

Analytic properties of the lattice Green's function

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Abstract. Theory of functions of a complex variable is applied to show that the lattice Green's function  $G_d(t;r)$  is an analytic function of the variable  $t$ , except when  $t$  is associated with a critical point. Singular behaviour of  $G_d(t;r)$  is given for  $t$  around its singular points  $\omega_c$  for the case where  $\omega_c$  is associated with the non-degenerate critical points. For the one-dimensional system, the singular behaviour is given also for the degenerate critical points. Possibility of cancellation of the singular behaviour is suggested for some of the sites  $r$ . The singular behaviour derived for  $\text{Im } G_d(t;0)$  is the same as given by Van Hove.

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## 1. Introduction

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

$$t G_d(t; r) - \sum_a J_a G_d(t; r+a) = \delta_{r,0}, \quad (1.1)$$

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

$$G_d(t; r) = \frac{1}{v_d} \int_{\Omega} dk \frac{e^{ik \cdot r}}{t - \omega_d(k)}, \quad (1.2)$$

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

$$\omega_d(k) = \sum_a J_a e^{ik \cdot a}, \quad (1.3)$$

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

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

$$g(s) = \text{Im } G_d(s - i\epsilon; 0), \quad (1.4)$$

where  $s$  takes on real values and  $\epsilon$  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  $\omega_d(k)$  in  $k$ -space. In the present paper, we present a general discussion of  $G_d(t;r)$  as a complex function of complex  $t$  on the basis of the general theory of a complex variable. The basic assumption is that  $\omega_d(k)$  occurring in (1.2) is an analytic function of each of the components of  $k$ , 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  $\omega_d(k)$  defined by (1.3) if  $J_a$  is of finite range: e.g. if there exists a distance  $R$  such that

$$J_a = 0 \quad \text{if} \quad |a| > R. \quad (1.5)$$

We notice that the lattice Green's 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  $G_d(t;r)$  is analytic with respect to  $t$  when  $t$  is not associated with the critical point  $k_c$  where  $t = \omega_d(k_c)$  and  $\partial\omega_d(k_c)/\partial k_c = 0$ . Sections 2, 3 and 4 are devoted to the linear, square, and cubic lattices, respectively. In section 5, the singular behaviour due to the non-degenerate critical point is given for  $G_d(t;r)$ . For one-dimensional lattice, the singular behaviour due to the degenerate critical point is given in section 2 and the Appendix. Section 6 is for conclusion.

## 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's function for this system is given by

$$G_1(t;n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dz \frac{\cos nz}{t - \omega_1(z)}, \quad (2.1)$$

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  $2\pi$ , and so is the integrand of (2.1). Hence the limits of the integration  $-\pi$  and  $\pi$  may be replaced by an arbitrary angle  $\sigma$  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  $z_0$ :

$$t - \omega_1(z_0) = 0 \quad (2.2)$$

or

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

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  $\text{Im } z_0$  is finite 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  $\Delta$  around the given value of  $t$ ,  $\text{Im } z_0$  remains finite; cf. Fig. 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  $\Delta$  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 e.g., Whittaker and Watson 1935).

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Fig. 1

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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 finite 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 finite distance from all the  $z_0$ 's; cf. Fig. 1(c). When  $-\pi$  and  $\pi$  are in an immediate neighbourhood of one of  $z_0$ 's, we choose the starting point of the integration to an angle  $\sigma$  which is not near to any of  $z_0$ 's; cf. Fig. 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  $\delta = 0$ ; cf. Fig. 1(e). As  $\omega_1(z)$  is an analytic function we have

$$t = \omega_1(z_0) \quad , \quad \frac{d}{dz_0} \omega_1(z_0) = 0 \quad (2.4)$$

for this case. Such 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  $\omega_c$  when the latter equation is satisfied by a real value of  $z_0$ .

Let a real  $z_0$  be a zero of  $v$ th order of the denominator of (2.1) and  $v \geq 2$ , when  $t = \omega_c$ . Then in the neighbourhood of  $z_0$  there are  $v$   $z$  for which  $\omega_1(z)$  is equal to  $t$  if  $t - \omega_c \approx 0$  by a well-known theorem of the theory of analytic functions (see e.g., Ahlfors 1953). In fact, when  $t - \omega_c \approx 0$ , the zero of  $t - \omega_1(z) = (t - \omega_c) + a(z - z_0)^v + 0(z - z_0)^{v+1}$  occurs at  $z = z_0 + [( \omega_c - t + 0(z - z_0)^{v+1} ) / a]^{1/v} = z_0 + [(\omega_c - t) / a]^{1/v} + 0(\omega_c - t)^{2/v}$ , where  $a$  is a non-zero 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  $\text{Im } t \approx 0$ . If we deform the path of integration to a finite 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 the route of the deformation of the path. If one deforms the path to the above of the real axis, one obtains the following contribution from each pole just above the real axis:

$$i \frac{\cos n z_0}{a^{1/v} v (\omega_c - t)^{1-1/v}} \{1 + 0[(\omega_c - t)^{1/v}]\} \quad (2.5)$$

or

$$-i \frac{\sin n z_0 \sin \{n [(\omega_c - t) / a]^{1/v} + 0(\omega_c - t)^{2/v}\}}{a^{1/v} v (\omega_c - t)^{1-1/v} \{1 + 0[(\omega_c - t)^{1/v}]\}} \quad (2.6)$$

according as  $\cos n z_0 \neq 0$  or  $\cos n z_0 = 0$ , where  $\text{Im}[(\omega_c - t) / a]^{1/v} > 0$ . In order to obtain the singular behaviour at  $t = \omega_c$ , 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  $z_0$ , 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 of 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 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  $v$ th roots  $[(\omega_c-t)/a]^{1/v}$  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  $v$ .

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  $\text{Im } t$  is not zero.

### 3. Square lattices

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

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

where the integrand is the lattice Green's function for a one-dimensional system:

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

Here  $m$  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

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

and  $\cos nz_0 \neq 0$ .

We now consider the integral (3.1) for a fixed  $t$  inside a neighbourhood  $\Delta$  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 finite 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  $\Delta$  and  $y$  on the path of integration. Then one confirms as in the pre-

ceding 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  $\delta$  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  $y=y_0$  is given by (3.3a). The corresponding condition for the point  $y_0 + \delta$  is the existence of real  $z_1$  such that

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

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:

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

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

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

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

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

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's 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 finite.

## 4. Cubic lattices

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

$$G_3(t; \ell, m, n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \cos \ell x G_2(t; m, n; x) \quad , \quad (4.1)$$

where

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

and  $\ell$ ,  $m$  and  $n$  are integers.

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

$$\left. \begin{aligned} t = \omega_3(x_0, y_0, z_0) \quad , \quad \frac{\partial \omega_3(x_0, y_0, z_0)}{\partial y_0} = \frac{\partial \omega_3(x_0, y_0, z_0)}{\partial z_0} = 0 \\ t = \omega_3(x_0 + \delta, y_1, z_1) \quad , \quad \frac{\partial \omega_3(x_0 + \delta, y_1, z_1)}{\partial y_1} = \frac{\partial \omega_3(x_0 + \delta, y_1, z_1)}{\partial z_1} = 0 \end{aligned} \right\} (4.3)$$

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  $G_3(t; \ell, m, n)$  must be analytic, etc., by the same argument as in the preceding section. As a result, we conclude that  $G_3(t; \ell, m, n)$  is singular at  $t$  only if there exists a set of real  $x_0$ ,  $y_0$  and  $z_0$  such that

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

and  $\cos \ell x_0 \neq 0$ ,  $\cos my_0 \neq 0$  and  $\cos nz_0 \neq 0$ .

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

### 5. Non-degenerate critical points

The conclusion of the preceding sections is that the lattice Green's function  $G(t;r)$  is analytic if  $\text{Im } t$  is finite. If  $\omega_c$  is one of the singularities, it is associated with a  $k_c$  with real components satisfying

$$\omega_c = \omega_d(k_c) \quad , \quad \frac{\partial \omega_d(k_c)}{\partial k_c} = 0 \quad . \quad (5.1)$$

(5.1) represents either (2.4), (3.7), or (4.4).  $k_c$  for which  $\partial \omega_d(k_c)/\partial k_c = 0$  is satisfied is called a critical point. It is called a "non-degenerate" critical point, if the determinant of the second derivatives, the Hessian, of  $\omega_d(k_c)$  is not zero.

We shall give the behaviour of  $G_d(t;r)$  at  $t$  near  $\omega_c$  which is associated only with non-degenerate critical points. We shall denote the total number of those critical points  $k_c$  that  $\omega_d(k_c)$  is equal to the given value  $\omega_c$ , by  $n$ , and the  $n$  values of  $k_c$  by  $k_c^{(1)}$ ,  $k_c^{(2)}$ , . . . and  $k_c^{(n)}$ . We divide the total region  $\Omega$  of the integration in (1.2) into small regions  $\Delta_i$  around  $k_c^{(i)}$ , and the remaining  $\Omega' = \Omega - \sum_{i=1}^n \Delta_i$ ;

$$G_d(t;r) = \frac{1}{v_d} \left\{ \int_{\Omega'} dk \frac{e^{ik \cdot r}}{t - \omega_d(k)} + \sum_{i=1}^n \int_{\Delta_i} dk \frac{e^{ik \cdot r}}{t - \omega_d(k)} \right\} . \quad (5.2)$$

If  $t$  is so near to  $\omega_c$  that  $|t - \omega_d(k)|$  is finite as far as  $k$  is outside of the small regions  $\Delta_i$ , 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  $\Delta_i$ , we expand  $\omega_d(k)$  in powers of  $k - k_c^{(i)}$ , choose suitable coordinates and write as

$$\omega_d(k) = \omega_c - \sum_{j=1}^d a_j \xi_j^2 + o(\xi^3) \quad (5.3)$$

(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  $\omega_d(k)$  at  $k_c^{(i)}$  and is denoted by  $\lambda$  ( $0 \leq \lambda \leq d$ ). When  $\omega_c$  is the maximum value of  $\omega_d(k)$ ,  $\lambda=d$ , and when  $\omega_c$  is the minimum,  $\lambda=0$ . If  $2 \leq d$  and  $0 < \lambda < d$ ,  $\omega_c$  corresponds to a saddle point of the plane or hyper-plane  $\omega_d(k)$  as a function  $k$ . The integrations with respect to  $\xi_j$  are taken over the region  $\Delta_i$ . The singular behaviours are expressed in terms of the parameters  $v_d$ ,  $A_d = \prod_{j=1}^d |a_j|^{1/2}$  and the Jacobian  $J$  of the variable transformation from  $k - k_c^{(i)}$  to  $\xi_j$ .  $C$  in the following expressions are complex constants.

(i) One dimension:

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

where  $\lambda = 0$  or  $1$ .  $(t - \omega_c)^{1/2}$  denotes the positive square root  $\sqrt{t - \omega_c}$  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

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

if  $t = s - i\epsilon$  ( $\epsilon \geq 0$ ). When we have only one of each of minimum and maximum values of  $\omega_1(k)$  where  $\lambda=0$  and  $1$ , respectively, the curves of the real and imaginary parts of the lattice Green's function  $G_1(s-i\epsilon;r)$

take the same singular characters as Fig. 2. One notices that (5.4) must be equivalent to (2.5) if  $n=0$  and  $\nu=2$ , where  $J=1$  and  $\nu_1=2\pi$ . A reduction of (2.5) to the form of (5.4) is given in the Appendix, for the case when  $\nu$  is even.

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Fig. 2

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(ii) Two dimension:

$$G_2(t;0,0) \approx C + \frac{\pi J}{i^\lambda A_2 \nu_2} \ln(t - \omega_c) \quad (5.6)$$

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

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

if  $t = s - i\epsilon$  ( $\epsilon \geq 0$ ). 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 Fig. 3; those curves were first given by Katsura and Inawashiro (1971).

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Fig. 3

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(iii) Three dimension:

$$G_3(t;0,0,0) \approx c + \frac{1}{i^\lambda} \frac{2\pi^2 J}{A_3 v_3} (t - \omega_c)^{\frac{1}{2}}, \quad (5.8)$$

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  $G_3(s-i\epsilon; r)$  take the same singular characters as given by Fig. 4.

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Fig. 4

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

In order to obtain the singular behaviour at a singularity  $\omega_c$ , a summation must be taken over all the contributions due to the critical points  $k_c^{(i)}$  associated with the singular point  $\omega_c$ . Occasion may happen that the singular behaviour is exactly cancelled. In the preceding sections, we found that if  $\cos k_c \cdot r = 0$ , the critical point does not result in a singularity. In that case, the singular behaviours at  $k_c$  and at  $-k_c$  are found to cancel with each other exactly; note that  $-k_c$  is a critical point if so is  $k_c$  for lattices with the 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  $G_2(s-i\epsilon; 0,0)$  and  $G_3(s-i\epsilon; 0,0,0)$  are in agreement with those given by Van Hove (1953).

## 6. Conclusion

The discussions of the lattice Green's function in the text are given for the linear, square and cubic lattices. For other lattices also, the lattice Green's 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 of several Brillouin zones in the reciprocal lattice space and the integrand is a periodic function in that space. As the consequence, we reach the same conclusion: The lattice Green's 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 non-degenerate critical points are given in section 5, where the leading terms only are listed. The higher-order terms and its analysis in comparison with the curves will be given in a separate paper.

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

It is shown in section 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

$$\pm i \frac{\cos nz_0}{v(\omega_c - t)[(\omega_c - t)/a]^{-1/v}} \quad (\text{A.1})$$

where the sum must be taken over all different  $v$ th roots satisfying

$$\text{Im} [(\omega_c - t)/a]^{1/v} \geq 0. \quad (\text{A.2})$$

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  $v$ .

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

$$i \frac{\cos nz_0}{v|a|^{1/v}(t - \omega_c)^{1-1/v}} \quad (\text{A.3})$$

where

$$\text{Im}(t - \omega_c)^{1/v} < 0. \quad (\text{A.4})$$

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

$$i \frac{\cos nz_0}{v|a|^{1/v}(\omega_c - t)^{1-1/v}} \quad (\text{A.5})$$

where

$$\operatorname{Im}(\omega_c - t)^{1/v} > 0. \quad (\text{A.6})$$

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

$$(\omega_c - t)^{1/v} = \frac{-1}{i_v} (t - \omega_c)^{1/v} \quad (\text{A.7})$$

from the  $v$ th roots  $(t - \omega_c)^{1/v}$  which satisfy (A.4), where  $i_v \equiv \exp(\pi i/v)$  and hence  $i_2 = i$ . Substituting (A.7) into (A.5), we obtain

$$\frac{i}{i_v} \frac{\cos nz_0}{v|a|^{1/v}(t - \omega_c)^{1-1/v}} \quad (\text{A.8})$$

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

$$\frac{i}{(i_v)^\lambda} \frac{\cos nz_0}{v|a|^{1/v}(t - \omega_c)^{1-1/v}} \quad (\text{A.9})$$

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

when  $v=2$  and  $n=0$ .

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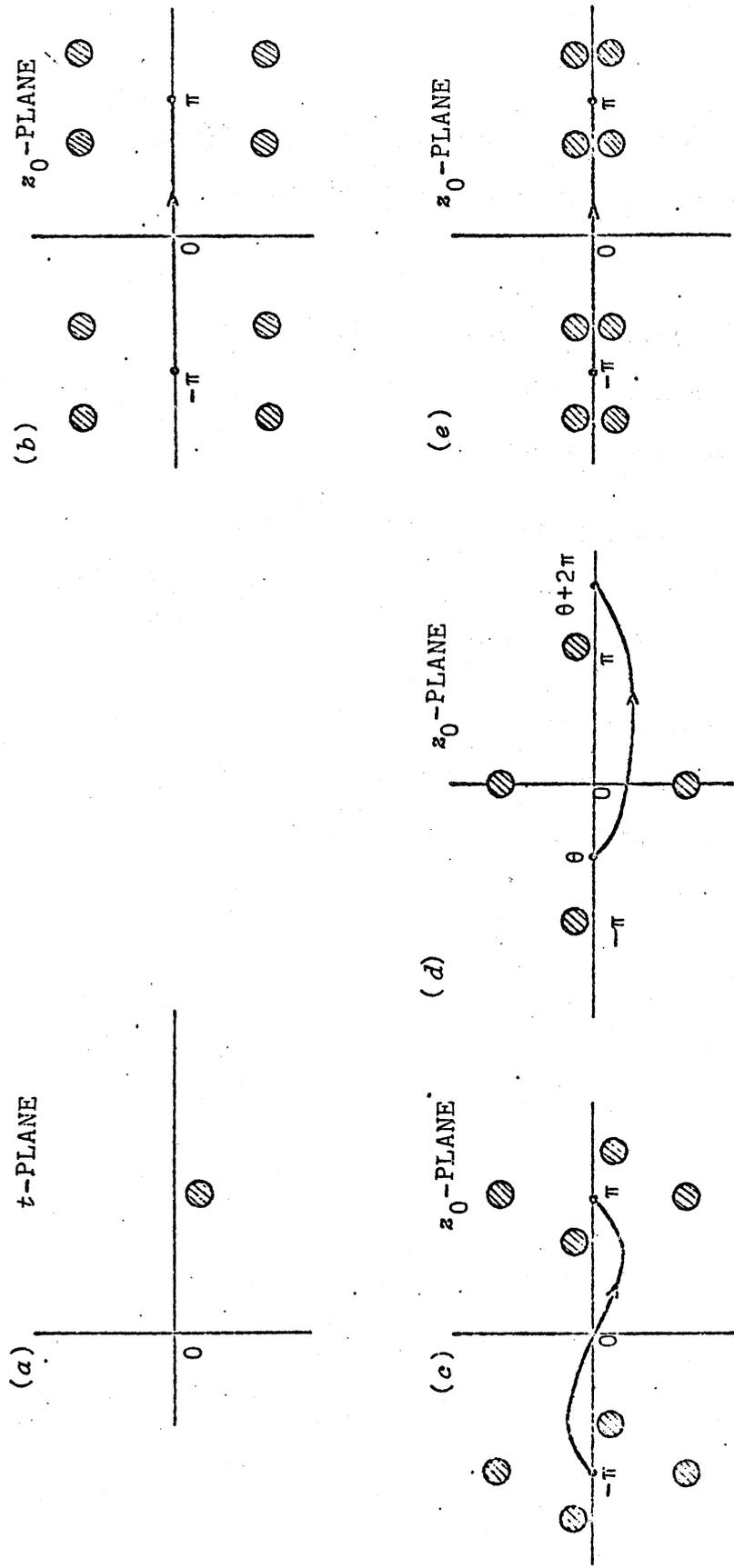
## Figure captions

Fig. 1. (a) Small region  $\Delta$  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  $\pi$  or from  $\sigma$  to  $\sigma+2\pi$  for (2.1)

Fig. 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.

Fig. 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. 1972).

Fig. 4. The real and imaginary parts of  $G_3(s-i\epsilon;1,0,0)$  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).



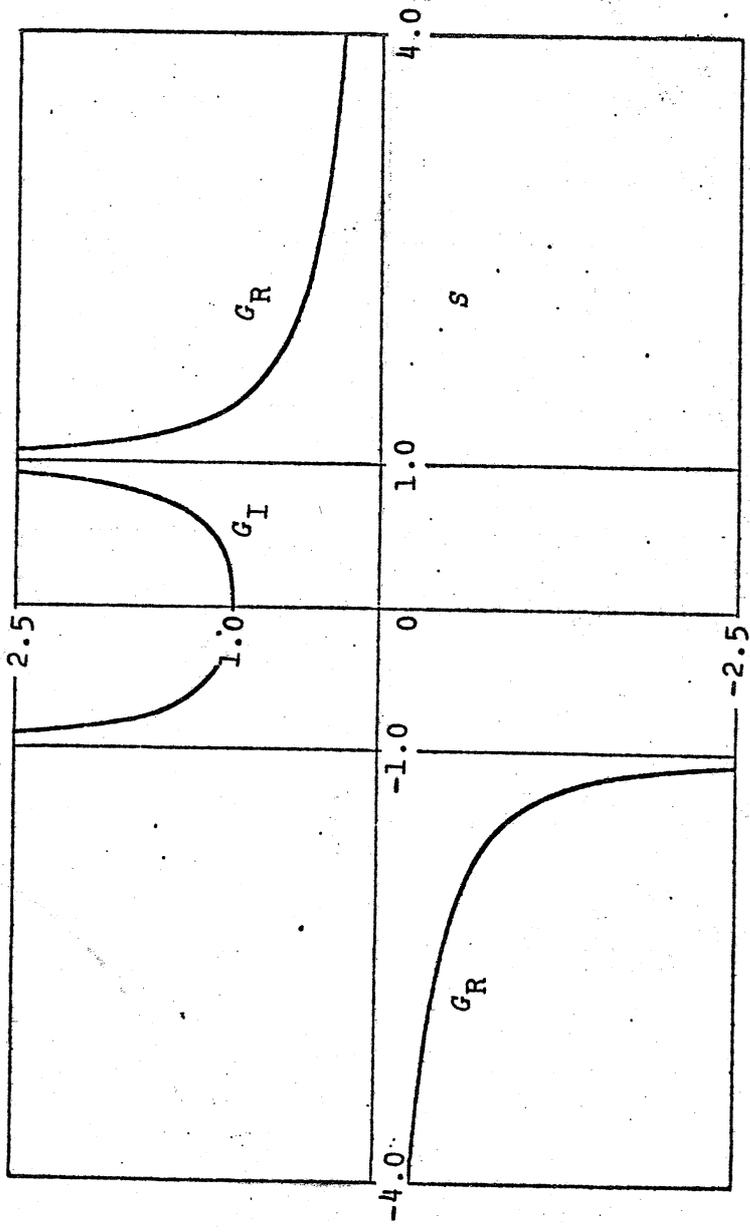


Fig. 2

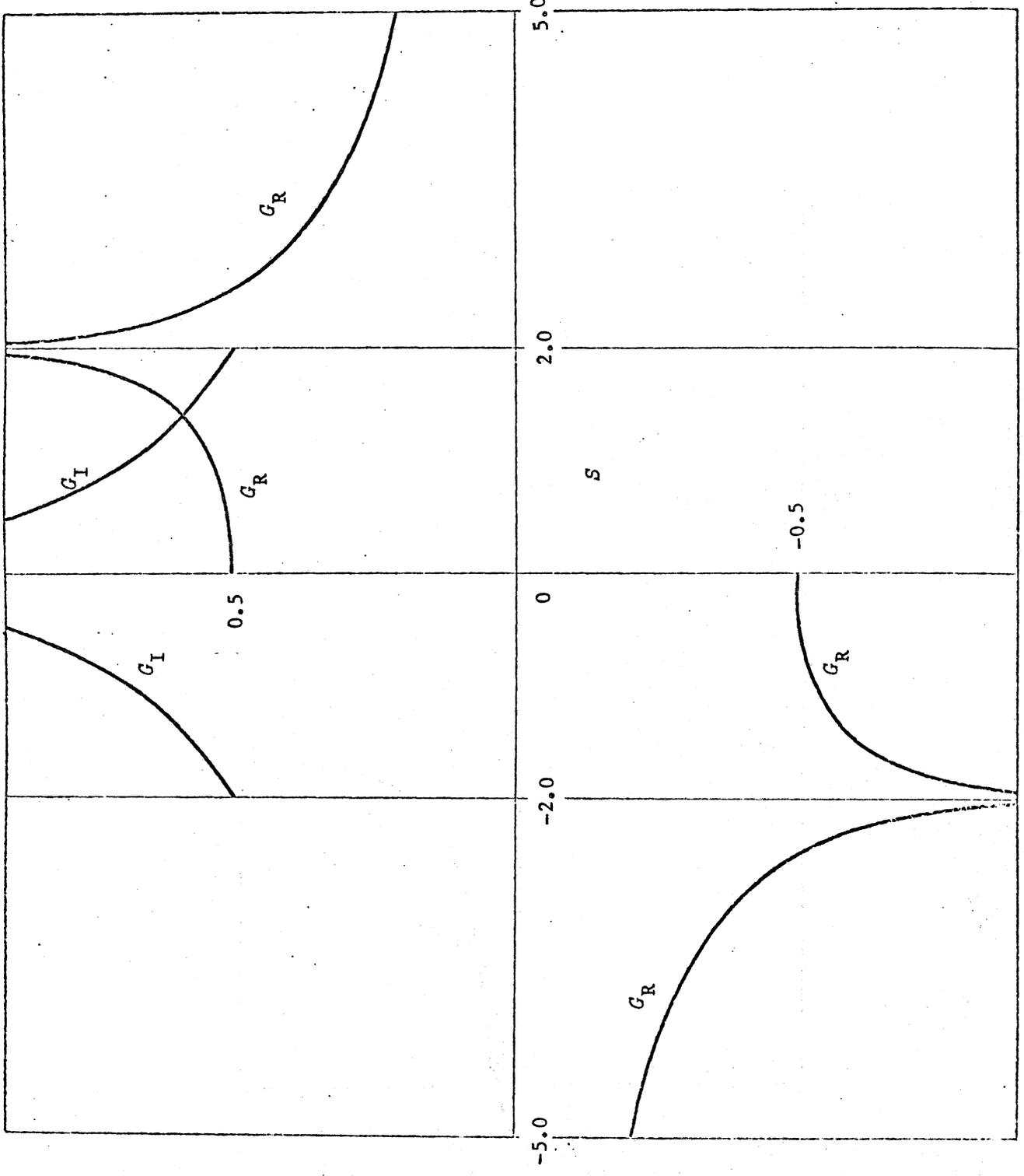


Fig. 3

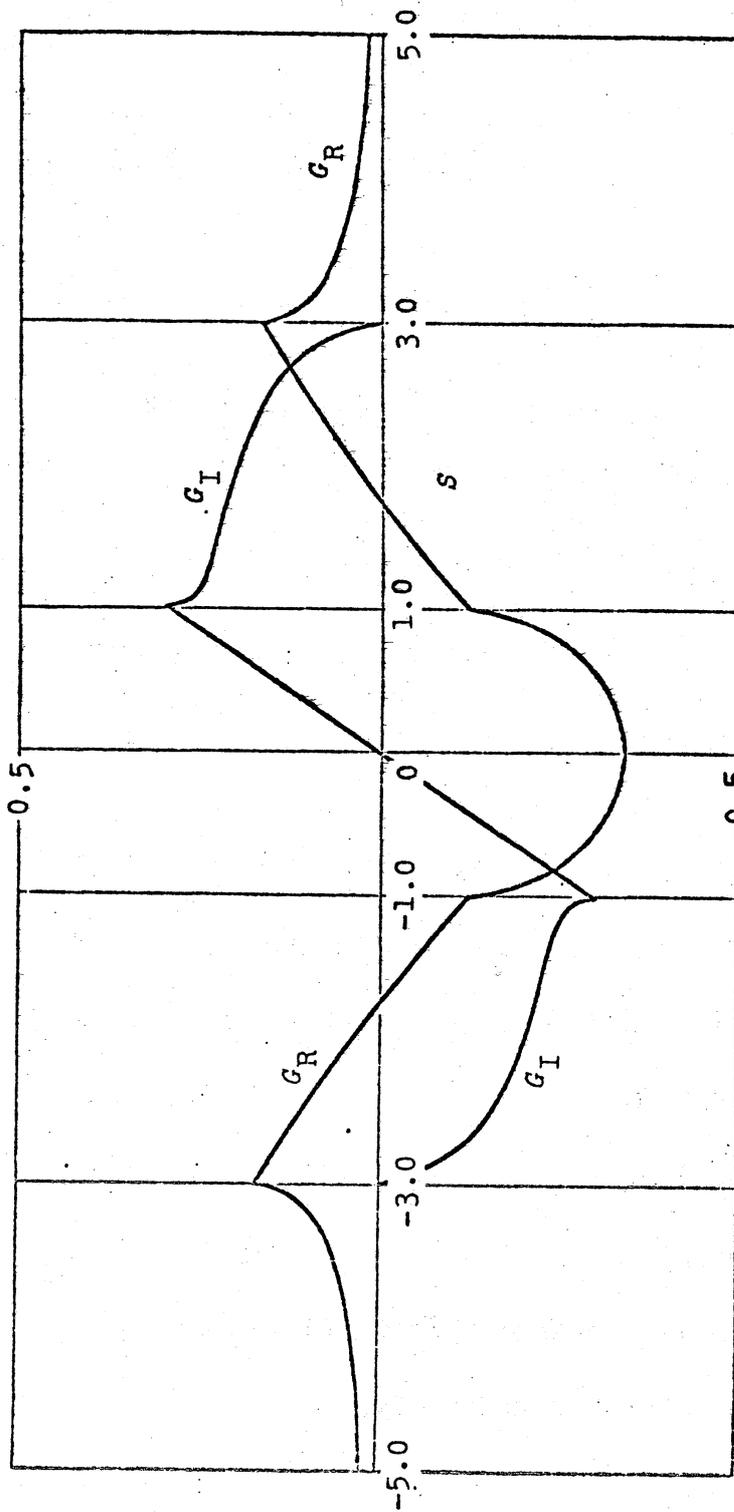


Fig. 4