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This Week's Citation Classic®

Ewald P P. Die Berechnung optischer und elektrostatischer Gitterpotentiale (Evaluation of optical and electrostatic lattice potentials).
Ann. Phys. Leipzig **64**:253-87, 1921.
[Institut für Theoretische Physik, Munich, Germany]

The theta function method is shown to allow a rapidly converging evaluation of lattice potentials and fields due to periodic arrangements of charges or dipoles, and, in particular, of the "field of excitation" created at the location of a charge or dipole by all others. [The *SCI*® indicates that this paper has been cited in over 555 publications since 1955.]

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Note: *Professor P.P. Ewald died in Ithaca, New York, on August 22, 1985, a few days before ISI® asked for his commentary on the above paper. His wife, Mrs. Ella Ewald, has requested us to respond.*

September 16, 1985

This paper is an offshoot of P.P. Ewald's much more significant work on the dynamical theory of optics and X rays in crystals,[1] a forerunner of all modern self-consistent treatments of waves in crystals, such as Bethe's theory of electron diffraction, for describing interactions of particles and waves in crystals.

Ewald himself has described its genesis.[2] While working on his thesis, after having constructed a lattice dipole potential as a sum of plane waves, he wrote: "My happiness over this first tangible result was not to last long: I found it impossible to subtract from this total potential that part that was contributed by the test dipole.... The impossibility of a direct subtraction comes from the fact that all individual dipole fields are jumbled together and recast into a sum of nonlocalised plane waves in which individual contributions can no longer be recognised. (I was not aware, at the time, that what I had obtained was a Fourier development of the total field.)

"Success in the removal of the field of the test dipole came through Sommerfeld's assistant, P. Debye. At a skiing holiday in Mittenwald, Easter 1911, Sommerfeld showed him our quandary. With one glance at the expression of the total potential, Debye said: 'This is quite simple; you have to use Riemann's method of bringing the denominator of the sum term into the exponent of an exponential function by introducing a new integration. The integrand then becomes a theta-function and you can apply the transformation theorem of the theta functions to it.' The whole 'consultation' probably lasted no more than a quarter of an hour. Debye was not only an avid reader of classical physics, but also had an extraordinary power of seeing through mathematical formalism. He did not know at the time in which of Riemann's papers this method occurred—nor did I ever find out.

"When I had finally understood Debye's advice, I transformed the total potential in the way he had suggested. This is a rather round-about way of obtaining the theta functions and in the publication I followed a more direct way by introducing the simple-integral representation of $\frac{1}{R}e^{ikR}$, which leads directly to theta functions....

"I later extended this method of calculating lattice potentials and Madelung constants from orthorhombic to general lattices. There, the theta function of the three space coordinates no longer splits into the product $\Theta(x)\cdot\Theta(y)\cdot\Theta(z)$. The transformation property of the space-theta was contained in the main text on theta function,[3] but in a horrible form. By using the concept of the reciprocal lattice, I could restate it in a way akin to the tools of the mathematical physicist. Since then, the theta function method has been the favored one for calculating lattice energies and potentials. The neat way in which the formal splitting of the integral for the potential produces two rapidly convergent parts was interpreted physically in a later paper of mine...."[4]

The method has since been incorporated in textbooks as diverse as Born and Huang[5] and Kittel,[6] as well as generalized. Currently, it has had an important role in modern band structure calculations.

1. **Ewald P P.** Zur Begründung der Kristalloptik. Teil I-III. *Ann. Phys. Leipzig* 49:1-38, 1916; 49:117-43, 1916; 54:519-97, 1917. (Cited 125, 105, and 150 times, respectively, since 1955.)
2. --------------. Postscript to L. Hollingsworth's English translation of *Ann. Phys. Leipzig* 49:1-38, 117-43, 1916; 54:519-97, 1917. Bedford, MA: Air Force Cambridge Research Laboratory, 1970. AFCRL Report 70-8580.
3. **Krazer A.** *Lehrbuch der Thetafunktionen.* Leipzig: Teubner, 1903. 509 p.
4. **Ewald P P.** Elektrostatische und Optische Potentiale im Kristallraum und im Fourierraum. *Nachr. Ges. Wiss. Göttingen Math.-Phys. Kl. Neue Folge. Fachgruppe II* 3:55-64, 1938.
5. **Born M & Huang K.** *Dynamical theory of crystal lattices.* Oxford: Clarendon Press, 1954. p. 248-55.
6. **Kittel C.** *Introduction to solid state physics.* New York: Wiley, 1956. p. 571-5.

