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Analytic properties of the lattice Green function

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Abstract. The theory of functions of a complex variable is applied to show that the lattice Green function $G_d(t; \boldsymbol{r})$ is an analytic function of the variable t, except when t is associated with a critical point. Here $\boldsymbol{r}$ denotes the position and t is the variable which represents the square of the frequency in lattice vibration problems, the energy in simplified problems of electron conduction and in spin wave theory. Singular behaviour of $G_d(t; \boldsymbol{r})$ is given for t around its singular points ω_c for the case where ω_c are associated with the nondegenerate critical points. For the one dimensional system, the singular behaviour is also given for the degenerate critical points. Possibility of cancellation of the singular behaviour is suggested for some of the sites $\boldsymbol{r}$. The singular behaviour derived for Im $G_d(t; 0)$ is the same as that given by Van Hove.

1. Introduction

We consider a regular lattice. The lattice Green function is defined as the solution of the difference equation of the form

$$tG_d(t; \boldsymbol{r}) - \sum_{\boldsymbol{a}} J_{\boldsymbol{a}} G_d(t; \boldsymbol{r}+\boldsymbol{a}) = \delta_{\boldsymbol{r},0} \tag{1.1}$$

where t is a complex variable, $\boldsymbol{r}$ denotes a lattice site, and $\boldsymbol{a}$ are vectors from the lattice site $\boldsymbol{r}$ to its neighbours. d denotes 1, 2, or 3 according as the lattice is one, two, or three dimensional. The boundary value of $G_d(t; \boldsymbol{r})$ is zero when $|\boldsymbol{r}| \to \infty$. The solution is of the form

$$G_d(t; \boldsymbol{r}) = \frac{1}{v_d} \int_\Omega \mathrm{d}\boldsymbol{k} \frac{\exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})}{t - \omega_d(\boldsymbol{k})} \tag{1.2}$$

where the integral is taken over the first or first several Brillouin zones in $\boldsymbol{k}$ space and the denominator v_d denotes the zone volume. $\omega_d(\boldsymbol{k})$ is given by

$$\omega_d(\boldsymbol{k}) = \sum_{\boldsymbol{a}} J_{\boldsymbol{a}} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{a}) \tag{1.3}$$

which is a periodic function of $\boldsymbol{k}$; the periods are the reciprocal lattice vectors $\boldsymbol{K}$, which satisfy $\boldsymbol{K} \cdot \boldsymbol{a} = 2\pi$ times an integer for all $\boldsymbol{a}$.

The lattice Green function $G_d(t; \boldsymbol{r})$ defined above occurs in the simplified problems of lattice vibrations (see eg equations (3.2) and (3.3) in a review article of Lifshitz and Kosevich 1966). In the article of Lifshitz and Kosevich (1966), variable ϵ is used in place of t and the notation $\omega_0(\boldsymbol{k})^2$ is used in place of the present $\omega_d(\boldsymbol{k})$. When we consider

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the problems within the band, $\omega^2 - \mathrm{i}\epsilon$ appears in the place of the variable t, where ω is the frequency of the vibration and ϵ is an infinitesimal positive number. The function $G_d(t; \boldsymbol{r})$ occurs also in simplified treatments of electron conduction and in the theory of spin wave scattering of the Heisenberg magnet, when t is related to the energy (see eg Koster and Slater 1954, and Wolfram and Callaway 1963). The present status of the theory of the function $G_d(t; \boldsymbol{r})$ is described in a recent review of Katsura *et al* (1971).

The imaginary part of the value at the origin of the lattice Green function, $\mathrm{Im}\, G_d(s - \mathrm{i}\epsilon; 0)$, is the level density $g(s)$ of the system of harmonically coupled oscillators

$$g(s) = \frac{1}{\pi} \mathrm{Im}\, G_d(s - \mathrm{i}\epsilon; 0) \tag{1.4}$$

where s takes on real values and ϵ is an infinitesimal positive number. General properties of the level density $g(s)$ have been discussed by Van Hove (1953) in terms of behaviours of the surface of constant $\omega_d(\boldsymbol{k})$ in $\boldsymbol{k}$ space. In the present paper, we present a general discussion of $G_d(t; \boldsymbol{r})$ as a complex function of complex t on the basis of the general theory of a complex variable. The basic assumption is that $\omega_d(\boldsymbol{k})$ occurring in (1.2) is an analytic function of each of the components of $\boldsymbol{k}$, say k_x, k_y, as well as k_z for the three dimensional case, when we assume complex values for these variables. This assumption is satisfied for $\omega_d(\boldsymbol{k})$ defined by (1.3) if $J_{\boldsymbol{a}}$ is of finite range: for example, if there exists a distance R such that

$$J_{\boldsymbol{a}} = 0 \qquad \text{if } |\boldsymbol{a}| > R. \tag{1.5}$$

We notice that the lattice Green functions for two and three dimensional lattices are integrals of the ones for one and two dimensional lattices, respectively. With this observation, we first investigate the one dimensional case in detail, and then proceed to the two and three dimensional cases. The purposes of the following three sections are to give a proof that $G_d(t; \boldsymbol{r})$ is analytic with respect to t when t is not associated with the critical point $\boldsymbol{k}_c$ where $t = \omega_d(\boldsymbol{k}_c)$ and $\partial\omega_d(\boldsymbol{k}_c)/\partial\boldsymbol{k}_c = 0$. §§ 2, 3 and 4 are devoted to the linear, square, and cubic lattices, respectively. In § 5, the singular behaviour due to the nondegenerate critical point is given for $G_d(t; \boldsymbol{r})$. For a one dimensional lattice, the singular behaviour due to the degenerate critical point is given in § 2 and the Appendix. § 6 is for conclusion.

In the general problems of lattice vibrations, we meet with a more complex lattice Green function (eg Maradudin *et al* 1958 and Maradudin 1965). The generalization of our results to that case is discussed in § 6.

2. One dimensional lattice

We consider a linear chain with equally spaced lattice sites. By using the spacing of the lattice sites as the unit of length, the lattice Green function for this system is given by

$$G_1(t; n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}z \frac{\cos nz}{t - \omega_1(z)} \tag{2.1}$$

where the variable t takes on complex values and n is an integer.

By definition (1.3), $\omega_1(z)$ is a periodic function of z with period 2π, and so is the integrand of (2.1). Hence the limits of the integration $-\pi$ and π may be replaced by an arbitrary angle σ and $\sigma + 2\pi$. The function $\omega_1(z)$ is assumed to be an analytic function of z for complex variable z. The integrand itself is, therefore, an analytic function of z except at the poles which can occur at the zeros of $t-\omega_1(z)$. We shall denote the zeros as z_0

$$t-\omega_1(z_0) = 0 \tag{2.2}$$

or

$$z_0 = \omega_1^{-1}(t). \tag{2.3}$$

For a real or a complex value of t, some of z_0 will be real and some others will be complex.

First we consider the case when $\operatorname{Im} z_0$ is nonzero for all z_0. The analytic function $t = \omega_1(z_0)$ and its inverse $z_0 = \omega_1^{-1}(t)$ induce continuous mappings. Hence when t is in a small region Δ around the given value of t, $\operatorname{Im} z_0$ remains nonzero (cf figure 1(a) and (b)). In that case, the integrand of (2.1) and its derivative with respect to t are analytic functions of both variables t and z for t inside of Δ and z on the path of the integration (2.1), and we confirm that $G(t; n)$ is analytic with respect to t at its given value (see eg Whittaker and Watson 1935).

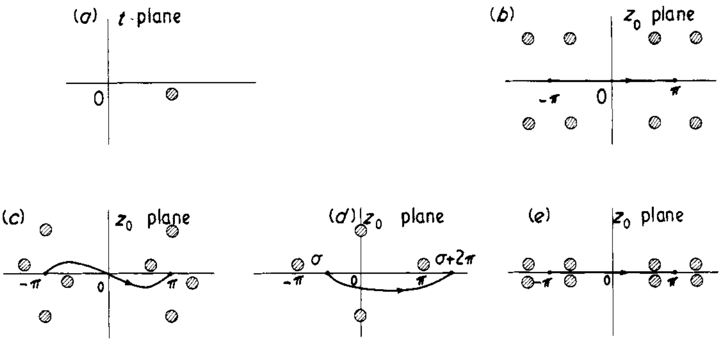

Figure 1. (a) Small region Δ in the t plane and (b)–(e) various cases of its mapping in the z_0 plane and the path of integral from $-\pi$ to π or from σ to $\sigma+2\pi$ for (2.1).

In the second place, we consider the case where some of z_0 occur on the real axis or in its immediate neighbourhood and they are isolated by a nonzero distance from each other. Then we can deform the path of the integration from the straight line to a curved line which is separated by a nonzero distance from all the z_0 (cf figure 1(c)). When $-\pi$ and π are in an immediate neighbourhood of one of z_0, we choose the starting point of the integration to an angle σ which is not near to any of z_0 (cf figure 1(d)). By such a choice of the path of integration, we confirm that the integral is analytic for this case also, where the same argument as in the preceding paragraph is used.

Now the cases excluded from the above discussions are the cases when two or more z_0 appear on the real axis or in its immediate neighbourhood with an infinitesimal distance between them; that is $t = \omega_1(z_0)$ and $\omega_1(z_0+\delta)-\omega_1(z_0) = 0$ where $\delta \simeq 0$ (cf figure 1(e)). As $\omega_1(z)$ is an analytic function we have

$$t = \omega_1(z_0) \qquad \frac{\mathrm{d}}{\mathrm{d}z_0}\omega_1(z_0) = 0 \tag{2.4}$$

for this case. This is the only case when we cannot prove that $G_1(t; n)$ is analytic with respect to t. The t given by the first equation of (2.4) will be denoted by ω_c when the latter equation is satisfied by a real value of z_0.

Let a real z_0 be a zero of νth order of the denominator of (2.1) and $\nu \geqslant 2$, when $t = \omega_c$. Then in the neighbourhood of z_0 there are ν values of z for which $\omega_1(z)$ is equal to t if $t - \omega_c \simeq 0$ by a well known theorem of the theory of analytic functions (see eg Ahlfors 1953). In fact, when $t - \omega_c \simeq 0$, the zero of

$$t - \omega_1(z) = (t - \omega_c) + a(z - z_0)^\nu + \mathrm{O}\{(z - z_0)^{\nu+1}\}$$

occurs at

$$z = z_0 + ([\omega_c - t + \mathrm{O}\{(z - z_0)^{\nu+1}\}]/a)^{1/\nu} = z_0\{(\omega_c - t)/a\}^{1/\nu} + \mathrm{O}\{(\omega_c - t)^{2/\nu}\}$$

where a is a nonzero constant. For a suitable choice of the $t - \omega_c$, some of the zeros appear above the real axis and some below the real axis if $\mathrm{Im}\, t \simeq 0$. If we deform the path of integration to a nonzero distance from z_0, the integral becomes an analytic function of t, but we have an additional contribution from the poles which were passed through in the deformation of the path. If one deforms the path to be above the real axis, one obtains the following contribution from each pole just above the real axis:

$$\mathrm{i}\frac{\cos nz_0}{a^{1/\nu}\nu(\omega_c - t)^{1-1/\nu}}[1 + \mathrm{O}\{(\omega_c - t)^{1/\nu}\}] \tag{2.5}$$

or

$$-\mathrm{i}\frac{\sin nz_0 \sin[n\{(\omega_c - t)/a\}^{1/\nu} + \mathrm{O}\{(\omega_c - t)^{2/\nu}\}]}{a^{1/\nu}\nu(\omega_c - t)^{1-1/\nu}[1 + \mathrm{O}\{(\omega_c - t)^{1/\nu}\}]} \tag{2.6}$$

according as $\cos nz_0 \neq 0$ or $\cos nz_0 = 0$, where $\mathrm{Im}\{(\omega_c - t)/a\}^{1/\nu} > 0$. In order to obtain the singular behaviour at $t \simeq \omega_c$, we have to take a summation of (2.5) or (2.6) over all z_0 which satisfy (2.4) for a given value of $t = \omega_c$. In particular we notice that, if (2.4) is satisfied at a point z_0, it is also satisfied at $-z_0$ for our lattice. When the contributions for z_0 and $-z_0$ are summed, (2.5) contributes twice that expression but (2.6) cancels exactly. That means we do not have a singularity if $\cos nz_0 = 0$ is satisfied even if (2.4) is satisfied.

We conclude this section by the following theorem: $G_1(t; n)$ is an analytic function of t except when there exists such a real z_0 that the equations $\omega_1(z_0) = t$ and $\omega_1'(z_0) = 0$ as well as $\cos nz_0 \neq 0$ are satisfied. If such is the case, the singular term is obtained by taking a summation of the contributions (2.5) over all νth roots $\{(\omega_c - t)/a\}^{1/\nu}$ with a positive imaginary part for all z_0 satisfying (2.4). An alternative expression for (2.5) is given in the Appendix for even values of ν.

For real z_0, $t = \omega_1(z_0)$ is real. Hence $G_1(t; n)$ can be singular at t on the real axis and is always analytic if $\mathrm{Im}\, t$ is not zero.

3. Square lattices

The lattice Green function for the square (rectangular) lattice is expressed as an integral

$$G_2(t; m, n) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}y \cos my G_1(t; n; y) \tag{3.1}$$

where the integrand is the lattice Green function for a one dimensional system

$$G_1(t; n; y) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}z \cos nz \frac{1}{t - \omega_2(y, z)} \tag{3.2}$$

where m and n are integers. The spacings of the layers occupied by the lattice sites are used as the units of length for the y and z directions, respectively. By using the arguments in the preceding section, we see that $G_1(t; n; y)$ defined by (3.2) is analytic with respect to t as well as with respect to y, except when a real value z_0 exists such that

$$t = \omega_2(y, z_0) \qquad \frac{\partial \omega_2(y, z_0)}{\partial z_0} = 0 \tag{3.3a}$$

and $\cos nz_0 \neq 0$.

We now consider the integral (3.1) for a fixed t inside a neighbourhood Δ of a given point on the t plane. If all the singular points of the function $G_1(t; n; y)$ as a function of y are either complex with a nonzero imaginary part or are isolated when they are on the real axis or in its immediate neighbourhood, one can choose the path of integration in such a way that the integrand of (3.1) and its derivative with respect to t are analytic functions of both variables t and y for t inside of Δ and y on the path of integration. Then one confirms as in the preceding section that the integral (3.1) is analytic as a function of t in the neighbourhood of the point in the t plane under consideration. The only points t at which the integral cannot be shown to be analytic are the cases where the two or more singularities of $G_1(t; n; y)$ as a function of y exist with an infinitesimal separation δ on the real axis or in its immediate neighbourhood. For such a case, we shall assume that those singularities occur at y_0 and $y_0+\delta$. The conditions that the integral $G_1(t; n; y)$ given by (3.2) is singular at $y = y_0$ are given by (3.3a). The corresponding condition for the point $y_0+\delta$ is the existence of real z_1 such that

$$t = \omega_2(y_0+\delta, z_1) \qquad \frac{\partial \omega_2(y_0+\delta, z_1)}{\partial z_1} = 0 \tag{3.3b}$$

and $\cos nz_1 \neq 0$.

Here we shall assume that y_0 and $y_0+\delta$ are the only singular points, on the real axis or in its neighbourhood, of $G_1(t; n; y)$, and that real z_0 and z_1 satisfying (3.3a) and (3.3b) are uniquely determined. Furthermore we assume that the z_0 and z_1 occurring in (3.3) are different from each other. In that case, we divide $G_1(t; n; y)$ into two parts as follows:

$$G_1(t; n; y) = G_1^{(1)}(t; n; y) + G_1^{(2)}(t; n; y) \tag{3.4}$$

$$G_1^{(1)}(t; n; y) = \frac{1}{2\pi} \int_{-\pi}^{(z_0+z_1)/2} dz \frac{\cos nz}{t - \omega_2(y, z)} \tag{3.5}$$

$$G_1^{(2)}(t; n; y) = \frac{1}{2\pi} \int_{(z_0+z_1)/2}^{\pi} dz \frac{\cos nz}{t - \omega_2(y, z)} \tag{3.6}$$

where we assume $z_0 < z_1$ without loss of generality. The first integral (3.5) has a singularity at $y = y_0$ and the second (3.6) at $y = y_0+\delta$. When (3.4) is substituted into (3.1), one finds that the contributions due to each of (3.5) and (3.6) and hence the total (3.1) are analytic with respect to t in the neighbourhood of the t under consideration.

We cannot show that $G_2(t; m, n)$ is analytic if $z_0 = z_1$. Then (3.3) reduces to

$$t = \omega_2(y_0, z_0) \qquad \frac{\partial \omega_2(y_0, z_0)}{\partial y_0} = 0 \qquad \frac{\partial \omega_2(y_0, z_0)}{\partial z_0} = 0 \tag{3.7}$$

and $\cos nz_0 \neq 0$. The above analysis is concluded by the theorem that, if and only if there exist a set of real y_0 and real z_0 which satisfy (3.7), $t = \omega_2(y_0, z_0)$ is a singular point of the lattice Green function $G_2(t; m, n)$.

When $\cos my_0 = 0$, we interchange the roles of y and z in the above discussion. Then one concludes that the t is not a singularity even if (3.7) is satisfied for a set of values of y_0 and z_0.

The argument given at the end of the preceding section is applied to show that $G_2(t; m, n)$ can be singular only at t on the real axis and is analytic if $\text{Im}\, t$ is not equal to zero.

4. Cubic lattices

We express the lattice Green function for the cubic (orthorhombic) lattices as follows:

$$G_3(t; l, m, n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}x \cos lx G_2(t; m, n; x) \tag{4.1}$$

where

$$G_2(t; m, n; x) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \mathrm{d}y \int_{-\pi}^{\pi} \mathrm{d}z \frac{\cos my \cos nz}{t - \omega_3(x, y, z)} \tag{4.2}$$

and l, m and n are integers.

When one proceeds as in the preceding section, one first sees that $G_3(t; l, m, n)$ can be singular only if

$$\begin{aligned} t &= \omega_3(x_0, y_0, z_0) \qquad & \frac{\partial\omega_3(x_0, y_0, z_0)}{\partial y_0} = \frac{\partial\omega_3(x_0, y_0, z_0)}{\partial z_0} = 0 \\ t &= \omega_3(x_0+\delta, y_1, z_1) \qquad & \frac{\partial\omega_3(x_0+\delta, y_1, z_1)}{\partial y_1} = \frac{\partial\omega_3(x_0+\delta, y_1, z_1)}{\partial z_1} = 0 \end{aligned} \tag{4.3}$$

and $\cos my_0 \neq 0$, $\cos nz_0 \neq 0$, $\cos my_1 \neq 0$ and $\cos nz_1 \neq 0$. If y_0 and y_1 are different, we divide the integral (4.2) over y into two parts and find that $G_3(t; l, m, n)$ must be analytic etc by the same argument as in the preceding section. As a result, we conclude that $G_3(t; l, m, n)$ is singular at t only if there exists a set of real x_0, y_0 and z_0 such that

$$\begin{gathered} t = \omega_3(x_0, y_0, z_0) \\ \frac{\partial\omega_3(x_0, y_0, z_0)}{\partial x_0} = \frac{\partial\omega_3(x_0, y_0, z_0)}{\partial y_0} = \frac{\partial\omega_3(x_0, y_0, z_0)}{\partial z_0} = 0 \end{gathered} \tag{4.4}$$

and $\cos lx_0 \neq 0$, $\cos my_0 \neq 0$ and $\cos nz_0 \neq 0$.

By the argument given at the end of § 2, one sees that the singularities of $G_3(t; l, m, n)$ occur only at real values of t.

5. Nondegenerate critical points

The conclusion of the preceding sections is that the lattice Green function $G(t; \boldsymbol{r})$ is analytic if $\text{Im}\, t$ is finite. If ω_c is one of the singularities, it is associated with a $\boldsymbol{k}_c$ with real components satisfying

$$\omega_c = \omega_d(\boldsymbol{k}_c) \qquad \frac{\partial\omega_d(\boldsymbol{k}_c)}{\partial\boldsymbol{k}_c} = 0. \tag{5.1}$$

(5.1) represents either (2.4), (3.7), or (4.4). A point $\boldsymbol{k}_c$ for which $\partial\omega_d(\boldsymbol{k}_c)/\partial\boldsymbol{k}_c = 0$ is satisfied is called a critical point. It is called a 'nondegenerate' critical point if the determinant of the second derivatives, the hessian, of $\omega_d(\boldsymbol{k}_c)$ is not zero.

We shall give the behaviour of $G_d(t; \boldsymbol{r})$ at t near ω_c which is associated only with nondegenerate critical points. We shall denote the total number of those critical points $\boldsymbol{k}_c$ for which $\omega_d(\boldsymbol{k}_c)$ is equal to the given value ω_c, by n, and the n values of $\boldsymbol{k}_c$ by $\boldsymbol{k}_c^{(1)}$, $\boldsymbol{k}_c^{(2)}, \dots$ and $\boldsymbol{k}_c^{(n)}$. We divide the total region Ω of the integration in (1.2) into small regions Δ_i around $\boldsymbol{k}_c^{(i)}$, and the remaining $\Omega' = \Omega - \Sigma_{i=1}^{n} \Delta_i$:

$$G_d(t; \boldsymbol{r}) = \frac{1}{v_d}\left(\int_{\Omega'} \mathrm{d}\boldsymbol{k}\frac{\exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})}{t-\omega_d(\boldsymbol{k})} + \sum_{i=1}^{n} \int_{\Delta_i} \mathrm{d}\boldsymbol{k}\frac{\exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})}{t-\omega_d(\boldsymbol{k})}\right). \tag{5.2}$$

If t is so near to ω_c that $|t-\omega_d(\boldsymbol{k})|$ is nonzero as long as $\boldsymbol{k}$ is outside of the small regions Δ_i, we confirm that the first term on the right hand side is analytic with the aid of an argument similar to that given in the preceding sections.

In evaluating the contributions from the integral over Δ_i, we expand $\omega_d(\boldsymbol{k})$ in powers of $\boldsymbol{k}-\boldsymbol{k}_c^{(i)}$, choose suitable coordinates and write as

$$\omega_d(\boldsymbol{k}) = \omega_c - \sum_{j=1}^{d} a_j\xi_i^2 + \mathrm{O}(\xi^3) \tag{5.3}$$

(Van Hove 1953). The coefficients a_j may be positive or negative. The total number of positive a_j is called the index of the critical point of $\omega_d(\boldsymbol{k})$ at $\boldsymbol{k}_c^{(i)}$ and is denoted by $\lambda\,(0 \leqslant \lambda \leqslant d)$. When ω_c is the maximum value of $\omega_d(\boldsymbol{k})$, $\lambda = d$, and when ω_c is the minimum, $\lambda = 0$. If $2 \leqslant d$ and $0 < \lambda < d$, ω_c corresponds to a saddle point of the plane or hyperplane $\omega_d(\boldsymbol{k})$ as a function $\boldsymbol{k}$. The integrations with respect to ξ_j are taken over the region Δ_i. The singular behaviours are expressed in terms of the parameters v_d, $A_d = \Pi_{j=1}^{d} |a_j|^{1/2}$ and the jacobian J of the variable transformation from $\boldsymbol{k}-\boldsymbol{k}_c^{(i)}$ to ξ_j. The terms C in the following expressions are complex constants.

(i) One dimension:

$$G_1(t; 0) \simeq C + \frac{\mathrm{i}}{\mathrm{i}^\lambda}\frac{\pi J}{A_1 v_1}\frac{1}{(t-\omega_c)^{1/2}} \tag{5.4}$$

where $\lambda = 0$ or 1. $(t-\omega_c)^{1/2}$ denotes the positive square root $(t-\omega_c)^{1/2}$ when $t-\omega_c$ is positive. When t is assumed to be a complex number with negative imaginary part, the argument of $t-\omega_c$ is between 0 and $-\pi$ and that of $(t-\omega_c)^{1/2}$ is chosen between 0 and $-\pi/2$, for the reason of analyticity. It follows that:

$$(t-\omega_c)^{1/2} = \begin{cases} (s-\omega_c)^{1/2} & s > \omega_c \\ -\mathrm{i}(\omega_c - s)^{1/2} & s < \omega_c \end{cases} \tag{5.5}$$

if $t = s - \mathrm{i}\epsilon\ (\epsilon \gtrsim 0)$. When we have only one of each of minimum and maximum values of $\omega_1(\boldsymbol{k})$ where $\lambda = 0$ and 1, respectively, the curves of the real and imaginary parts of the lattice Green function $G_1(s-\mathrm{i}\epsilon; \boldsymbol{r})$ take the same singular characters as figure 2. One notices that (5.4) must be equivalent to (2.5) if $n = 0$ and $v = 2$, where $J = 1$ and $v_1 = 2\pi$. A reduction of (2.5) to the form of (5.4) is given in the Appendix, for the case when v is even.

(ii) Two dimensions:

$$G_2(t; 0, 0) \simeq C + \frac{\pi J}{\mathrm{i}^\lambda A_2 v_2}\ln(t-\omega_c) \tag{5.6}$$

where $\lambda = 0, 1$ or 2. $\ln(t-\omega_c)$ is real when $t-\omega_c$ is positive. If t is complex with negative imaginary part, the imaginary part of $\ln(t-\omega_c)$ is chosen between 0 and $-\pi$ for the analyticity of the function. In particular, one has

$$\ln(t-\omega_c) = \begin{cases} \ln(s-\omega_c) & s > \omega_c \\ \ln(\omega_c - s) - \pi i & s < \omega_c \end{cases} \tag{5.7}$$

if $t = s - i\epsilon (\epsilon \gtrsim 0)$. When we have only one of each of these critical points with $\lambda = 0, 1$ and 2, respectively, we have the same singular characters for the real and imaginary parts of $G_2(s-i\epsilon, r)$ as the curves given in figure 3; those curves were first given by Katsura and Inawashiro (1971).

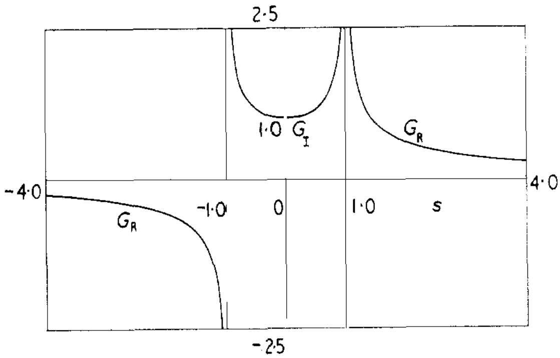

Figure 2. The real and imaginary parts of $G_1(s-i\epsilon; 0)$ for the one dimensional lattice with the nearest neighbour interaction; G_R and G_I denote the real and the imaginary part, respectively.

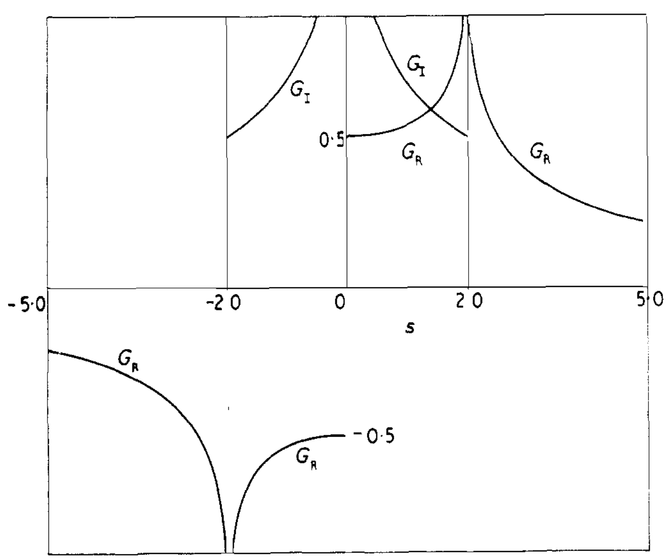

Figure 3. The real and imaginary parts of $G_2(s-i\epsilon; 0, 0)$ for the square lattice with nearest neighbour interaction; G_R and G_I denote the real and the imaginary part, respectively (from Horiguchi *et al* 1971).

(iii) Three dimensions:

$$G_3(t;0,0,0) \simeq C + \frac{\mathrm{i}}{\mathrm{i}^{\lambda}} \frac{2\pi^2 J}{A_3 v_3}(t-\omega_c)^{1/2} \tag{5.8}$$

where $\lambda = 0, 1, 2$ or 3. When we have one of each of the critical points with $\lambda = 0, 1, 2$ and 3, respectively, the curves for the real and imaginary parts of $G_3(s-\mathrm{i}\epsilon; \boldsymbol{r})$ take the same singular characters as given by figure 4.

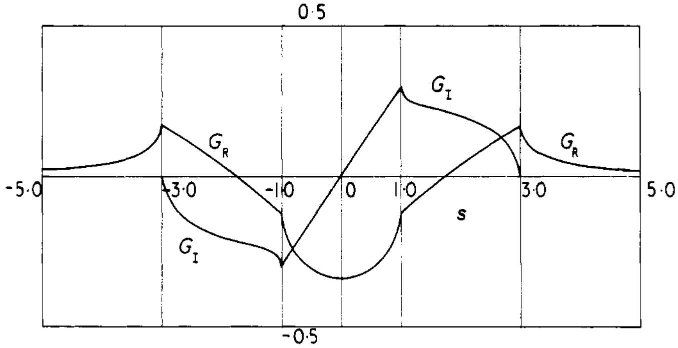

Figure 4. The real and imaginary parts of $G_3(s-\mathrm{i}\epsilon;\ 1, 0, 0)$ for the simple cubic lattice with the nearest neighbour interaction; G_R and G_I denote the real and the imaginary part, respectively (from Horiguchi 1971).

The singular behaviours (5.4), (5.6) and (5.8) due to the critical point $\boldsymbol{k}_c^{(i)}$ are for $G_d(t; \boldsymbol{r} = 0)$. If $\boldsymbol{r} \neq 0$, the right hand sides of these equations must be multiplied by the constant $\exp(\mathrm{i}\boldsymbol{k}_c^{(i)} \cdot \boldsymbol{r})$.

In order to obtain the singular behaviour at a singularity ω_c, a summation must be taken over all the contributions due to the critical points $\boldsymbol{k}_c^{(i)}$ associated with the singular point ω_c. It may happen that the singular behaviour is exactly cancelled. In the preceding sections, we found that if $\cos(\boldsymbol{k}_c \cdot \boldsymbol{r}) = 0$, the critical point does not result in a singularity. In that case, the singular behaviours at $\boldsymbol{k}_c$ and at $-\boldsymbol{k}_c$ are found to cancel with each other exactly; note that $-\boldsymbol{k}_c$ is a critical point if $\boldsymbol{k}_c$ is for lattices with inversion symmetry as considered in the preceding sections. Another example of such cancellation will be discussed in a subsequent paper.

The singular behaviours of the imaginary part of the expressions obtained for $G_2(s-\mathrm{i}\epsilon; 0, 0)$ and $G_3(s-\mathrm{i}\epsilon; 0, 0, 0)$ are in agreement with those given by Van Hove (1953).

6. Conclusion

The discussions of the lattice Green function in the text are given for the linear, square and cubic lattices. For other lattices also, the lattice Green function is expressed as a multiple integral over real variables and the integrand can be regarded as an analytic function of those variables when complex values are assumed to them. Then we can apply the same argument to the integral. It may become necessary in the arguments to recall the fact that the region of the integration is the first one or several Brillouin zones in the reciprocal lattice space and the integrand is a periodic function in that space. In consequence, we reach the same conclusion : the lattice Green function becomes singular, only if the integrand has a pole of second or higher order as a function of each integration variable at a set of real values of the variables.

The singular behaviours due to the nondegenerate critical points are given in § 5. For the one dimensional lattice, the singular behaviours due to the nondegenerate critical points are given in § 2.

Before concluding this paper, we notice that the only assumption in the course of the arguments in the text is that $\omega_d(\boldsymbol{k})$ as a function of each of the components of $\boldsymbol{k}$ is analytic within a region of nonzero width surrounding the real axis. For instance, the arguments are valid even if $\omega_d(\boldsymbol{k})$ has branch points in so far as all of the imaginary parts of the branch points are not equal to zero.

In the general problem of lattice vibrations, we consider a lattice composed of cells involving a number of atoms. The lattice Green function which occurs in that case takes the form

$$G_{\alpha\beta}(t;l\kappa;l'\kappa') = \frac{1}{(M_\kappa M_{\kappa'})^{1/2}} \sum_j \frac{1}{v_d} \int_\Omega \mathrm{d}\boldsymbol{k} \frac{w_\alpha(\kappa|\boldsymbol{k}j) w_\beta^*(\kappa'|\boldsymbol{k}j)}{t-\omega_j(\boldsymbol{k})^2} \times \exp\{\mathrm{i}\boldsymbol{k}\,.\,(\boldsymbol{x}(l\kappa)-\boldsymbol{x}(l'\kappa'))\} \tag{6.1}$$

where $\boldsymbol{x}(l\kappa)$ is the equilibrium position of the κth atom in lth cell, M_κ is the mass of the κth atom, $\omega_j(\boldsymbol{k})$ is the frequency of jth mode with wavevector $\boldsymbol{k}$, and $w_\alpha(\kappa|\boldsymbol{k}j)$ is the αth component of the unit polarization vector of the κth atom for the mode specified by $(\boldsymbol{k}j)$ (see eg equation (2.1.18) of a review article of Maradudin 1965).

We shall assume that $\omega_j(\boldsymbol{k})^2$ and $w_\alpha(\kappa|\boldsymbol{k}j)$ are analytic functions of the components of $\boldsymbol{k}$, when the components take complex values. Then we can apply the arguments given in the text to each of the integrals over $\boldsymbol{k}$ occurring in (6.1). From the analytic behaviour of the integral for each value of j, we obtain the same conclusion as stated above for the total function (6.1). The leading terms of the singular behaviours at the nondegenerate critical points are obtained by using the results of § 5, by introducing the factor appropriate for the critical point and summing the singular behaviours due to different j.

As mentioned above, the conclusion is extended to the cases when $\omega_j(\boldsymbol{k})^2$ and $w_\alpha(\kappa|\boldsymbol{k}j)$ are analytic within a region of nonzero width surrounding the real axis. For instance, the conclusion is valid for the lattice Green function occurring in a problem of the simple cubic diatomic lattice where $\omega_j(\boldsymbol{k})^2$ has branch points with nonzero imaginary part (see eg Maradudin *et al* 1958).

Appendix. Reduction of (2.5) and (2.6) to the form of (5.4)

It is shown in § 2 that the leading term with singular behaviour at $\omega_c = \omega_1(z_0)$ is obtained as the sum of contributions of all the poles around z_0 just above the real axis, or as the sum due to those just below the real axis. The contribution from each pole is given by

$$\pm\mathrm{i}\frac{\cos nz_0}{\nu(\omega_c-t)\{(\omega_c-t)/a\}^{-1/\nu}} \tag{A.1}$$

where the sum must be taken over all different νth roots satisfying

$$\mathrm{Im}\{(\omega_c-t)/a\}^{1/\nu} \gtrless 0. \tag{A.2}$$

The results obtained by adopting the upper and the lower sign, respectively, must be the same. We restrict the following discussion to even values of ν.

If $a < 0$, we shall choose the lower signs and then (A.1) with (A.2) reads as follows:

$$\mathrm{i}\frac{\cos nz_0}{\nu|a|^{1/\nu}(t-\omega_c)^{1-1/\nu}} \tag{A.3}$$

where

$$\mathrm{Im}(t-\omega_c)^{1/\nu} < 0. \tag{A.4}$$

When $a < 0$, $\lambda = 0$ and (A.3) coincides with (5.4).

If $a > 0$, we use the upper signs in (A.1) and (A.2), and we have

$$\mathrm{i}\frac{\cos nz_0}{\nu|a|^{1/\nu}(\omega_c-t)^{1-1/\nu}} \tag{A.5}$$

where

$$\mathrm{Im}(\omega_c-t)^{1/\nu} > 0. \tag{A.6}$$

We notice here that, when $\mathrm{Im}\, t = \mathrm{Im}(t-\omega_c)$ is negative, all the νth roots $(\omega_c-t)^{1/\nu}$ which satisfy (A.6) are obtained by the relation

$$(\omega_c-t)^{1/\nu} = \frac{-1}{\mathrm{i}_\nu}(t-\omega_c)^{1/\nu} \tag{A.7}$$

from the νth roots $(t-\omega_c)^{1/\nu}$ which satisfy (A.4), where $\mathrm{i}_\nu \equiv \exp(\pi \mathrm{i}/\nu)$ and hence $\mathrm{i}_2 = \mathrm{i}$. Substituting (A.7) into (A.5), we obtain

$$\frac{\mathrm{i}}{\mathrm{i}_\nu}\frac{\cos nz_0}{\nu|a|^{1/\nu}(t-\omega_c)^{1-1/\nu}}. \tag{A.8}$$

The singular behaviour of $G_1(t; n)$ at $t \simeq \omega_c = \omega_1(z_0)$ is now given by the sum of (A.8) over all $(t-\omega_c)^{1/\nu}$ satisfying (A.4), for the case of $a > 0$. (A.3) and (A.8) are combined to the form

$$\frac{\mathrm{i}}{(\mathrm{i}_\nu)^\lambda}\frac{\cos nz_0}{\nu|a|^{1/\nu}(t-\omega_c)^{1-1/\nu}} \tag{A.9}$$

where $\lambda = 0$ or 1 according as $a < 0$ or $a > 0$. (A.9) with (A.4) gives (5.4) when $\nu = 2$ and $n = 0$.

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