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IDENTITY RELATIONS FOR A CERTAIN TYPE OF LATTICE SUMS

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The identity between two expressions of the potential in a crystal made of point charges is proved by applying Cauchy's theorem of residues to a suitable function. The procedure can be easily generalized, and the results may be applied to calculating in a more efficient way a certain type of lattice sums.

1. Introduction

In a previous paper [1] we found an expression for the electrostatic potential in a crystal consisting of a triclinic lattice of point charges immersed in a uniform neutralizing background, using the "planewise summation method". The result corresponds to a slab-shaped specimen cut parallel to a given pair of crystal axes. Actually, there exist three such expressions, because the crystal planes over which the summation is performed can be chosen either as the *ab*, as the *bc* or as the *ac* crystal planes. The three values corresponding to the above slabs differ from each other by additive constants, which we evaluated therein. In this way, the following identity can be written down for the sums on the two-dimensional reciprocal lattice*:

$$\frac{1}{b\sin\gamma}\sum_{\mu_1,\mu_2}{}' \frac{\mathrm{e}^{-2\pi\mathrm{i}(j_a\mu_1+j_b\mu_2)}}{h_{c,\mu}}\left\{\frac{\mathrm{e}^{-j_c(H_{c,\mu}+\mathrm{i}X_{c,\mu})}}{1-\mathrm{e}^{-(H_{c,\mu}+\mathrm{i}X_{c,\mu})}}+\frac{\mathrm{e}^{-(1-j_c)(H_{c,\mu}-\mathrm{i}X_{c,\mu})}}{1-\mathrm{e}^{-(H_{c,\mu}-\mathrm{i}X_{c,\mu})}}\right\}+\frac{2\pi c\cos\delta_c}{ab\sin\gamma}\left[(j_c-\tfrac{1}{2})^2-\tfrac{1}{12}\right]$$
$$=\frac{1}{c\sin\alpha}\sum_{\mu_1,\mu_2}{}' \frac{\mathrm{e}^{-2\pi\mathrm{i}(j_b\mu_1+j_c\mu_2)}}{h_{a,\mu}}\left\{\frac{\mathrm{e}^{-j_a(H_{a,\mu}+\mathrm{i}X_{a,\mu})}}{1-\mathrm{e}^{-(H_{a,\mu}+\mathrm{i}X_{a,\mu})}}+\frac{\mathrm{e}^{-(1-j_a)(H_{a,\mu}-\mathrm{i}X_{a,\mu})}}{1-\mathrm{e}^{-(H_{a,\mu}-\mathrm{i}X_{a,\mu})}}\right\}+\frac{2\pi a\cos\delta_a}{bc\sin\alpha}\left[(j_a-\tfrac{1}{2})^2-\tfrac{1}{12}\right] \quad (1)$$

(see the first of eqs. (67), where use is made of (44), (46), (47) and (49), of [1]; the second of eqs. (67) is obtained from the first one by cyclic permutation of the crystal directions ***a***, ***b*** and ***c***). The parameters appearing in eq. (1) are defined as follows: a, b, c, α, β, γ, δ_a and δ_c are shown in fig. 1; j_a, j_b and j_c are the fractional coordinates of a lattice point Q with respect to the field point P (i.e., $\boldsymbol{r}_{\mathrm{PQ}} = j_a\boldsymbol{a} + j_b\boldsymbol{b} + j_c\boldsymbol{c}$), the lattice point being the one for which $0 \leq j_a, j_b, j_c < 1$ (in the case of (1) j_a and j_c must be non-zero);

$$h_{c,\mu} = \left(2\pi\frac{c}{a}\cos\delta_c\right)^{-1} H_{c,\mu} = \frac{1}{\sin\gamma}\sqrt{\mu_1^2 - 2\frac{a}{b}\mu_1\mu_2\cos\gamma + a^2\mu_2^2/b^2}\,; \quad (2a)$$

$$h_{a,\mu} = \left(2\pi\frac{a}{b}\cos\delta_a\right)^{-1} H_{a,\mu} = \frac{1}{\sin\alpha}\sqrt{\mu_1^2 - 2\frac{b}{c}\mu_1\mu_2\cos\alpha + b^2\mu_2^2/c^2}\,; \quad (2b)$$

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* When dealing with a sum over n indices $(l_1, \ldots, l_n)$, the n indices run through all integers and we employ the symbol Σ' in order to indicate that the term with $l_1 = l_2 = \cdots = l_n = 0$ is omitted.

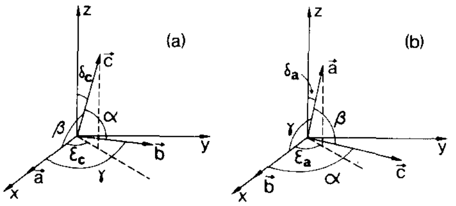

Fig. 1. Orientation of the primitive vectors with respect to the coordinate axes when the summation is performed over the *ab* (case (a)) or the *bc* (case (b)) crystal planes.

$$X_{c,\mu} = 2\pi(\xi_{c,1}\mu_1 + \xi_{c,2}\mu_2)\,; \tag{3a}$$

$$X_{a,\mu} = 2\pi(\xi_{a,1}\mu_1 + \xi_{a,2}\mu_2)\,; \tag{3b}$$

$$\xi_{c,1} = \frac{c}{a}\sin\delta_c(\cos\varepsilon_c - \sin\varepsilon_c\cot\gamma) = \frac{c}{a}\frac{\cos\beta - \cos\alpha\cos\gamma}{\sin^2\gamma}\,; \tag{4a}$$

$$\xi_{c,2} = \frac{c}{b}\frac{\sin\delta_c\sin\varepsilon_c}{\sin\gamma} = \frac{c}{b}\frac{\cos\alpha - \cos\beta\cos\gamma}{\sin^2\gamma}\,; \tag{4b}$$

$$\xi_{a,1} = \frac{a}{b}\sin\delta_a(\cos\varepsilon_a - \sin\varepsilon_a\cot\alpha) = \frac{a}{b}\frac{\cos\gamma - \cos\alpha\cos\beta}{\sin^2\alpha}\,; \tag{4c}$$

$$\xi_{a,2} = \frac{a}{c}\frac{\sin\delta_a\sin\varepsilon_a}{\sin\alpha} = \frac{a}{c}\frac{\cos\beta - \cos\alpha\cos\gamma}{\sin^2\alpha}\,; \tag{4d}$$

(ε_a and ε_c are shown in fig. 1).

Eq. (1) was arrived at by evaluating the same quantity (the potential in a crystal made of point charges plus a neutralizing background plus suitable dipole layers) in two different ways (i.e., in two differently cut slabs): in other words, the conclusion that both sides of eq. (1) form an identity in the parameters j_a, j_b, j_c, α, β, γ, c/a and b/a was reached by relying upon a physical argument.

We have found a mathematical proof of eq. (1). In so doing, we have found that this equation is actually the sum of an infinite number of identities. The latter, which too can be given a physical interpretation, are particular cases of more general identities involving a certain type of one-dimensional sums.

Our procedure can be easily further generalized so that it can conceivably be applied to other sums of physical interest.

2. Derivation of the identities needed to prove eq. (1)

Let us consider the function of the complex variable z

$$F(z) = \frac{1}{U(z)}\frac{\mathrm{e}^{-2\pi\mathrm{i}j'Az}}{1-\mathrm{e}^{-2\pi\mathrm{i}Az}}\left\{\frac{\mathrm{e}^{-2\pi j\{CU(z)+\mathrm{i}(k_1z+k_2z')\}}}{1-\mathrm{e}^{-2\pi\{CU(z)+\mathrm{i}(k_1z+k_2z')\}}} + \frac{\mathrm{e}^{-2\pi(1-j)\{CU(z)-\mathrm{i}(k_1z+k_2z')\}}}{1-\mathrm{e}^{-2\pi\{CU(z)-\mathrm{i}(k_1z+k_2z')\}}}\right\} \tag{5}$$

with

$$U(z) = (z^2 - 2uz'z + z'^2)^{1/2}\,; \tag{6}$$

j, j', A, C, u, k_1, k_2 and z' are constant parameters which, for the purposes of this paper, are assumed to be real and to fulfill the following conditions:

$$0<j, j'<1\,; \qquad A, C \neq 0\,; \qquad -1<u<1\,. \tag{7a, b, c}$$

From now on, any reference to conditions (7) will include the understanding that all the above parameters are real.

The analytic properties of $F(z)$ are slightly different according to whether $z' \neq 0$ or not. We shall consider the two cases separately. Notice that, otherwise than is possibly suggested by (6), $F(z)$ has no cut, because it does not depend on which sign is chosen for $U(z)$.

In the following we shall write

$$Q[j; f(z)] \equiv \frac{e^{-jf(z)}}{1-e^{-f(z)}}\,. \tag{8}$$

2.1. *The case $z' \neq 0$*

Due to conditions (7a, b) $F(z)$ tends exponentially to zero when $z \to \infty$, irrespective of the direction. $F(z)$ has simple poles at

$$z = z_m = m/A\,, \qquad (m = 0, \pm1, \pm2, \ldots) \tag{9}$$

arising from $Q(j'; 2\pi i A z)$, and at

$$z = z_{n,\pm} = \frac{(C^2u - k_1k_2)z' + k_1 n \pm iC\Delta_n}{C^2 + k_1^2}\,, \qquad (n = 0, \pm1, \pm2, \ldots)\,, \tag{10}$$

with

$$\Delta_n = \sqrt{\{C^2(1-u^2) + k_1^2 + k_2^2 + 2uk_1k_2\}z'^2 - 2n(uk_1 + k_2)z' + n^2}\,, \tag{11}$$

arising from $Q\{j; 2\pi[CU(z) \pm i(k_1z + k_2z')]\}$. The values $z_{n,\pm}$ are the two roots of the equation

$$C^2U^2(z) = -(k_1z + k_2z' - n)^2\,, \tag{12a}$$

which is equivalent to

$$CU(z) \pm i(k_1z + k_2z') = \pm ni\,. \tag{12b}$$

Condition (7c) implies that the argument of the root in (11) is positive definite. This ensures that no poles (9) and (10) coincide.

The factor $1/U(z)$ introduces no additional poles if $\{k_1(u \pm \sqrt{u^2-1}) + k_2\}z' \neq l$ $(l = 0, \pm1, \pm2, \ldots)$, because in such a case $\lim F(z) \neq 0$ when $U(z) \to 0$. On the other hand, if $\{k_1(u \pm \sqrt{u^2-1}) + k_2\}z' = l$ (which because of (7c) is equivalent to $k_1 = 0$, $k_2z' = l$), it is seen that the two roots of $U(z) = 0$ coincide with the values $z_{n,\pm}$ for $n = l$.

The residues of $F(z)$ are

$$R_m = \frac{1}{U_m}\frac{e^{-2\pi i j' m}}{2\pi i A}\{Q(j; 2\pi[CU_m + i(k_2z' + k_1m/A)]) + Q(1-j; 2\pi[CU_m - i(k_2z' + k_1m/A)])\}\,, \tag{13}$$

with

$$U_m = \sqrt{(m/A)^2 - 2uz'm/A + z'^2}\,,$$

at the poles (9) and

$$R_{n,\pm} = \pm \frac{e^{-2\pi i jn}}{2\pi i \Delta_n} Q(j'; 2\pi i A z_{n,\pm}) \tag{14}$$

at the poles (10). Notice that all the R_m and $R_{n,\pm}$ are finite: in fact, neither U_m nor Δ_n can vanish because of condition (7c); due to this and to (7b) neither $CU_m \pm i(k_2 z' + k_1 m/A)$ nor $iAz_{n,\pm}$ can be equal to an integer times i.

Applying Cauchy's theorem of residues to $F(z)$, with a circumference whose radius tends to infinity as integration curve, leads to the first of the general identities we derive in this paper:

$$\begin{aligned}\frac{1}{A}\sum_{m=-\infty}^{\infty} \frac{e^{-2\pi i j' m}}{U_m}\{Q(j; 2\pi[CU_m + i(k_2 z' + k_1 m/A)]) + Q(1-j; 2\pi[CU_m - i(k_2 z' + k_1 m/A)])\} \\ = -\sum_{n=-\infty}^{\infty} \frac{e^{-2\pi i jn}}{\Delta_n}\{Q(j'; 2\pi i A z_{n,+}) - Q(j'; 2\pi i A z_{n,-})\}\,.\end{aligned} \tag{15}$$

2.2. *The case $z' = 0$*

The function $F(z)$ reduces to

$$F_0(z) = \frac{1}{z} Q(j'; 2\pi i A z)\{Q[j; 2\pi(C + ik_1)z] + Q[1-j; 2\pi(C - ik_1)z]\}\,. \tag{16}$$

Its analytic properties are the same as those of $F(z)$, save for the poles $m = 0$ and $n = 0$ in eqs. (9) and (10) respectively, which are replaced by a triple pole at $z = 0$.

The residues of $F_0(z)$ are

$$R_m = \frac{e^{-2\pi i j' m}}{2\pi i m}\{Q[j; 2\pi(C + ik_1)m/A] + Q[1-j; 2\pi(C - ik_1)m/A]\} \tag{17}$$

at the poles (9) (excluding $m = 0$),

$$R_{n,\pm} = \pm \frac{e^{-2\pi i jn}}{2\pi i n} Q(j'; 2\pi i A z_{n,\pm}) \tag{18}$$

at the poles (10) (excluding $n = 0$), which now reduce to

$$z_{n,\pm} = \pm ni/(C \pm ik_1)\,,$$

and

$$R_0 = \frac{C}{iA}\left\{[(j - \tfrac{1}{2})^2 - \tfrac{1}{12}] - \frac{A^2}{C^2 + k_1^2}[(j' - \tfrac{1}{2})^2 - \tfrac{1}{12}]\right\} \tag{19}$$

at $z = 0$. The latter residue is obtained from

$$R_a = \frac{1}{(n-1)!} \lim_{z \to a} \left\{ \frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}} [(z-a)^n f(z)] \right\}$$

for a pole of order n of $f(z)$ at $z = a$ and from

$$\lim_{z \to 0} \left\{ \frac{\mathrm{d}^2}{\mathrm{d}z^2} \frac{z^2\, \mathrm{e}^{-\alpha_1 z}}{(1-\mathrm{e}^{-\alpha_2 z})(1-\mathrm{e}^{-\alpha_3 z})} \right\} = \frac{1}{\alpha_2 \alpha_3} \left\{ \alpha_1^2 - \alpha_1(\alpha_2 + \alpha_3) + \frac{\alpha_2^2 + \alpha_3^2}{6} + \frac{\alpha_2 \alpha_3}{2} \right\}.$$

Again, we see that all the residues are finite and that no poles (9) and (10) coincide (except for $m = n = 0$).

Cauchy's theorem of residues applied as before yields the second identity:

$$\sum_m{}' \frac{\mathrm{e}^{-2\pi \mathrm{i} j' m}}{m} \{Q[j; 2\pi(C + \mathrm{i}k_1)m/A] + Q[1-j; 2\pi(C - \mathrm{i}k_1)m/A]\} + \frac{2\pi C}{A}[(j-\tfrac{1}{2})^2 - \tfrac{1}{12}]$$
$$= \sum_n{}' \frac{\mathrm{e}^{-2\pi \mathrm{i} j n}}{n} \{Q[1-j'; 2\pi nA/(C+\mathrm{i}k_1)] + Q[j'; 2\pi nA/(C-\mathrm{i}k_1)]\} + \frac{2\pi AC}{C^2 + k_1^2}[(j'-\tfrac{1}{2})^2 - \tfrac{1}{12}]. \tag{20}$$

In the sum over n the terms due to the poles $z_{n,+}$ have been rewritten making use of

$$Q(j; f) = -Q(1-j; -f). \tag{21}$$

3. Application to the potential of the triclinic point-charge lattice

We choose the following values for the parameters appearing in $F(z)$:

$$j' = j_a, \qquad j = j_c, \qquad A = 1, \qquad C = \frac{c}{a}\frac{\cos \delta_c}{\sin \gamma}, \tag{22a, b, c, d}$$

$$u = \cos \gamma, \qquad k_1 = \xi_{c,1} = \frac{c^2 \sin^2 \alpha}{a^2 \sin^2 \gamma} \xi_{a,2}, \qquad k_2 = \frac{b}{a} \xi_{c,2}. \tag{22e, f, g}$$

If eqs. (22) hold, it can be shown that

$$C^2(1-u^2) + k_1^2 + k_2^2 + 2uk_1k_2 = c^2/a^2, \tag{23a}$$

$$uk_1 + k_2 = \frac{c}{a} \cos \alpha, \tag{23b}$$

$$C^2 u - k_1 k_2 = \frac{c^2}{a^2} \frac{\cos \gamma - \cos \alpha \cos \beta}{\sin^2 \gamma}, \tag{23c}$$

$$C^2 + k_1^2 = \frac{c^2 \sin^2 \alpha}{a^2 \sin^2 \gamma}, \tag{23d}$$

$$\frac{1}{C \pm \mathrm{i}k_1} = \frac{a}{c} \frac{\cos \delta_a}{\sin \alpha} \mp \mathrm{i}\xi_{a,2}. \tag{23e}$$

Now we substitute all the above into eq. (15), where we also take

$$z' = \frac{a}{b}\mu_2 \qquad (\mu_2 = 0, \pm 1, \pm 2, \ldots)$$

and replace m and n by μ_1. In this way, denoting by $\tilde{\mu}$ the set (μ_2, μ_1) (e.g., $2\pi(\xi_{a,1}\mu_2 + \xi_{a,2}\mu_1) \equiv X_{a,\tilde{\mu}}$), we have

$$U_m = \sin\gamma\, h_{c,\mu}\,, \qquad \Delta_n = \frac{c}{b}\sin\alpha\, h_{a,\tilde{\mu}}\,,$$

$$z_{n,\pm} = \xi_{a,1}\mu_2 + \xi_{a,2}\mu_1 \pm \mathrm{i}\frac{a}{b}\cos\delta_a\, h_{a,\tilde{\mu}}$$

so that

$$2\pi\mathrm{i} z_{n,\pm} = \mp H_{a,\tilde{\mu}} + \mathrm{i}X_{a,\tilde{\mu}}$$

(see eqs. (2), (4)). Eq. (15) takes the form

$$\begin{aligned}
&\sum_{\mu_1} \frac{\mathrm{e}^{-2\pi\mathrm{i}j_a\mu_1}}{\sin\gamma\, h_{c,\mu}} \{Q(j_c; H_{c,\mu} + \mathrm{i}X_{c,\mu}) + Q(1-j_c; H_{c,\mu} - \mathrm{i}X_{c,\mu}) \\
&\quad = \sum_{\mu_1} \frac{\mathrm{e}^{-2\pi\mathrm{i}j_c\mu_1}}{(c/b)\sin\alpha\, h_{a,\tilde{\mu}}} \{Q(1-j_a; H_{a,\tilde{\mu}} - \mathrm{i}X_{a,\tilde{\mu}}) + Q(j_a; H_{a,\tilde{\mu}} + \mathrm{i}X_{a,\tilde{\mu}})\}\,,
\end{aligned} \tag{24}$$

where we applied eq. (21) to the first term of the r.h.s. Now we multiply both sides by $\exp(-2\pi\mathrm{i}j_b\mu_2)$ where j_b is an arbitrary real constant, sum over μ_2 from $-\infty$ to $+\infty$, excluding $\mu_2 = 0$, and interchange μ_1 with μ_2 in the r.h.s. We get

$$\begin{aligned}
&\sum_{\mu_2}{}' \sum_{\mu_1} \frac{\mathrm{e}^{-2\pi\mathrm{i}(j_a\mu_1 + j_b\mu_2)}}{b\sin\gamma\, h_{c,\mu}} \{Q(j_c; H_{c,\mu} + \mathrm{i}X_{c,\mu}) + Q(1-j_c; H_{c,\mu} - \mathrm{i}X_{c,\mu})\} \\
&\quad = \sum_{\mu_1}{}' \sum_{\mu_2} \frac{\mathrm{e}^{-2\pi\mathrm{i}(j_b\mu_1 + j_c\mu_2)}}{c\sin\alpha\, h_{a,\mu}} \{Q(j_a; H_{a,\mu} + \mathrm{i}X_{a,\mu}) + Q(1-j_a; H_{a,\mu} - \mathrm{i}X_{a,\mu})\}\,.
\end{aligned} \tag{25}$$

Now we consider eq. (20), where we make the same substitutions as above (eqs. (22), (23)) and replace m and n by μ_1 and μ_2 respectively:

$$\begin{aligned}
&\sum_{\mu_1}{}' \frac{\mathrm{e}^{-2\pi\mathrm{i}j_a\mu_1}}{\mu_1} \left\{Q\left[j_c; 2\pi\left(\frac{\cos\delta_c}{\sin\gamma}\frac{c}{a} + \mathrm{i}\xi_{c,1}\right)\mu_1\right] + Q\left[1-j_c; 2\pi\left(\frac{\cos\delta_c}{\sin\gamma}\frac{c}{a} - \mathrm{i}\xi_{c,1}\right)\mu_1\right]\right\} \\
&\quad + \frac{c}{a}\frac{2\pi\cos\delta_c}{\sin\gamma}[(j_c - \tfrac{1}{2})^2 - \tfrac{1}{12}] \\
&\quad = \sum_{\mu_2}{}' \frac{\mathrm{e}^{-2\pi\mathrm{i}j_c\mu_2}}{\mu_2} \left\{Q\left[1-j_a; 2\pi\left(\frac{\cos\delta_a}{\sin\alpha}\frac{a}{c} - \mathrm{i}\xi_{a,2}\right)\mu_2\right] + Q\left[j_a; 2\pi\left(\frac{\cos\delta_a}{\sin\alpha}\frac{a}{c} + \mathrm{i}\xi_{a,2}\right)\mu_2\right]\right\} \\
&\quad + \frac{a}{c}\frac{2\pi\cos\delta_a}{\sin\alpha}[(j_a - \tfrac{1}{2})^2 - \tfrac{1}{12}]\,.
\end{aligned} \tag{26}$$

Finally, we add up eqs. (25) and (26): in this way we obtain eq. (1), so that we have proved the desired result.

4. Physical interpretation of the results of the previous section

Eqs. (24)–(26) can be given a physical interpretation in terms of the Fourier decomposition of the charge density located on the straight lines in the b direction of a crystal.

Let us have an infinite set of charges q, equally spaced by a distance b, on a straight line. If s is the abscissa on that line, then the charge per unit length is

$$\rho(s) = q \sum_{\lambda=-\infty}^{\infty} \delta(s - \lambda b) = \frac{q}{b} \sum_{\mu=-\infty}^{\infty} \mathrm{e}^{-2\pi \mathrm{i} \mu s/b} \equiv \sum_{\mu=-\infty}^{\infty} \rho_\mu(s) \tag{27}$$

(see eq. (A.10) of ref. [2]). Let us apply this decomposition to the straight lines parallel to the $\boldsymbol{b}$ direction of the triclinic lattice, and let us consider just one component $\rho_\mu(s)$. We shall develop with some detail the case $\mu \neq 0$. We shall consider two different slabs, one of them cut parallel to the ab and the other to the bc crystal planes (cases 1 and 2 respectively; for the orientation of the primitive vectors see figs. 1a and 1b respectively).

Case 1

The space charge density is given by

$$\rho_\mu(\boldsymbol{r}; abc) = \frac{q}{b \sin\gamma} \sum_{\lambda_1, \lambda_3} \delta(x - \lambda_1 a - lb\cos\gamma - \lambda_3 c \sin\delta_c \cos\varepsilon_c)\delta(z - \lambda_3 c\cos\delta_c)\,\mathrm{e}^{-2\pi \mathrm{i}\mu l}, \tag{28}$$

where

$$l = (y - \lambda_3 c \sin\delta_c \sin\varepsilon_c)/b \sin\gamma .$$

The potential $V_\mu(j; abc)$ of this charge distribution at a point $\boldsymbol{r}_P = -(j_a\boldsymbol{a} + j_b\boldsymbol{b} + j_c\boldsymbol{c})$ can be easily evaluated by considering in a separate way the contribution of each crystal plane parallel to the slab and following the same procedure as for a point-charge lattice [1]. The potential of a λ_3 plane turns out to be*

$$V_\mu^{(\lambda_3)}(j; abc) = \frac{q}{4\pi\varepsilon_0} \frac{1}{b\sin\gamma} \sum_{\mu_1} \mathrm{e}^{-2\pi\mathrm{i}\{j_a\mu_1 + j_b\mu + (\lambda_3 + j_c)(\xi_{c,1}\mu_1 + \xi_{c,2}\mu)\}} \frac{\mathrm{e}^{-2\pi h_{c,\mu}|\lambda_3 + j_c|\cos\delta_c c/a}}{h_{c,\mu}} . \tag{29}$$

Carrying out the λ_3 summation we obtain $V_\mu(j; abc)$:

$$\frac{4\pi\varepsilon_0}{q} V_\mu(j; abc) = \frac{1}{b\sin\gamma} \sum_{\mu_1} \mathrm{e}^{-2\pi\mathrm{i}(j_a\mu_1 + j_b\mu)} h_{c,\mu}^{-1} \left\{ \frac{\mathrm{e}^{-j_c(H_{c,\mu} + \mathrm{i}X_{c,\mu})}}{1 - \mathrm{e}^{-(H_{c,\mu} + \mathrm{i}X_{c,\mu})}} + \frac{\mathrm{e}^{-(1-j_c)(H_{c,\mu} - \mathrm{i}X_{c,\mu})}}{1 - \mathrm{e}^{-(H_{c,\mu} - \mathrm{i}X_{c,\mu})}} \right\} . \tag{30}$$

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* Here and in eq. (30) $h_{c,\mu}$, $H_{c,\mu}$ and $X_{c,\mu}$ are given by (2a) and (3a) with μ replacing μ_2; analogously, in eqs. (32), (33) $h_{a,\mu}$, $H_{a,\mu}$ and$X_{a,\mu}$ are given by (2b) and (3b) with μ replacing μ_1.

Case 2

Now the x axis coincides with the $\boldsymbol{b}$ direction. The charge density is

$$\rho_\mu(\boldsymbol{r}; bca) = \frac{q}{b} \sum_{\lambda_2,\lambda_3} \delta(y - \lambda_2 c \sin\alpha - \lambda_3 a \sin\delta_a \sin\varepsilon_a)\delta(z - \lambda_3 a \cos\delta_a)\,\mathrm{e}^{-2\pi\mathrm{i}\mu l}\,, \tag{31}$$

where

$$l = \frac{1}{b}(x - \lambda_2 c \cos\alpha - \lambda_3 a \sin\delta_a \cos\varepsilon_a)\,.$$

Proceeding in an analogous way as in case 1 we obtain

$$V_\mu^{(\lambda_3)}(j; bca) = \frac{q}{4\pi\varepsilon_0}\frac{1}{c\sin\alpha}\sum_{\mu_2} \mathrm{e}^{-2\pi\mathrm{i}\{j_b\mu + j_c\mu_2 + (\lambda_3 + j_a)(\xi_{a,1}\mu + \xi_{a,2}\mu_2)\}}\,\frac{\mathrm{e}^{-2\pi h_{a,\mu}|\lambda_3 + j_a|\cos\delta_a a/b}}{h_{a,\mu}}\,, \tag{32}$$

$$\frac{4\pi\varepsilon_0}{q}\,V_\mu(j; bca) = \frac{1}{c\sin\alpha}\sum_{\mu_2} \mathrm{e}^{-2\pi\mathrm{i}(j_b\mu + j_c\mu_2)}h_{a,\mu}^{-1}\left\{\frac{\mathrm{e}^{-j_a(H_{a,\mu} + \mathrm{i}X_{a,\mu})}}{1 - \mathrm{e}^{-(H_{a,\mu} + \mathrm{i}X_{a,\mu})}} + \frac{\mathrm{e}^{-(1-j_a)(H_{a,\mu} - \mathrm{i}X_{a,\mu})}}{1 - \mathrm{e}^{-(H_{a,\mu} - \mathrm{i}X_{a,\mu})}}\right\}. \tag{33}$$

Now let us go back to eq. (24), where we make the following changes: we replace μ_2 by μ, multiply both sides by $\exp(-2\pi\mathrm{i}j_b\mu)$ and substitute the summation index μ_1 in the r.h.s. by μ_2. The left- and the right-hand sides of the equation so obtained coincide with the left-hand sides of eqs. (30) and (33) respectively. In this way, a physical interpretation of eq. (24) is obtained, namely

$$V_\mu(j; abc) = V_\mu(j; bca)\,. \tag{34}$$

Actually, it is not a priori evident that the above quantities should be equal. In fact, the potential created by the above-considered charge distribution (eqs. (28) and (31)) does, in principle, depend on the shape of the specimen (in our case, on the way the slab is cut) because the unit cell has a non-vanishing quadrupole tensor $\boldsymbol{Q}_\mu^{(\rho)}$. A shape-independent potential $V_{E,\mu}(j)$ can be introduced, as in [1], by superimposing on the slab surface a dipole density whose quadrupole tensor is equal to $-\boldsymbol{Q}_\mu^{(\rho)}$. It can be seen that (we take the cell orientation as in case 1)

$$\boldsymbol{Q}_\mu^{(\rho)} = \frac{(-1)^\mu q b^2}{2\pi^2\mu^2}\begin{pmatrix} \cos^2\gamma & \cos\gamma\sin\gamma & 0 \\ \cos\gamma\sin\gamma & \sin^2\gamma & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{35}$$

so that, using eqs. (I.3) of [1], the dipole layers must be given by

$$\tau_a = \tau_c = 0\,, \qquad \tau_b = \frac{(-1)^{\mu-1} q b^2}{4\pi^2\mu^2 v}\cos^2\delta_b \tag{36a, b}$$

(τ_i is the density of surface dipole moment on the $a_k a_l$ face, with $k, l \neq i$). Using

$$V_{E,\mu}(j) = V_\mu(j; abc) - \tau_c/\varepsilon_0 = V_\mu(j; bca) - \tau_a/\varepsilon_0$$

(by analogy with eqs. (64)–(66) of [1]) and eq. (36a) we verify that the equality (34) holds true.

A similar interpretation could be found for eq. (26) as for (24): in this case one should consider the $\mu = 0$ component of the point-charge lattice decomposition, introduce a uniform neutralizing background in order to avoid a divergent value for the potential and take into account the shape dependence.

5. Conclusion

The analytic properties of the function $Q\{j; f(z)\}$ (eq. (8)) make it well suited for the derivation of identities between a certain type of lattice sums. The function $F(z)$ we defined in eq. (5) and with which we proved the identities between sums related to the potential of a triclinic point-charge lattice is just an example of that. Of course, one could obtain other identities by considering different combinations of Q-functions, or different factors (instead of $1/U(z)$). As these identities relate two series with different rates of convergence, they could be used to save computation time when evaluating a sum of this type.

References

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