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Lattice sum of electric field gradients in tetragonal crystals

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Abstract. A new method to calculate the lattice contribution to electric field gradients at a nuclear site in tetragonal crystals is developed. The crystal is regarded as an assembly of positive ions at lattice points embedded in a uniform background of negative charge (point charge model). The method uses Euler-Maclaurin formula and makes the plane-wise summation in the direct crystal space unlike most of the previous methods utilising Fourier transform to reciprocal space. The numerical values obtained using the above approach agree well with previous results.

Keywords. Electric field gradient; lattice sum; convergence; tetragonal crystals; Euler-Maclaurin formula.

1. Introduction

Electric field gradients (EFG) have played an important role in providing insight of the electric charge distribution surrounding a nuclear site, shielding-antishielding mechanism, electron-phonon interactions etc. This quantity can be experimentally measured using Mössbauer effect, NQR, PAC etc techniques. A large number of such measurements were made during recent years and interesting systematic trends of EFG were pointed out (Christiansen *et al* 1976; Raghavan *et al* 1976). An excellent review on the subject has been presented by Kaufman and Vianden (1979).

The EFG in a metal is conventionally separated into ionic and electronic parts, the former being due to the positive ions of the lattice outside the atom containing the nucleus of interest and the latter due to conduction electrons. The distortion of the otherwise spherical atomic core due to the electric field of lattice ions is taken into account by multiplying the lattice EFG by the 'Sternheimer antishielding factor' (Sternheimer 1954, 1954a) $(1-\gamma_\infty)$. The total EFG is thus written as

$$eq = eq_{\text{latt}}(1-\gamma_\infty) + eq_{\text{electron}}. \tag{1}$$

The lattice contribution eq_{latt} is represented by a sum over lattice points

$$eq_{\text{latt}} = \sum_a{}' \frac{Ze}{4\pi\epsilon_0} \frac{3z_a^2 - r_a^2}{r_a^5}, \tag{2}$$

where z_a is the z-coordinate and r_a the distance of ath lattice point from the origin situated at the nucleus of interest. The summation runs through all the lattice points except the one containing origin and this is indicated by a ' prime ' over the summation.

The interest in the lattice EFG has been greatly enhanced after the identification of the so called ' universal correlation ' (Raghavan *et al* 1976) between the lattice and electronic parts of EFG. This correlation may be expressed as

$$eq = eq_{\mathrm{latt}} (1 - \gamma_{\infty}) (1 - K), \tag{3}$$

where $K = 2 \sim 5$. Thus the complicated electronic contributions may be estimated from the knowledge of (2). This offers a great simplification as the first principle calculation of the electronic part needs a knowledge of electronic wavefunctions and crystal potentials, which are available for only relatively few metals.

The sum in (2) is known to converge extremely slowly. Techniques have been developed to improve the convergence. The basic idea of the method developed by Simmons and Slichter (1961) is to divide the crystal into electrically neutral polyhedra and sum the contributions from the multipole moments of each external cell. Another rapidly converging procedure involving transformation to reciprocal lattice space was introduced by Ewald (1921) and was further developed by Nijboer and de Wette (1957, 1958). This method has since been widely applied to get the lattice EFG (de Wette 1961; Das and Pomerantz 1961; de Wette and Schacher 1965; Dickmann and Schacher 1967; etc.). We here report a new method to evaluate the sum in (2) in the direct lattice space itself for a simple tetragonal lattice. The results match with those given by de Wette (1961) employing the Fourier transform methods.

2. Theoretical formulation

The sum in (2) is conditionally convergent. It means that its value depends on the shape of the boundary of the infinite crystal (de Wette 1961). The EFG at a lattice point which receives contributions from positive charges as well as from negative background, however, is not an ambiguous quantity and is independent of the shape. This EFG may be written as

$$eq = \int \frac{\rho(\mathbf{r})}{4\pi \epsilon_0} \frac{3z^2 - r^2}{r^5} \mathrm{d}^3 \mathbf{r} + \frac{Ze}{4\pi \epsilon_0} \sum_a{}' \frac{3z_a^2 - r_a^2}{r_a^5}. \tag{4}$$

Assuming a uniform negative background making the crystal electrically neutral, $\rho(\mathbf{r}) = Ze/v$, where v is the volume of the unit cell. Both the terms are conditionally convergent and the values of the terms depend on the order of summation inside Σ' and the boundary shape of crystal in the integration. We can choose the order of summation that is most advantageous, but the integration has to be done accordingly. We follow the order used by de Wette (1961), *i.e.* we choose the z axis along the c axis of the tetragonal crystal and make summation in the planes $z = 0, \pm c, \pm 2c$, etc. and then add these partial sums. This summation order means that we take the shape of the crystal to be a slab of infinite thickness with faces perpendicular to the c axis.

The integration in (4) is

$$\int \frac{3z^2 - r^2}{r^5} \mathrm{d}^3\,\mathbf{r} = -\,8\pi/3 \tag{5}$$

for such a slab-shaped crystal (de Wette 1961). The sum over the lattice is

$$S_0 = \frac{Ze}{4\pi\epsilon_0\,a^3} \sum_{n_3=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_1=-\infty}^{\infty} \frac{2n_3^2\,\alpha^2 - n_1^2 - n_2^2}{\{n_1^2 + n_2^2 + n_3^2\,\alpha^2\}^{5/2}} \quad \text{(except origin)} \tag{6}$$

for a tetragonal crystal where $\alpha = c/a$. The summations over n_1 and n_2 are to be carried out before summation over n_3.

2.1 *Contribution of baseplane* ($z = 0$)

The contribution to

$$\left(\frac{4\pi\epsilon_0\,a^3}{Ze}\,S_0\right)$$

from the baseplane is

$$A_0 = \sum_{n_2=-\infty}^{\infty} \sum_{n_1=-\infty}^{\infty} \frac{-1}{(n_1^2 + n_2^2)^{3/2}}, \quad \text{(except origin)} \tag{7}$$

$$= -4 \sum_{n_2=1}^{\infty} \sum_{n_1=0}^{\infty} \frac{1}{(n_1^2 + n_2^2)^{3/2}}.$$

The Euler-Maclaurin (EM) formula (Hildebrand 1956) is

$$\sum_{n=M}^{N} f(n) = \int_M^N f(x)\,\mathrm{d}x + \tfrac{1}{2}\{f(N) + f(M)\} + \int_M^N P_1(x)\,\frac{\mathrm{d}f(x)}{\mathrm{d}x}\,\mathrm{d}x$$

where $P_1(x) = x - 1/2$ for $0 < x < 1$ and is defined outside this region by $P_1(x + 1) = P_1(x)$.

Applying this to summation over n_1 and replacing the dummy index n_2 by n, we get

$$\sum_{n_1=0}^{\infty} \frac{1}{(n_1^2+n_2^2)^{3/2}} = \int_0^{\infty} \frac{\mathrm{d}x}{(x^2+n^2)^{3/2}} + \frac{1}{2n^3} + \int_0^{\infty} P_1(x) \frac{-3x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

$$= \frac{1}{n^2} + \frac{1}{2n^3} - \int_0^{\infty} \frac{3\,P_1(x)\,x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

$$\text{Hence } A_0 = -4\sum_{n=1}^{\infty} \frac{1}{n^2} - 2\sum_{n=1}^{\infty} \frac{1}{n^3} + 12\sum_{n=1}^{\infty}\int_0^{\infty} \frac{P_1(x)\,x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

$$= -4\zeta(2) - 2\zeta(3) + 12\sum_{n=1}^{\infty}\int_0^{\infty} \frac{P_1(x)\,x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

$$= -8{\cdot}9838500 + \epsilon(\infty), \qquad (8)$$

where $\zeta(2) = \pi^2/6$ and $\zeta(3) = 1{\cdot}20205690\ldots.$ are Riemann zeta functions at 2 and 3 respectively and $\epsilon(\infty)$ is the term involving integral in the expression of A_0. To estimate $\epsilon(\infty)$ we apply the above procedure to the finite sum

$$A_0(N) = \sum_{n_2=-N}^{N} \sum_{n_1=-N}^{N} \frac{-1}{(n_1^2+n_2^2)^{3/2}},$$
(except origin)

and get

$$A_0(N) = \sum_{n=1}^{N} \frac{-4N}{n^2(N^2+n^2)^{1/2}} - 2\sum_{n=1}^{N}\frac{1}{n^3}$$

$$-2\sum_{n=1}^{N} \frac{1}{(N^2+n^2)^{3/2}} + 12\sum_{n=1}^{N}\int_0^{N} \frac{P_1(x)\,x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

or

$$\epsilon(N) = 12\sum_{n=1}^{N}\int_0^{N} \frac{P_1(x)\,x\,\mathrm{d}x}{(x^2+n^2)^{5/2}}$$

$$= -4\sum_{n_2=1}^{N}\sum_{n_1=0}^{N} \frac{1}{(n_1^2+n_2^2)^{3/2}} + 4N\sum_{n=1}^{N} \frac{1}{n^2(N^2+n^2)^{1/2}}$$

$$+2\sum_{n=1}^{N}\frac{1}{n^3} + 2\sum_{n=1}^{N}\frac{1}{(N^2+n^2)^{3/2}}. \qquad (9)$$

As will be discussed later, our results are expected to have an accuracy up to the fifth decimal place. The quantity $|\epsilon(\infty)-\epsilon(N)|$ is discussed in the appendix and it is shown that $\epsilon(80)$ gives a good enough approximation of $\epsilon(\infty)$ for the present calculations. Evaluating the right side of (9) with $N = 80$ we get $\epsilon(80) = -0{\cdot}04976934$ and using this for $\epsilon(\infty)$ in (8) we get

$$A_0 = -9{\cdot}033619, \tag{10}$$

which compares well with the corresponding value ($-$ 9·033621) obtained by de Wette (1961).

2.2 *Contribution of plane $z = n_3 a = k$*

The contribution of plane $z = n_3 a = k$ to $\left(\frac{4\pi\epsilon_0 a^3}{Ze} S_0\right)$ is

$$A_k = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \frac{2k^2-(n_1^2+n_2^2)}{(k^2+n_1^2+n_2^2)^{5/2}}$$

$$= 4 \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \frac{2k^2-(n_1^2+n_2^2)}{(k^2+n_1^2+n_2^2)^{5/2}}$$

$$-4 \sum_{n=0}^{\infty} \frac{2k^2-n^2}{(k^2+n^2)^{5/2}} + \frac{2}{k^3}. \tag{11}$$

Using EM formula we have

$$\sum_{n=0}^{\infty} \frac{3k^2-A^2-n^2}{(A^2+n^2)^{5/2}} = \frac{2k^2-A^2}{A^4} + \frac{3k^2-A^2}{2A^5}$$

$$+ \int_0^{\infty} \frac{3P_1(x)\, x\, (x^2+A^2-5k^2)}{(A^2+x^2)^{7/2}} \mathrm{d}x. \tag{12}$$

Making use of this result in the summation over n_2 in the double summation in (11) and replacing the dummy index n_1 by n, we have,

$$A_k = 4 \sum_{n=0}^{\infty} \left\{\frac{2k^2}{(k^2+n^2)^2} - \frac{1}{k^2+n^2}\right\} - 2 \sum_{n=0}^{\infty} \frac{3k^2-k^2-n^2}{(k^2+n^2)^{5/2}}$$

$$+ \frac{2}{k^3} + 12 \sum_{n=0}^{\infty} \int_0^{\infty} \frac{P_1(x)\, x\, (x^2+n^2-4k^2)}{(x^2+n^2+k^2)^{7/2}} \mathrm{d}x. \tag{13}$$

The first and second series in this equation can be exactly summed using Cauchy formulae for contour integration

$$\sum_{n=0}^{\infty} \frac{1}{(k^2+n^2)^2} = \frac{\pi}{4}\left\{\frac{\coth(\pi k)}{k^3} + \frac{\pi \operatorname{cosech}^2(\pi k)}{k^2}\right\} + \frac{1}{2k^4}$$

and,
$$\sum_{n=0}^{\infty} \frac{1}{k^2+n^2} = \frac{1+\pi k \coth(\pi k)}{2k^2}.$$

The third series of (13) can be expanded using the result (12) and then A_k becomes

$$A_k = 2\pi^2 \operatorname{cosech}^2(\pi k) + \epsilon_k(\infty) \tag{14}$$

where
$$\epsilon_k(\infty) = -6\int_0^{\infty} \frac{P_1(x)\, x\,(x^2-4k^2)}{(k^2+x^2)^{7/2}}\,\mathrm{d}x$$

$$+12\sum_{n=0}^{\infty}\int_0^{\infty} \frac{P_1(x)\, x\,(x^2+n^2-4k^2)}{(x^2+n^2+k^2)^{7/2}}\,\mathrm{d}x.$$

Again to evaluate $\epsilon_k(\infty)$ we apply the above procedure to the finite sum:

$$A_k(N) = \sum_{n_1=-N}^{N}\sum_{n_2=-N}^{N} \frac{2k^2-n_1^2-n_2^2}{(k^2+n_1^2+n_2^2)^{5/2}}$$

and get,

$$\epsilon_k(N) = -6\int_0^{N} \frac{P_1(x)\, x\,(x^2-4k^2)}{(k^2+x^2)^{7/2}}\,\mathrm{d}x$$

$$+12\sum_{n=0}^{N}\int_0^{N} \frac{P_1(x)\, x\,(x^2+n^2-4k^2)}{(k^2+n^2+x^2)^{7/2}}\,\mathrm{d}x$$

$$=4\sum_{n_1=0}^{N}\sum_{n_2=0}^{N} \frac{2k^2-n_1^2-n_2^2}{(k^2+n_1^2+n_2^2)^{5/2}} - 4\sum_{n=0}^{N} \frac{2k^2-n^2}{(k^2+n^2)^{5/2}}$$

$$+\frac{2}{k^3} - \left\{4\sum_{n=0}^{N} \frac{k^2N(2N^2+3k^2+3n^2)}{(N^2+k^2+n^2)^{3/2}(k^2+n^2)^2}\right.$$

$$+\frac{1}{2}\frac{2k^2-n^2-N^2}{(k^2+n^2+N^2)^{5/2}}-\frac{N}{(k^2+n^2+N^2)^{1/2}\,(k^2+n^2)}\Big\}$$

$$+\frac{2k^2-N^2}{(k^2+N^2)^{5/2}}+\frac{2N\,(2N^2+3k^2)}{k^2\,(k^2+N^2)^{3/2}}-\frac{2N}{k^2\,(k^2+N^2)^{1/2}}. \tag{15}$$

We evaluate $\epsilon_k\,(N)$ for $N = 80$ and substitute it for $\epsilon_k\,(\infty)$ in (4) as we did to calculate the contribution due to base plane.

3. Results and discussion

The different terms in (15) have different orders of magnitude. The largest order is for the third series of (15) and its value for $k = 1$ is $-$ 10·46462 as given by computer in an eight digit mantissa calculation. Thus the accuracy of this term is 10^{-5}. As the absolute errors add in addition or subtraction the values of $\epsilon(k)$ thus obtained may be accurate only up to the fifth decimal place. We made calculations for three crystals with $c/a = 1$, 1·1 and 1·5. Contributions due to planes $|z| > 4$ are found to ' zero ' within the mentioned error limits.

Table 1. Lattice EFG in tetragonal crystals in units of $Ze/(4\pi\,\epsilon_0\,a^3)$.

c/a	$k = n_3\,c/a$	$2\pi^2$ cosec h$^2\,\pi k$	ϵ_k	$\epsilon_k + 2\pi^2$ cosech$^2\,\pi k$
1	1	0·14800	0·17947	0·32747
	2	0·00028	0·00028	0·00056
	3	0·00000	0·00000	0·00000
	4	0·00000	0·00000	0·00000
	$B_0 = 0·32803$		$2B_0 = 0·65606$	$A_0 + 2B_0 =$ $-$ 8·37756
1·1	1·1	0·07882	0·09166	0·17048
	2·2	0·00008	0·00008	0·00016
	3·3	0·00000	0·00000	0·00000
	4·4	0·00000	0·00000	0·00000
	$B_0 = 0·17064$		$2B_0 = 0·34128$	$A_0 + 2B_0 =$ $-$ 8·69234
1·5	1·5	0·00637	0·00674	0·01311
	3·0	0·00000	0·00000	0·00000
	4·5	0·00000	0·00000	0·00000
	6·0	0·00000	0·00000	0·00000
	$B_0 = 0·01311$		$2B_0 = 0·02622$	$A_0 + 2B_0 =$ $-$ 9·00740

Values from de Wette (1961) for the three cases are $-$ 8·37758, $-$ 8·69234 and $-$ 9·00740 respectively.

The contribution to $(4\pi\epsilon_0 a^3/Ze)\, S_0$ from baseplane is $A_0 = -9{\cdot}03362$ (equation (10)) and from other planes is $2\,B_0$ where B_0 is the sum of contribution from the plane $z = c$, $2c$, $3c$ and $4c$. These values are given in table 1 together with the values of de Wette (1961) for comparison. It is seen that the present values are in excellent agreement with the previous calculations.

The EFG in point change model eq_{ion} is obtained by adding the contribution of negative background to $(A_0 + 2B_0)$. For $c/a = 1$, this EFG is zero. This is expected from symmetry as the crystal reduces to a simple cubic for this value of c/a.

4. Conclusion

Euler Maclaurin summation formula is used to sum the extremely slowly convergent lattice sum of electric field gradient at a nuclear site in simple tetragonal lattice. The summation is carried out in the direct lattice space itself, contrary to the popular methods employing Fourier transforms to work in reciprocal space. To reproduce the known results up to five decimal places it is sufficient to make numerical summation of certain series up to $N = 80$.

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Appendix

Estimation of $\epsilon(\infty) - \epsilon(N)$

The contribution from baseplane to the EFG is given by(8) containing $\epsilon(\infty)$. For computations, $\epsilon(\infty)$ was replaced by $\epsilon(N)$. In this appendix, we estimate the error introduced by using a finite N and show that to get an accuracy up to the fifth decimal place, it is sufficient to take $N = 80$.

Let $f(x) = x/(n^2 + x^2)^{5/2}$ and the prime denote differentiation with respect to x. Then,

$$\epsilon(\infty) - \epsilon(N) = 12 \left\{ \sum_{n=1}^{\infty} \int_0^{\infty} P_1(x) f(x)\, \mathrm{d}x - \sum_{n=1}^{N} \int_0^{N} P_1(x) f(x)\, \mathrm{d}x . \right\} \quad \text{(A1)}$$

The Bernaulli's polynomials $P_k(x)$ have the following properties,

$$P_k'(x) = P_{k-1}(x)\,; \quad P_{2k}(0) = \frac{B_{2k}}{(2k)!},$$

$$P_{2k+1}(0) = 0; \qquad |P_k(x)| \leqslant \frac{2\,\zeta(k)}{(2\pi)^k},$$

$$P_k(x) = P_k(x+1)\,,$$

where B_{2k} are the Bernoulli's numbers and $\zeta(x)$ is the Riemann zeta function. In particular $P_2(0) = 1/12$ and $|P_3(x)| < 1/100$. Using these properties, we have for α and β integers,

$$\int_\alpha^\beta P_1(x)\ f(x)\ \mathrm{d}x = [P_2(x)\ f(x)]_\alpha^\beta - \int_\alpha^\beta P_2(x) f'(x)\,\mathrm{d}x$$

$$= \frac{1}{12}\,[f(\beta) - f(\alpha)] + \int_\alpha^\beta P_3\,(x) f''\,(x)\,\mathrm{d}x$$

Also $f(0) = f(\infty) = 0$.

Hence,

$$\epsilon(\infty) - \epsilon(N)$$

$$= -\sum_{n=1}^{N} \frac{N}{(n^2 + N^2)^{5/2}} + 12 \sum_{n=1}^{\infty} \int_0^\infty P_3\,(x) f''\,(x)\,\mathrm{d}x$$

$$- 12 \sum_{n=1}^{N} \int_0^N P_3\,(x) f''\,(x)\,\mathrm{d}x$$

$$= -N \sum_{n=1}^{N} \frac{1}{(n^2 + N^2)^{5/2}} + 12 \sum_{n=1}^{N} \int_N^\infty P_3\,(x) f''\,(x)\,\mathrm{d}x$$

$$+ 12 \sum_{n=N+1}^{\infty} \int_0^\infty P_3\,(x) f''\,(x)\,\mathrm{d}x$$

$$= -N\,\Sigma_1 + 12\,\Sigma_2 + 12\,\Sigma_3. \tag{A2}$$

In Σ_1, the terms decrease as n increases. Hence

$$\int_1^{N+1} \frac{\mathrm{d}x}{(x^2 + N^2)^{5/2}} < \Sigma_1 < \int_0^N \frac{\mathrm{d}x}{(x^2 + N^2)^{5/2}},$$

or,
$$\Sigma_1 = \int_0^N \frac{\mathrm{d}x}{(x^2 + N^2)^{5/2}} - q_1$$

$$= \frac{5}{6\sqrt{2}\,N^4} - q_1 \text{ with } 0 < q_1 < \frac{1}{N^5}. \tag{A3}$$

In $\Sigma_2, f''(x)$ is always positive. Hence,

$$|\Sigma_2| \leqslant \sum_{n=1}^{N} \int_{N}^{\infty} |P_3(x)| f''(x)\,dx \leqslant \frac{1}{100} \sum_{n=1}^{N} \frac{4N^2 - n^2}{(n^2 + N^2)^{7/2}}$$

$$= \frac{N^2}{20} \sum_{n=1}^{N} \frac{1}{(n^2 + N^2)^{7/2}} - \frac{1}{100} \sum_{n=1}^{N} \frac{1}{(n^2 + N^2)^{5/2}}.$$

Using method same as that to estimate Σ_1, we get,

$$|\Sigma_2| \leqslant \frac{1}{20 N^4} \cdot \frac{43}{60\sqrt{2}} - \frac{1}{100 N} \cdot \frac{5}{6\sqrt{2} N^3} - q_2 + \frac{q_1}{100 N},$$

$$= \frac{11}{400\sqrt{2} N^4} - q_2 + \frac{q_1}{100 N} \text{ with } 0 < q_2 < \frac{1}{20 N^5}. \tag{A4}$$

In $\Sigma_3, f''(x)$ is negative for $0 < x < \sqrt{3}\, n/2$ and is positive for $\sqrt{3}\, n/2 < x < \infty$. Hence,

$$|\Sigma_3| \leqslant \frac{1}{100} \sum_{n=N+1}^{\infty} \left\{ \int_{\sqrt{3}\,n/2}^{\infty} f''(x)\,dx - \int_{0}^{\sqrt{3}\,n/2} f''(x)\,dx \right\}$$

$$= \frac{1}{100} \left\{ 1 + \frac{512}{343\sqrt{7}} \right\} \sum_{n=N+1}^{\infty} \frac{1}{n^5} \leqslant \frac{0.004}{N^4}. \tag{A5}$$

Using (A3), (A4) and (A5) in (A2),

$$\epsilon(\infty) - \epsilon(N) = -\frac{5}{6\sqrt{2} N^3} + q \text{ with } |q| < \frac{2}{N^4}$$

or,

$$|\epsilon(\infty) - \epsilon(80)| \leqslant 1.15 \times 10^{-6} + 4.9 \times 10^{-8}$$

$$< 1.2 \times 10^{-6}$$

Thus for calculations up to the fifth decimal place it is sufficient to take $N = 80$. The nature of expressions $\epsilon_k(\infty) - \epsilon_k(N)$ are also similar and in view of the small contributions A_k from planes $n_3 > 0$, $N = 80$ will set an appropriate limit for the present calculations.

References

Christiansen J, Heubes P, Keitel R, Klinger W, Loeffler W, Sandner W and Witthuhn W 1976 *Z. Phys.* **B24** 177

Das T P and Pomerantz M 1961 *Phys. Rev.* **123** 2070

de Wette F W 1961 *Phys. Rev.* **123** 103

de Wette F W and Schacher G E 1965 *Phys. Rev.* **137** A78 and A92

Dickmann D B and Schacher G E 1967 *J. Comput. Phys.* **2** 87

Ewald P P 1921 *Ann. Phys. (Leipz).* **64** 253

Hildebrand F B 1956 *Introduction to numerical analysis* (New Delhi: Tata McGraw-Hill) p. 152

Kaufman E N and Vianden R J 1979 *Rev. Mod. Phys.* **51** 161

Nijboer B R A and de Wette F W 1957 *Physica* **23** 309

Nijboer B R A and de Wette F W 1958 *Physica* **24** 422

Raghavan P, Kaufman E N, Raghavan R S, Ansaldo E J and Naumahn R A 1976 *Phys. Rev.* **B13** 2835

Simmons W W and Slichter C P 1961 *Phys. Rev.* **121** 1580

Sternheimer R M 1954 *Phys. Rev.* **95** 736

Sternheimer R M 1954a *Phys. Rev.* **96** 951