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Gilat G & Raubenheimer L J. Accurate numerical method for calculating frequency-distribution functions in solids. *Phys. Rev.* **144**:390-5, 1966.
[Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN]

The paper describes an efficient method of calculating densities of states g(ν) in cubic crystals. The irreducible part of the Brillouin zone is divided into a finite number of cells. In every cell, the constant energy surface is approximated by a set of parallel planes which allows for analytic calculation of g(ν). [The *SCI®* indicates that this paper has been cited in over 440 publications since 1966.]

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"In 1963, while spending a postdoctoral year at Chalk River, Canada, I was introduced by G. Dolling to the then new field of inelastic neutron scattering. Part of the data analysis of the experiments consisted of calculating the phonon density of states g(ν) and for this the local computer was booked for a whole night in order to generate several million matrix diagonalizations. This was necessary to obtain a relatively accurate histogram of g(ν) where one could observe the Van Hove singularities. This 'brute force' method did not appeal to me and I began to consider alternative methods. Soon enough, it became evident that the gradient $\vec{\nabla}\,\nu(\vec{k})$ must play some role in such a scheme, but it was not quite clear in what manner. However, certain progress was made where the gradient was employed to generate many results using the perturbation approach instead of matrix diagonalization so that a satisfactory histogram of g(ν) was computed within several minutes instead of hours.[1] Although this certainly was a success, I still was not very happy, since this new method was based on numerical shortcuts rather than on an analytic approach.

"It took another two years—by then I had moved to Oak Ridge National Laboratory—until the main idea was conceived. What was missing in the picture was the role of constant energy surfaces of phonons throughout the Brillouin zone. Those could be approximated within small cells, cubic as they were, by sets of parallel planes so that their particular contribution to g(ν) was proportional to the area of the plane associated with a given ν and confined within the cell. We called this the 'cross-section area' of the cell (cube). This idea was actually a breakthrough for such calculations, since the cross-section area could be calculated analytically for each cell. It took Louis Raubenheimer and myself several more weeks to obtain all the pertinent expressions and the method was ready. Soon afterward it was extended to orthorhombic crystals.[2]

"As I see it, the main significance of this paper was that it became the basis for high-resolution calculations of spectral properties in solids derivable from theoretical models. This method made it possible to perform elaborate and complex computations of phonon and electronic densities of states within relatively short computer times which could not have been envisaged before then. Within several years many developments and ramifications followed, but they all used the same idea of cross-section area.

"A few of the more important developments were: (a) the extension of the method to so-called real-part functions;[3] (b) the inclusion of transition probabilities within the framework of the method, which enabled the computation of spectral functions;[4] and (c) the replacement of the cubic small cell by a tetrahedron, which proved to be very useful.[5,6]

"I believe that the reason this paper is highly cited is mainly its usefulness. It did not offer any new insight into the physics of the solid state, but enabled accurate calculations that sometimes led to an unexpected prediction. This actually happened when an accurate calculation of g(ν) of aluminum led to a prediction of a low temperature specific heat anomaly which was observed later."[7]

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1. **Gilat G & Dolling G.** A new sampling method for calculating the frequency distribution function of solids. *Phys. Lett.* 8:304-7, 1964. (Cited 75 times.)
2. **Raubenheimer L J & Gilat G.** Accurate numerical method of calculating frequency distribution functions in solids. II. Extension to hcp crystals. *Phys. Rev.* **157**:586-99, 1967. (Cited 85 times.)
3. **Gilat G & Bohlin L.** High resolution method for calculating spectra of solids—II. *Solid State Commun.* 7:1727-30, 1969. (Cited 15 times.)
4. **Gilat G & Kam Z.** High-resolution method for calculating spectra of solids. *Phys. Rev. Lett.* **22**:715-17, 1969.
5. **Jepson O & Anderson O K.** The electronic structure of h.c.p. ytterbium. *Solid State Commun.* 9:1763-7, 1971. (Cited 150 times.)
6. **Lehmann G & Taut M.** On the numerical calculation of the density of states and related properties. *Phys. Status Solidi B—Basic Re.* 54:469-77, 1972. (Cited 235 times.)
7. **Berg W T.** Heat capacity of aluminum between 2.7 and 20°K. *Phys. Rev.* **167**:583-6, 1968.