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LETTER TO THE EDITOR

Van Hove singularities

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Abstract. Two methods of determining Van Hove singularities of non-degenerate electronic energy bands in non-magnetic crystals are compared. The equivalence of the two methods is shown.

A method to identify Van Hove singularities in electronic energy bands of non-magnetic crystals has been formulated by Cracknell (1973) and compared with a second method used by Kudryavtseva (1967, 1968, 1969). It was concluded (Cracknell 1973) that there are some 'apparent disagreements' between the two methods. In a later publication, Cracknell (1974) pointed out that the analysis of Van Hove singularities in Cracknell (1973) is in fact applicable only to non-degenerate energy bands. There was, however, no re-comparison of the two methods. It is the purpose of this letter to point out the equivalence of the two methods in the case of non-degenerate energy bands.

The symmetry group of a non-magnetic crystal is the direct product of the symmetry space group of the crystal and the time reversal group consisting of the identity and time reversal. Energy bands $E(\boldsymbol{k})$ at wavevector $\boldsymbol{k}$ are classified by co-representations of the magnetic little group of the wavevector $\boldsymbol{k}$ (Cracknell 1974). In the case of a non-degenerate energy band, the energy band $E(\boldsymbol{k})$ at wavevector $\boldsymbol{k}$ is associated with a one-dimensional irreducible co-representation $\boldsymbol{D}$ of the magnetic little group of the wavevector $\boldsymbol{k}$, a type 'a' co-representation (Bradley and Davies 1968), ie where $D(u) = \Delta(u)$, $D(a) = \Delta(aa_0^{-1})P$, and $PP^* = \Delta(a_0^2)$. Since, in this case, $\Delta(u)$ is a one-dimensional irreducible representation and P a complex number, $\Delta(u)\Delta(u)^* = 1$ and $PP^* = 1$. Consequently, the criterion for a Van Hove singularity in $E(\boldsymbol{k})$ at $\boldsymbol{k}$ used by Kudryavtseva (1967, 1968, 1969) becomes

$$\sum_R \chi^{\mathrm{v}}(R) - \sum_R \chi^{\mathrm{v}}(R_2R) = 0 \qquad (1)$$

where χ^{v} denotes the character of the vector representation, the sum is over all rotations (proper or improper) R of the point group of the crystal such that $R\boldsymbol{k} \doteq \boldsymbol{k}$, and R_2 is a rotation of the point group of the crystal such that $R_2\boldsymbol{k} \doteq -\boldsymbol{k}$. One may write $-\chi^{\mathrm{v}}(R_2R) = \chi^{\mathrm{v}}(IR_2R)$, where I denotes spatial inversion, and rewrite equation (1) as

$$\sum_S \chi^{\mathrm{v}}(S) = 0 \qquad (2)$$

where S is an element of the point group $\boldsymbol{R} + IR_2\boldsymbol{R}$, and where $\boldsymbol{R}$ denotes the group of all rotations R.

From equation (2) one concludes—and this is the criterion for determining Van Hove singularities in non-denerate energy bands using the method used by Kudryavtseva (1967, 1968, 1969)—that there is a Van Hove singularity in a non-degenerate energy band $E(\boldsymbol{k})$ at $\boldsymbol{k}$ if the vector representation of the point group $\boldsymbol{R} + IR_2\boldsymbol{R}$ does not contain the identity representation. Alternatively one can reinterpret equation (2)—and this is the form of the criterion for determining Van Hove singularities as given by Cracknell (1973)—as follows: There is a Van Hove singularity in a non-degenerate energy band $E(\boldsymbol{k})$ at $\boldsymbol{k}$ if there is no vector invariant under the point group $\boldsymbol{R} + IR_2\boldsymbol{R}$.

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