n^2)^{1/2}$$
$$\times(t^2+a^2)^{1/2}]\,dt.$$

The sum splits into two parts:

$$\sum\sum_{-\infty}^{+\infty}\sum = \sum_{-\infty}^{+\infty}\sum{}'\sum_{p=-\infty}^{+\infty} + 2\sum_{p=1}^{\infty}\quad (m=n=0).$$

In the first term a Schlömilch series appears which is summed in accordance with (5). The second term is easily summed by elementary manipulations on geometric progressions. We find

$$S = -2\ln[1-\exp(-a)] + 2\sum_{-\infty}^{\infty}\sum{}'\{K_0[a(m^2+n^2)^{1/2}]$$
$$+ 2K_0[(a^2+4\pi^2)^{1/2}(m^2+n^2)^{1/2}]$$
$$+ 2K_0[(a^2+16\pi^2)^{1/2}(m^2+n^2)^{1/2}] + \cdots\}.$$

This series quickly converges through the whole range of a values. The use of the K_0 function may be avoided by using the procedure described in Sec. III.D. One finds

$$S = (4\pi/a)[\exp a - 1]^{-1} + 16\pi\sum_1^{\infty}\sum_0^{\infty}[a^2+(2k\pi)^2+(2l\pi)^2]^{-1/2}$$
$$\times\{\exp[a^2+(2k\pi)^2+(2l\pi)^2]^{1/2} - 1\}^{-1}$$
$$+ 4\sum_1^{\infty}\sum(m^2+n^2)^{-1/2}\exp[-a(m^2+n^2)^{1/2}]$$

When a is small, the behavior of the last term has been studied by Glasser[6] who gives its approximate value. The other terms are easily evaluated since they involve only elementary functions.

IV. BRIEF DISCUSSION OF THE NUMERICAL RESULTS

It is interesting to compare the various numerical α values occurring in the literature since they do not always coincide! Let us consider the most important example: α(NaCl). Most of the authors give the value 1.7476 in their textbooks on solid state physics. Kittel[11] and Dekker[12] give more accurate values: 1.747 558. They obtained that value from the classical paper of Shermann.[13] Comparing with our result, we note a discrepancy of 6.10^{-6}. Sakamoto[14] and earlier Emersleben[15] have calculated the same quantity by Ewald's method; they have found a value in agreement with ours. The same remark holds for CsCl: the traditional value[11,12,13] is 2.035 356 but we find 2.035 361. For ZnS the literature is less accurate (3.782 92) so that the discrepancy does not exist.

V. CONCLUSIONS

It is possible to reformulate the above theory by using the language of the theory of integral transforms.[10] Having to sum the series $S = \sum_z(\pm)u(z)$, we introduce the Hankel transform (or order s) of the function $z^s u(z)$:

$$F(t) = \int_0^\infty z\,J_s(zt)z^s u(z)\,dz.$$

The inversion theorem tells us that

$$z^s u(z) = \int_0^\infty t\,J_s(zt)F(t)\,dt.$$

After slight manipulation we can write

$$S = 2^{-s}\int_0^\infty t^{s+1}\left[\sum_z(\pm)J_s(zt)/(zt/2)^s\right]F(t)\,dt.$$

A Schlömilch series appears which is summed according to (4) or (5). Performing the integration, the final result takes the form of a new series whose convergence may be improved with respect to the convergence of $\sum(\pm)u(z)$. This paper has shown by several classical examples that the method is effective and useful. It furnishes a very good method for computing lattice sums in ionic crystals. No other method gives simple results as in Eqs. (14)–(16) with such an accuracy. Among all the existing methods leading to the evaluation of very accurate lattice sums, this method appears to be one of the simplest.

Very recently we have further refined the above results. In particular, the use of Schlömilch series allows us to find numerous summation formulas for K_s functions like those described in Appendix B. Calculations and related applications will be reported in a future paper. A possible application is the expression of α in term of elementary functions only (without reference to the zeta and the beta function of Riemann).

Example: One has the curious formula

$$\alpha(\text{NaCl}) = (9/2)\ln 2 - (\pi/2)$$
$$+ 12\sum_1^{\infty}\sum\{[(2j-1)^2+(2k-1)^2]^{-1/2}$$
$$\times\text{csch}\,\pi[(2j-1)^2+(2k-1)^2]^{1/2}$$
$$-(4j^2+4k^2)^{-1/2}\,\text{csch}\,\pi(4j^2+4k^2)^{1/2}\}.$$

Four terms give:

$$(9/2)\ln 2-(\pi/2)+(12\sqrt{2})\,\mathrm{csch}\,\pi\sqrt{2}-(12/\sqrt{8})\,\mathrm{csch}\,\pi\sqrt{8}+(24\sqrt{10})\,\mathrm{csch}\,\pi\sqrt{10}=1.747\,56(28)$$

accurate to 10^{-6}.

Similar formulas hold for the other crystallographic structures. They will be reported in a future paper with other possible applications.

APPENDIX A

Certain double series containing K_s functions can be summed exactly in terms of Riemann zeta and beta functions. If $s>0$ one has

$$\sum_{l,m=1}^{\infty}\sum(-1)^{m+1}m^{1/2-s}(2l-1)^{s-1/2}K_{s-1/2}[(2l-1)m\pi]=\pi^{-s}2^{s-5/2}\Gamma(s)[2(1-2^{1-s})\zeta(s)\beta(s)-(1-2^{1-2s})\zeta(2s)].$$

The proof of this formula is left to the reader. He will start with the formula[6]

$$\sum_{m,n=1}^{\infty}\sum(-1)^{m+n}(m^2+n^2)^{-s}=(1-2^{1-2s})\zeta(2s)-(1-2^{1-s})\beta(s)\zeta(s).$$

He will evaluate the double series by the new method. The result will follow. This series occurs in the evaluation of $\alpha(\mathrm{NaCl})$ (with $s=1/2$).

APPENDIX B

Using the method presented in Sec. III.D, the reader will have no difficulty to prove that

$$\sum_{-\infty}^{+\infty}\sum K_0\{z[4m^2+(2n+1)^2]^{1/2}\}=(\pi/2z)\,\mathrm{csch}\,z+\pi\sum_{k=1}^{\infty}(z^2+k^2\pi^2)^{-1/2}\,\mathrm{csch}(z^2+k^2\pi^2)^{1/2}$$

and that

$$\sum_{0}^{\infty}\sum K_0\{z[(2m+1)^2+(2n+1)^2]^{1/2}\}=(\pi/8z)\,\mathrm{csch}\,z-(\pi/4)\sum_{k=1}^{\infty}(-1)^{k+1}(z^2+k^2\pi^2)^{-1/2}\times\mathrm{csch}(z^2+k^2\pi^2)^{1/2}.$$

The first equation leads to the refined value of $\alpha(\mathrm{CsCl})$ while the second leads to $\alpha(\mathrm{ZnS})$.

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