Addition theorem for Bloch wave vectors for energy bands of inequivalent one-dimensional lattices

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An addition theorem is derived which describes how the Bloch wave vectors, for a given energy, of two pure one-dimensional lattices are to be combined to obtain the Bloch wave vector for a composite lattice formed of the two pure lattices. Applications are discussed. The theorem is valid for an ordered or a disordered lattice, but the detailed nature of the energy bands of a disordered lattice is determined by the details of the structure of the disordered array.

INTRODUCTION

In 1949 Saxon and Hutner stated a proposition relating forbidden energy-band gaps in the energy bands of two periodic one-dimensional potentials to the gaps in the energy bands of a one-dimensional lattice potential constructed by following, at random, the potential in one cell by a cell with the same potential, or the other potential.[1] Their proposition was that, for energies for which both pure periodic lattices have imaginary Bloch wave vectors, that is, for "forbidden" energies, the composite lattice would also have a gap in the allowed energy. Luttinger proved the theorem under the special condition that the potentials be representable by symmetric delta functions of different amplitude.[2] Others have discussed the proposition and arrived at similar or contrary conclusions.[3–8]

What is needed is something more general than the Saxon-Hutner-Luttinger (SHL) proposition; one needs an addition theorem which describes how the Bloch wave vectors, for given energy, for two inequivalent lattices are to be combined to derive the Bloch wave vector for the lattice formed by taking each component lattice in sequence.

Transfer matrix: The complex representation

The transfer-matrix formalism is used here. This is, possibly, an unfamiliar but long-established and mathematically understood technique. It is also known as the "matrizant" method[9–13] or the reciprocal-matrix method.[14–19] It was first applied to the present problem by Kramers in 1935,[20] and it was also used by Saxon and Hutner[1] and Luttinger.[2] Saxon and Hutner used a complex representation for which the basis vectors are $\exp(\pm ikx)$. Luttinger used the real representation for which the basis vectors are an amplitude and a slope of a function. The complex representation is used here. The basis-vector wave vector k can be related to the energy, as Saxon and Hutner do, but it need not be since the energy scale is arbitrary, being determined by the zero chosen for the potential. Thus the energy transformation,

$$V'(x)=V(x)-E+k^2 \quad (1)$$

may be used to allow any energy, including zero, to be considered with the complex representation.

The properties of the transfer matrix R are readily established from scattering theory.[1] R has elements $R_{11}=R_{22}^*$, $R_{12}=R_{21}^*$, and $R_{11}R_{22}-R_{12}R_{21}=1$. It is a two-dimensional three-parameter representation with unit determinant. The eigenvalues thus have a product of 1, and may be written as $\exp(i\mu d)$, and $\exp(-i\mu d)$, where μ the characteristic, or Bloch, wave vector, is either real or imaginary, and d is the unit-cell length. The trace of R is $2\cos(\mu d)$. For real μ the wave function propagates on the lattice with bounded amplitude. For imaginary μ the wave-function amplitude increases without bound, and the energy associated with it is said to be "forbidden." One exceptional state exists for $\mu=0$ or π. In this case only one bounded solution exists and it has eigenvalues of ± 1; the second unbounded solution cannot be obtained by any linear transformation on the original basis vectors.

Addition theorem

Consider two periodic lattice potentials, V_M and V_N, and a lattice with m cells of the M potential followed by n cells of the N potential. The transfer matrix relating the wave function at the beginning of the section to the wave function at the end of the section will be $R_N^n R_M^m$. Except for the single state at the interface of the real and imaginary wave vectors, that is, except for the trace equal to ± 2 representation, a similarity transformation U exists which will diagonalize the pure-lattice representations,

$$URU^{-1}=\Lambda=\begin{bmatrix}\lambda & 0\\ 0 & \lambda^{-1}\end{bmatrix} . \tag{2}$$

For the complex representation U will be a representation in SU(2),

$$U=\begin{bmatrix}a & b\\ -b^* & a^*\end{bmatrix} \quad \begin{matrix} a=\cos\beta\exp(i\alpha)\\ b=\sin\beta\exp(i\gamma) \end{matrix} . \tag{3}$$

A similarity transformation which will refer Λ_M to the same basis vectors as Λ_N will be $U_N U_M^{-1}$, with elements a_{MN} and b_{MN},

$$(U_N R_N U_N^{-1})(U_N U_M^{-1}\Lambda_M U_M U_N^{-1}) = U_N R_N R_M U_N^{-1} . \tag{4}$$

So one finds that the trace of the product matrix will be

$$\mathrm{tr}[U_N R_N^n R_M^m U_N^{-1}] = \lambda_N^n[(aa^*)_{MN}\lambda_M^m+(bb^*)_{MN}\lambda_M^{-m}] + \lambda_N^{-n}[(bb^*)_{MN}\lambda_M^m+(aa^*)_{MN}\lambda_M^{-m}]. \tag{5}$$

The trace determines the wave vector of the composite lattice to be

$$\cos[(md_M+nd_N)\mu_{MN}] = \cos(md_M\mu_M)\cos(nd_N\mu_N) - \cos(2\beta_{MN})\sin(md_M\mu_M)\sin(nd_N\mu_N) , \tag{6}$$

with

$$\cos(2\beta_{MN})=(aa^*-bb^*)_{MN} .$$

This is the desired addition theorem.

For a lattice of several potentials with random sequence, the theorem can be applied successively to reduce one pair of wave vectors to their effective value. Then this effective wave vector can be combined with a third wave vector for the three segments, and so on.

APPLICATION AND DISCUSSION

As to the Saxon-Hutner-Luttinger theorem, we note that the energy gaps are characterized by real eigenvalues. If λ is an eigenvalue of R it follows that the elements of the diagonalizing transformation U are related by

$$\frac{a}{b}=\frac{\lambda-R_{22}}{R_{12}} \tag{7}$$

and so,

$$\frac{a^*}{b^*}=\frac{\lambda^*-R_{11}}{R_{21}} . \tag{8}$$

With λ real then,

$$\frac{aa^*}{bb^*}=\frac{(\lambda-R_{11})(\lambda-R_{22})}{R_{12}R_{21}}=1 . \tag{9}$$

Hence for λ real, $\beta=\pi/4$. In this case $U_N U_M^{-1}$ will have $aa^*=1$ and $bb^*=0$. Hence,

$$\cos[(md_M+nd_N)\mu_{MN}] = \cosh[md_M|\mu_M|+nd_N|\mu_N|] \tag{10}$$

for μ_M and μ_N imaginary.

It is clear that μ_{MN} must also be imaginary, and that the composite has a forbidden energy gap where the two pure lattices both have gaps. This proves the Saxon-Hutner conjecture, vindicates Luttinger's proof, and contradicts other findings.

We can extend the proposition for the case with both pure lattices having complex eigenvalues. In this case one sees immediately from Eq. (6) that for $\beta_{MN}=\pm\pi/4$ or 0, μ_{MN} is certainly real also. Intermediate cases can be examined by rewriting Eq. (6) as,

$$\cos[(md_M+nd_N)\mu_{MN}] = \sin^2\beta_{MN}\cos(md_M\mu_M-nd_N\mu_N) + \cos^2\beta_{MN}\cos(md_M\mu_M+nd_N\mu_N) . \tag{11}$$

It is evident that an extremum exists when both the μ-dependent terms have the same extremum, and then the magnitude of the sum is 1. Hence the overlapping allowed bands are also allowed in the composite random lattice.

If one wave vector, μ_M, for example, is imaginary and the other, μ_N , is real, some energies allowed in the pure N lattice but forbidden in the M lattice become allowed or forbidden in the composite, depending upon whether the magnitude of the right-hand side of Eq. (6) or (11) is greater than or less than 1. If V_M and V_N are equivalent potentials, then the equations reduce properly since in this case $\beta_{MN}=0$.

Since the addition theorem uses only quantities derived from a single unit cell of the pure lattice, it is valid for an ordered or a disordered lattice. The detailed nature of the energy bands of a disordered lattice is determined by the precise structure of the disordered lattice. What is needed in this case is a third parameter in addition to energy and wave vector, a morphology, or complexion parameter. Since allowed and forbidden states can be combined to obtain allowed or forbidden states in the composite, it will be seen that localized forbidden states can exist at energies allowed for the total composite lattice; and localized allowed states can exist at energies forbidden for the total composite lattice.

It also follows that a pure-lattice potential can be considered as a composite by breaking the unit cell, arbitrarily, into two or more characteristic features or parts. In this way the predictions of the addition theorem can be intuitively understood. For a sinusoidal potential, for example one can divide the unit cell into regions in which the energy is greater than or less than the potential. For the region with energy everywhere less than the potential, the eigenvalue will certainly be real. The region with energy greater than the potential may have an eigenvalue that is complex. The composite of these two regions can have both forbidden and allowed energies as one knows from experience. This result is compatible with the result one obtains from the addition theorem as applied to the composite of the portions of one unit cell. This procedure of breaking the unit cell up into several parts is also of use when one, for example, discusses the quantum defect, that is, the effect of changing the potential in a localized region of the unit cell.

It does not seem necessary to point out that to demonstrate these results by using wave functions and matching them in slope and magnitude at the cell boundaries is certainly much more difficult, to carry out, to report on as an author, and to follow as a reader. These results are applicable to other one-dimensional systems such as transmission lines with varying physical parameters, or cascades of inequivalent two-port filter networks.[21]

This device, the transfer matrix, can be applied to study lattices of higher dimension. Some results obtained will be published elsewhere. Many electron effects and correlation effects have not been considered here, as is the convention in the discussion of this theorem.

[1]D.S. Saxon and R. A. Hutner, Philips Res. Rep. 4, 81 (1949)

[2]J. M. Luttinger, Philips Res. Rep. 6, 303 (1951).

[3]T. A. Hoffman, Acta Phys. Acad. Sci. Hung. 1, 5, (1952); 1, 175 (1952); 2, 97 (1952); 2, 107 (1952); 2, 195 (1952).

[4]H. M. James and A. S. Ginzbarg, J. Phys. Chem. 57, 840 (1953).

[5]E. H. Kerner, Phys. Ref. 95, 687 (1954).

[6]R. E. Borland, Proc. Phys. Soc. 78, 926 (1961); Proc. R. Soc. London 274, 529 (1963).

[7]R. J. Rubin, J. Math. Phys. 9, 2252 (1968).

[8]L. Dworin, Phys. Rev. 138A, 1121 (1965).

[9]G. Peano, Math. Ann. 32, 455 (1888).

[10]M. Bocher, Am. J. Math. 24, 311 (1902)

[11]H. F. Baker, Proc. London Math. Soc. Ser. 2 2, 293 (1904).

[12]L. A. Pipes, in *Modern Mathematics for the Engineer*, edited by E. F. Beckenbach (McGraw-Hill, New York, 1953), Chap. 13.

[13]R. A. Frazer, W. J. Duncan, and A. R. Collar, *Elementary Matrices* (Cambridge University Press, London, 1957).

[14]G. Hamel, Math. Ann. 73, 371 (1912).

[15]O. Haupt, Math. Ann. 76, 67 (1914).

[16]J. C. Slater, Phys. Rev. 45, 794 (1934); 87, 807 (1952).

[17]W. Shockley, Phys. Rev. 56, 317 (1939).

[18]H. M. James, Phys. Rev. 76, 1602 (1949); 76, 1611 (1949).

[19]F. Seitz, *Modern Theory of Solids* (McGraw-Hill, New York, 1940), Chap. 8.

[20]H. A. Kramers, Physica (Utrecht) 2, 483 (1935).

[21]L. Brillouin, *Wave Propagation in Periodic Structures* (Dover, New York, 1953), Chaps. IX and X.