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C.H. Hodges

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Van Hove singularities and continued fraction coefficients

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VAN HOVE SINGULARITIES AND CONTINUED FRACTION COEFFICIENTS

C. H. HODGES

C.N.R.S., Groupe des Transitions de Phases,
B.P. 166, 38042 Grenoble Cedex, France

Résumé. — On établit un rapport entre les singularités internes de Van Hove dans une bande et le comportement asymptotique des coefficients de la fraction continue qui décrit la densité d'états de cette bande. Ainsi, on peut démontrer que les coefficients oscillent autour de leurs bornes infinies avec une fréquence liée à la position de la singularité dans la bande, résultat déjà obtenu empiriquement par Gaspard et Cyrot-Lackmann. En outre, la méthode employée ici permet de déduire l'amplitude, la phase et la loi d'amortissement de ces oscillations.

Abstract. — A relation is derived between the internal Van Hove singularities in a band and the asymptotic behaviour of the coefficients of the continued fraction which represents the density of states. Thus one may show that these coefficients oscillate about their infinite limit values with a frequency related to the position of the singularity within the band, a result first obtained empirically by Gaspard and Cyrot-Lackmann. The present method enables one to derive in addition the amplitude, phase and decay law of these oscillations.

The continued fraction [1] provides a powerful method of representing or approximating densities of states (e.g. for electrons or phonons) in periodic or aperiodic systems, without the necessity of calculating individual eigenvalues and eigenfunctions. It expresses the Green function of the system, whose imaginary part gives the density of states, in terms of real coefficients a_n, b_n ([1]), which may be calculated from a knowledge of the moments of the density of states [2] or by a process of tridiagonalising the Hamiltonian [3]. This method is applicable to a Hamiltonian (or dynamic matrix), expressed in a local, tight-binding representation, where the spectrum of eigenvalues is bounded and forms a band. It has recently been widely applied to the study of d bands in transition metals, both in the bulk and at the surface [e.g. 4, 5].

For an infinite (or semi-infinite) system, as $n \to \infty$ the coefficients a_n and b_n tend to limits a_∞, b_∞, which are related to the band extrema [3]. This permits the evaluation of the *tail* of the continued fraction which would give a smooth, continuous, semi-elliptical density of states. Structure is imposed on this density of states by the deviation for finite n of the a_n, b_n from

their asymptotic limits a_∞, b_∞. In particular, it is observed that internal Van Hove singularities in the band are related to the way in which a_n, b_n approach their limits. Gaspard and Cyrot-Lackmann found empirically [2] by studying particular cases in three dimensions that the deviations

$$a'_n = a_n - a_\infty , \quad b'_n = b_n - b_\infty$$

oscillate with a frequency related to the position E_s of the singularity and decay asymptotically at a rate governed by the sharpness of the singularity. Pottier has shown [6] how to derive this relation by treating the deviations a'_n, b'_n as a perturbation on the semi-infinite chain $a_n = a_\infty$, $b_n = b_\infty$. Using a similar sort of idea, I shall show how to prove this result directly and very simply from the relations defining the continued fraction, and shall also derive quite generally the precise form of the asymptotic decay and its amplitude. I shall confine myself to a consideration of internal singularities in three dimensional structures.

As a function of complex energy z, the continued fraction is defined by :

$$R(z) = b_0^2/x_0$$
$$x_0 = (z - a_0) - b_1^2/x_1$$
$$x_1 = (z - a_1) - b_2^2/x_2, \text{ etc.}$$
$$x_n = (z - a_n) - b_{n+1}^2/x_{n+1}, \text{ etc.} \tag{1}$$

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([1]) In this article, the notation of reference [3] will be followed as far as possible. Note that the coefficient b_n of reference [2] is equal to the square of b_n in reference [3].

The denominators $x_n(z)$ have the analytic properties :

$$|x_n(z)| \to \infty \quad \text{as} \quad |z| \to \infty$$

$$x_n(z^*) = x_n(z)^*$$

$$\text{Im } x_n > 0 \quad \text{if} \quad \text{Im } z > 0 . \qquad (2)$$

This gives $R(z)$, which is either the trace of, or a local diagonal matrix element of the Green function, the conventional analytic properties. In particular the density of states $N(E)$ which is positive is given by, [3],

$$N(E) = - \pi^{-1}[\text{Im } R(z)]_{z=E+0i} =$$

$$= \pi^{-1}[\text{Im } R(z)]_{z=E-0i} . \qquad (3)$$

The tail of the continued fraction may be *summed* by solving (1) in the asymptotic *limit* where $a_n = a_\infty$, $b_n = b_\infty$ and $x_n = x_{n+1} = x$ [3]. For energies lying within the band, $a_\infty - 2 b_\infty < E < a_\infty + 2 b_\infty$, x is complex and given by

$$x = b_\infty \, e^{i\varphi}$$

$$\varphi = \arccos \left(\frac{E - a_\infty}{2 b_\infty} \right), \quad - \pi < \varphi < \pi . \qquad (4)$$

The two solutions of (4) are chosen to give the correct analytic properties (2). Thus

$$\text{for} \quad z = E + 0i , \qquad 0 < \varphi < \pi$$

and

$$\text{for} \quad z = E - 0i , \qquad - \pi < \varphi < 0 .$$

The relation between the Van Hove singularities and the continued fraction coefficients may be deduced by linearizing (1) in the asymptotic *region*, i.e. where the deviations a'_n, b'_n and $x'_n = x_n - x$ are small, *but n is finite*. To first order in these deviations, one obtains :

$$x'_n = - a'_n - 2 \, e^{-i\varphi} b'_{n+1} + e^{-2i\varphi} x'_{n+1} , \qquad (5)$$

and its solution with the boundary condition $x'_\infty = 0$

$$x'_n = - \sum_{m=0}^{\infty} e^{-2mi\varphi}(a'_{n+m} + 2 \, e^{-i\varphi} b'_{n+m+1}) . \qquad (6)$$

Thus for $l > n$ and n in the asymptotic region :

$$a'_l = - (2 \pi)^{-1} \int_{-\pi}^{+\pi} x'_n(\varphi) \, e^{(2l-2n)i\varphi} \, d\varphi$$

$$b'_l = - (4 \pi)^{-1} \int_{-\pi}^{+\pi} x'_n(\varphi) \, e^{(2l-2n-1)i\varphi} \, d\varphi . \qquad (7)$$

The asymptotic behaviour of a'_l, b'_l ($l \gg n$) will be determined by the singularities in x'_n, which, since n is finite, must be at same energy as those of $R(z)$. Thus x'_n is singular at

$$\varphi = \varphi_s = \arccos \left(\frac{E_s - a_\infty}{2 b_\infty} \right)$$

and asymptotically a'_l, b'_l oscillate with a factor

$$\cos (2 \, l\varphi_s) = (- 1)^l \cos w_s \, l$$

where

$$w_s = 2 \arcsin \left(\frac{E_s - a_\infty}{2 b_\infty} \right) . \qquad (8)$$

This is Gaspard's and Cyrot-Lackmann's result [2].

To determine the amplitude and rate of the asymptotic decay, it is necessary to relate the singularities in x'_n to those of $R(z)$. For a three dimensional Van Hove singularity $R(z)$ has a singular part

$$\pm A\pi(E_s - z)^{1/2} \quad \text{or} \quad \pm A\pi(z - E_s)^{1/2}$$

as may be verified from eq. (3), A being the strength of the singularity. Using eq. (1), R can be written as a function of $x_n = x + x'_n$ and expanded thus :

$$R = R_n(x + x'_n) \simeq R_n(x) + \left(\frac{dR}{dx_n} \right) x'_n + \cdots \quad (9)$$

where

$$\frac{dR}{dx_n} = - \prod_{m=0}^{n} [b_m^2/x_m^2]_{x_n=x} . \qquad (10)$$

For finite n, since x is smooth, R_n and dR/dx_n are also smooth, and the singular part of R is therefore contained in x'_n. In the asymptotic limit $l \to \infty$, the Fourier transform eq. (7) is dominated by the square root singularity in x'_n which gives an $l^{-3/2}$ behaviour. One finds in this limit :

$$a'_l \to Fl^{-3/2} \cos (2 \, l\varphi_s + \eta)$$

$$b'_l \to \tfrac{1}{2} Fl^{-3/2} \cos (2 \, l\varphi_s - \varphi_s + \eta) \qquad (11)$$

where

$$F \, e^{i\eta} = e^{i\theta} \tfrac{1}{2} AC \, | \, \pi b_\infty \sin \varphi_s \, |^{1/2} \qquad (12)$$

and :

$$C = \frac{x_0^2}{b_0^2} L_{n\to\infty}^t \left[\prod_{m=1}^{n} \left(\frac{x_m}{x} \frac{b_\infty}{b_m} \right)^2 \right]_{\varphi=\varphi_s} . \qquad (13)$$

In eq. (12) θ takes the values $\pi/4$, $- \pi/4$, $3 \pi/4$, $- 3 \pi/4$ corresponding to the four types of Van Hove singularity in three dimensions, S_2, minimum, S_1, maximum [7], respectively. Note the convergence of the constant C in (13) with increasing n.

Relation (11) has been tested for the simple cubic s-band studied by Gaspard and Cyrot-Lackmann (the ferromagnetic case of ref. [2]). Extrapolating the coefficients b_l given by these authors enables an estimate of C, the amplitude F and phase η. The strength A of the internal saddle point singularities has been given by Cyrot-Lackmann [8] for the simple cubic s-band. In figure 1, the deviation

$$[(b_l/b_\infty)^2 - 1] \, l^{3/2}$$

obtained from the calculated values of b_l^2, [2], is compared to that given by eq. (11)-(13). This figure
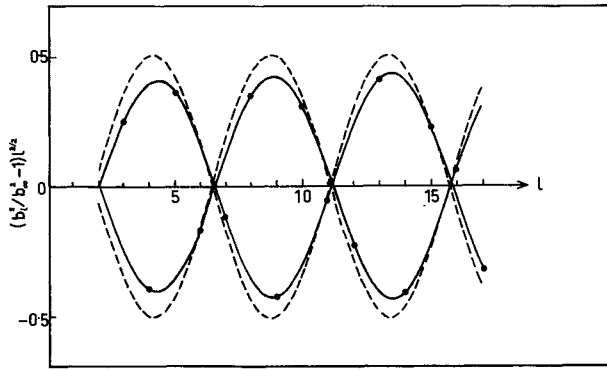
FIG. 1. — Shows the oscillatory behaviour of $(b_l^2/b_\infty^2 - 1)\, l^{3/2}$. The points (interpolated by the full line) are calculated using the values of b_l given in ref. [2]. The dashed line represents the asymptotic behaviour given by eq. (11)-(13) of the text. The amplitude and phase of the oscillations are slowly approaching their asymptotic values with increasing l.

indicates that for $l < 17$, the deviation has not yet reached its exact asymptotic amplitude and phase, but that the general $l^{-3/2}$ decay law is well obeyed.

In this work, the case of 2 and 1 dimensional internal singularities for which $R(z)$ has a divergent, logarithmic or inverse square root behaviour, has not been considered. Neither have singularities at the band edge E_0 when the density of states has the more general form $(E_0^2 - E^2)^\nu$ with $\nu \neq 1/2$. For this latter

case, the deviations a_l', b_l' do not oscillate since in eq. (11) $\varphi_s = 0$ or π. For such singularities Gaspard and Cyrot-Lackmann [2] showed b_l^2 to have the form $(0.25 - \nu^2)\, b_\infty^2/l^2$ for large l. If ν is close to $1/2$, it is not difficult to show that the present method leads to the same result.

Some final remarks may be made concerning the use of eq. (11) to extrapolate the continued fraction coefficients. Since this equation applies to the linearized regime, the effect of different singularities will be a sum of terms of the type (11) with different values of φ_s, F and η. If the number of singularities is not too large, one might try to fit a series of coefficients c_n by a sum over singularities α

$$c_n = \sum_\infty F_\alpha \cos\left(n\varphi_{s,\alpha} + \eta_\alpha\right) \qquad (14)$$

where

$$c_n = l^{3/2}\, a_l' \qquad \text{for} \qquad n = 2\,l\,,$$

and

$$c_n = 2\, l^{3/2}\, b_l' \qquad \text{for} \qquad n = 2\,l - 1\,.$$

Whether such a scheme would be feasible for a case of physical interest remains to be seen.

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