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Kellermann E W. Theory of the vibrations of the sodium chloride lattice.
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Using a method developed by P.P. Ewald, a quickly convergent representation of Born's treatment suggested for the calculation of the frequency equations for a vibrating crystal was found, and a special application was made to sodium chloride. It appears that correct solutions for the whole frequency spectrum of the crystal can be obtained only by taking account of the electrodynamic boundary conditions, namely that the crystal as a whole does not emit radiation. This then also leads to the correct solution for the frequency of the residual rays and the elastic constants of sodium chloride can be calculated. [The *SCI®* indicates that this paper has been cited in over 525 publications since 1955.]

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Although Born's treatment of the vibrations of crystal lattices had been largely developed in his *Atomtheorie des festen Zustandes*[1] and his article (with Maria Göppert-Mayer) in the *Handbuch der Physik*,[2] the formulae developed by him resisted successful exploitation through the calculation of the frequency spectrum (now known as the phonon spectrum) of a real crystal, in spite of Blackman's pioneering work on two-dimensional models.[3] How the problem was eventually solved in this paper may be of interest to the science historian for two reasons: it gives an insight into Born's way of interacting with his research students, and it shows how (in my opinion) a graduate research student, trained at first as an experimentalist, could find a solution that had escaped some eminent theoreticians.

It was on the occasion of a colloquium given by Ewald at Edinburgh that Born suggested to me that Ewald's Fourier representation of lattices[4] might well be applied to Born's coefficients derived for the calculation of the frequencies. I began the work and eventually solved the mathematical and the tedious numerical problems in finding solutions for a large number of frequencies, which meant calculating the roots of a number of sixth-order determinants large enough to cover the frequency range adequately. However, the results were disappointing because the frequencies, instead of being real, turned out to be complex numbers.

Born was convinced that I had made a mistake, but I did not agree. I had found, experimentally, that by changing the formula given in the *Handbuch* article, I could obtain realistic results and proceeded to tell Born that I thought there was a mistake in his article! His reaction was almost predictable: *"Das verstehen Sie nicht,"* accusing me of ignorance in no uncertain terms. However, after a short period of depression, I managed to find proof for my assertion. I could show that the assumption made in Born and Göppert-Mayer's article, omitting the zero term of the Fourier representation of the coefficients, was correct if it applied only to vibrations with infinitely long waves (i.e., "long" compared with the dimensions of the crystal), otherwise it had to be included. It could be proved that this exception was not arbitrary, but that it followed from the electrodynamic boundary condition that the crystal as a whole must not emit radiation. Applying this condition yielded real values for the frequencies as well as the frequency for the "residual rays" (*Reststrahlen*).

Born immediately accepted this argument and very generously insisted that the resulting paper should be published under my name alone in the *Transactions of the Royal Society*; he also showed me a letter "communicating" the paper to the secretary, which stated that his own treatment in the *Handbuch* had not been correct, but that by developing the correct expression, I had been able to solve this important problem.

The importance of this paper rests on the possibility opened up by it of calculating from its final formulae the phonon spectrum, the elastic constants, and the specific heat of real crystals. All these are verifiable experimentally and were found to agree with the measurements as well as with the experiments on X-ray scattering. The lattice theory was thus firmly established. Also, it was no longer necessary to rely on Debye's semi-empirical treatment of the specific heat, which cannot account accurately for the behaviour of crystals at low temperature.

1. **Born M.** *Atomtheorie des festen Zustandes (Dynamik der Kristallgitter).* Leipzig: Teubner, 1923. 789 p.
2. **Born M & Göppert-Mayer M.** Dynamische Gittertheorie der Kristalle. *Handbuch der Physik* **24**(Pt.2):623-790, 1933.
3. **Blackman M.** On anomalous vibrational spectra. *Proc. Roy. Soc. A* **164**:162-79, 1938.
4. **Ewald P P.** Elektrostatische und Optische Potentiale im Kristallraum und im Fourierraum. *Nachr. Gesell. Göttingen Neue Folge Fachgruppe II* **3**:55-64, 1938.