Note on Electronic State of Random Lattice. III

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This paper is the continuation of a systematic study of the electronic states of a random lattice by the Green's function method. In this article, the second-order correction to the self energy part of the one electron Green's function is given by taking into account the exact average over a random distribution of impurities. With the low concentration approximation, the same result is also derived through an alternative method (the Matsubara-Toyozawa method).

§ 1. Introduction

As was mentioned in the Introduction and review of the second paper of this series,[1] there are several essential points in the problem of a random lattice which have not yet been given any satisfactory explanation. Among them, one of the most interesting properties of a random lattice is that the energy or frequency spectrum of a random lattice shows a very fine structure with many peaks; this fact is quite suggestive in many respects. The fine structure is, on the one hand, to be expected from the fact that the eigenvalues produced by the islands of impurities inbedded in the ideal lattice correspond to the energies or frequencies at which the peaks appear in the level density of a random system; this was first numerically predicted by Dean et al.,[2] and later proved generally by Hori and Fukushima.[3] Another piece of evidence for the appearance of fine structure is the discovery of the special frequencies[4] in the energy or frequency distribution of a random lattice at which the level density always vanishes under some given condition. The physical significance or content of this fact, however, has not yet been completely clarified.

The aim of the present article is to see how the above problem may be clarified by the Green's function technique, in the hope of finding a general way to treat higher-dimensional cases. In view of the fact that nothing like the true fine structure has been attained through the perturbational methods so far carried out[5] or from the results of expansion in powers of the concentration c by means of the Green's function method,[6] it is suspected that it is precisely the exact treatment of $P_s(c)$ — the coefficients of the cumulant average introduced in II — which is the key to the achievement of a correct understanding.

With this in mind, the second-order self-energy part $\Sigma(2)$ is treated in the present paper, by taking exact account of $P_s(c)$. This is a correction which

is better than $\Sigma(1)$ by one step; the formulation of $\Sigma(1)$ was given in II. An attempt to obtain the explicit expression for the second-order correction $\Sigma(2)$ is important in the sense that this leads to the investigation, through the Green's function method, of the connection between the local modes produced by a cluster of two impurity atoms with the peaks in the energy spectrum of a random system. In this connection, the local modes of an impurity and a cluster of two impurities are evaluated in § 2, while in § 3 it is shown how the second-order self-energy part $\Sigma(2)$ may be calculated by Edwards' method[7] if we deal with $P_s(c)$ accurately.

The complete correspondence between the results for $\Sigma(1)$ reached by Edwards' method and by the M–T method[8] has been given in I[9] under the assumption that $P_s(c) = c$. This restriction for $P_s(c)$ can be removed so that the proof is made on a more general basis; the detailed discussion of this will appear in one of the succeeding papers. The main purpose of having constructed $\Sigma(1)$ through two methods is to provide two different formulations so that one of them may be chosen for a given problem in consideration of the properties or the content of the problem. Besides, when we want to improve the approximation, we shall see that in general one of them will prove to be more suitable for use than the other, in accordance with the nature of the approximation and with the manner of improving it. This is the idea of re-evaluating $\Sigma(2)$ using the M–T method to show that we get the same result as that obtained by Edwards' method. Here again, for the sake of simplicity, the same restriction is laid down on $P_s(c)$; this does not affect the generality of the proof. Lastly, in § 5, further aspects of the problem are briefly considered.

§ 2. A single impurity and two impurities

Before we begin the general discussion of the second-order correction, it is as well to review the simple cases in which systems with only one impurity atom and two impurity atoms are treated. Knowledge of these simple systems will turn out to be useful when we discuss the correspondence between the localized modes and the many fine peaks appearing in the frequency spectrum of a random lattice.

First, let us consider the case of a single impurity inserted into an otherwise ideal lattice and assume that this one impurity atom attracts electrons with a potential of the delta-function type

$$v(\boldsymbol{r} - \boldsymbol{R}_0) = - V_0' \delta(\boldsymbol{r} - \boldsymbol{R}_0). \tag{2·1}$$

For the sake of simplicity, a one-band approximation is adopted so that the matrix elements of the potential are free from the indices n which denote various bands; thus, for this potential, Eq. (2·10) in II becomes

$$V_{\boldsymbol{k}\boldsymbol{k}'} = - V_0' \exp[-i(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}_0] u_{\boldsymbol{k}}(\boldsymbol{R}_0) u_{\boldsymbol{k}'}(\boldsymbol{R}_0). \tag{2·2}$$

Further simplification is introduced by assuming that $u_k(r)$ is constant everywhere in the space, i.e.

$$u_k(r) = \text{constant} = 1/\sqrt{\Omega}, \tag{2.3}$$

where Ω is the normalization volume. With this wave function, Eq. (2·2) is rewritten simply as

$$V_{kk'} = -V_0 \exp[-i(k-k')\cdot R_0] \tag{2.4}$$

where $V_0 = V_0'/\Omega$. It does not spoil the generality of the formulation even if R_0 is taken to be the origin. With all these considerations, the secular equation given by Eq. (2·7) in II reduces to

$$(\varepsilon_k - E)A_k - V_0 \sum_{k'} A_{k'} = 0. \tag{2.5}$$

Solving Eq. (2·5) for $\sum_k A_k$, we have an equation which determines E:

$$\sum_k \frac{1}{\varepsilon_k - E} = \frac{1}{V_0}. \tag{2.6}$$

All the solutions but one are found at $E \approx \varepsilon_k$, and the exceptional one is a discrete level below the band. It is easy to show that this discrete level is a localized mode.

Next, we formulate the problem of a system with two impurity atoms of the same kind at $R_0 = 0$ and $R_1 = R$. The potential in this case is

$$V(r) = -V_0'\{\delta(r) + \delta(r-R)\}. \tag{2.7}$$

With the same approximations as were used for the single-impurity system discussed above, the matrix element of the potential (2·7) is given by

$$V_{kk'} = -V_0\{1 + \exp[-i(k-k')\cdot R]\}, \tag{2.8}$$

and the secular equation becomes

$$(\varepsilon_k - E)A_k - V_0\{\sum_{k'} A_{k'} + \sum_{k'} \exp[-i(k-k')\cdot R]A_{k'}\} = 0. \tag{2.9}$$

To find the new eigenvalues, we first introduce $A(R)$ by the definition

$$A(R) = \sum_k \exp(ik\cdot R)A_k, \tag{2.10}$$

and then solve Eq. (2·9) for $A(0)$ and $A(R)$. Thus we have

$$\{1 + V_0 f(E, 0)\}A(0) + V_0 f(E, -R)A(R) = 0,$$

$$V_0 f(E, R)A(0) + \{1 + V_0 f(E, 0)\}A(R) = 0, \tag{2.11}$$

where

$$f(E, R) = \sum_k \frac{\exp(ik\cdot R)}{E - \varepsilon_k} = \sum_k G_0(k) \exp(ik\cdot R) \tag{2.12}$$

and $G_0(k)$ is an unperturbed Green's function defined by Eq. (2·20) in II.

The resulting secular equation for E is

$$[1 + V_0 f(E, 0)]^2 - V_0^2 |f(E, \boldsymbol{R})|^2 = 0, \qquad (2 \cdot 13)$$

where we have used the relation

$$f(E, -\boldsymbol{R}) = f^*(E, \boldsymbol{R}). \qquad (2 \cdot 14)$$

Incidentally, the secular equation $(2 \cdot 6)$ which determines the discrete level for the single-impurity case is written in the new formalism as

$$1 + V_0 \sum_k G_0(\boldsymbol{k}) = 1 + V_0 f(E, 0) = 0. \qquad (2 \cdot 15)$$

§ 3. Many impurities

With the preparations made in § 2, it is now much easier to understand the problem of many impurities distributed completely at random in the host lattice. On using the same assumptions as in § 2 that only one band is involved and that the potential of the impurities is of an attractive delta-function type, the equation for the one-electron Green's function is given by (see Eq. $(2 \cdot 19)$ in II)

$$G_{kk'}(E) = G_0(\boldsymbol{k}) \delta_{kk'} - V_0 G_0(\boldsymbol{k}) \sum_{k''} \rho(\boldsymbol{k} - \boldsymbol{k}'') G_{k''k'}(E), \qquad (3 \cdot 1)$$

where $G_{kk'}(E) = [G(E)]_{kk'}$. In order to make clear the relation between the equations and the corresponding diagrams, let us write down the leading terms of the expansion of $G_{kk'}(E)$:

$$G_{kk'}(E) = \delta_{kk'} [G_0(\boldsymbol{k}) - G_0(\boldsymbol{k}) N P_1(c) V_0 G_0(\boldsymbol{k})$$

$$+ \{ N^2 P_1^2(c) V_0^2 G_0^3(\boldsymbol{k}) + N P_2(c) V_0^2 G_0^2(\boldsymbol{k}) \sum_{k'} G_0(\boldsymbol{k}') \}$$

$$+ \cdots]. \qquad (3 \cdot 2)$$

Note that Eq. $(3 \cdot 2)$ is the matrix element of the true Green's function after the average over the impurity sites has been carried out, and it is obvious that the averaged Green's function $G_{kk'}(E)$ is diagonal with respect to k so that $G_{kk'}(E)$ is written as $G(\boldsymbol{k}) \delta_{kk'}$.

In II, we have seen that all the diagrams up to third order in V_0 are taken into account if the first order self-energy part is calculated self-consistently. The lowest-order diagram discarded from the first-order correction is the fourth-order diagram shown in Fig. 1(a). All the rest of the fourth-order diagrams are included in $\Sigma(1)$. Out of all the fifth-order diagrams, only the one diagram given in Fig. 1(b) is omitted from the first-order self-energy part. On collecting all this information, it may be suspected that, when we want to take one more step towards a better approximation, the diagrams which should be retained are those pictured in Fig. 2(a). If the potential is strong and short range, multiple scattering in higher order predominates, so that it is necessary to sum

all the diagrams shown in Fig. 2(b). This is actually the case for the present problem since the potential under consideration is of the delta-function type which is extremely short range.
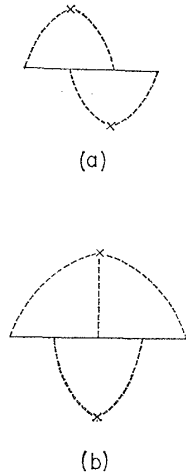

(a)

(b)

Fig. 1. The fourth and fifth-order digrams discarded in Σ(1).
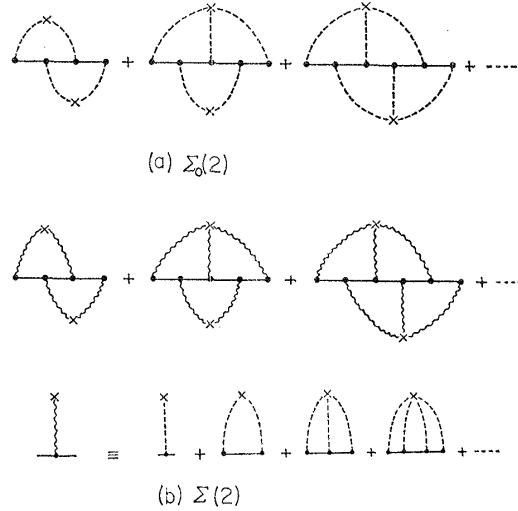

(a) Σ_0(2)

(b) Σ(2)

Fig. 2. The diagrams to be included in the second-order self-energy part. (a) Σ_0(2) (b)Σ(2)

With this goal in mind, we first sum the diagrams in Fig. 2(a). For the moment, $P_s(c)$ is approximated by c. By making use of the prescriptions given in Fig. 2 of II, the contribution from the first diagram in Fig. 2(a) is shown to be

$$(-V_0)^4 N^2 c^2 \sum_{k_1 k_2 k_3} \delta(k-k_1+k_2-k_3)\delta(k_1-k_2+k_3-k') G_0(k_1) G_0(k_2) G_0(k_3)$$

$$= \delta(k-k') Nc^2 V_0^4 \sum_R \exp(-ik\cdot R)f(E,R)|f(E,R)|^2,$$

while the second diagram gives the contribution

$$(-V_0)^5 N^2 c^2 \sum_{k_1\cdots k_4} \delta(k-k_1+k_2-k_3+k_4-k')\delta(k_1-k_2+k_3-k_4) \prod_{i=1}^4 G_0(k_i)$$

$$= -\delta(k-k') Nc^2 V_0^5 \sum_R |f(E,R)|^4,$$

where we have used Eq. (2·12) and the identity

$$N\delta(k_1-k_2+k_3-k_4) = \sum_R \exp[-i(k_1-k_2+k_3-k_4)\cdot R].$$

From these, it is immediately inferred that the contribution from the diagrams in Fig. 2(a) is expressed by the sum of the infinite series

$$\delta(k-k') Nc^2 V_0 \sum_R \{\exp(-ik\cdot R) \sum_{n=1}^{\infty} V_0^{2n+1} f(E,R)|f(E,R)|^{2n}$$

$$-\sum_{n=1}^{\infty} V_0^{2n+2}|f(E,R)|^{2n+2}\},$$

which yields

$$\sum_{kk'}^{(a)}(2) = \delta(k-k') Nc^2 V_0^4 \sum_R \frac{|f(E, R)|^2 \exp(-ik\cdot R) f(E, R) - V_0|f(E, R)|^2}{1 - V_0^2 |f(E, R)|^2}.$$

$$(3\cdot3)$$

Next, let us evaluate the second-order self-energy part represented by Fig. 2(b). Each diagram of the series in Fig. 2(b) is actually an infinite sum of diagrams. For instance, the first diagram in Fig. 2(b) is the infinite sum of those diagrams, a typical one of which is drawn in Fig. 3(a). In this diagram s_1 is the multiplicity of the scattering by the first impurity before any scattering by the second impurity sets in, while t_1 is the multiplicity of the scattering by the second impurity which takes place between two separate interactions of an electron with the first impurity and so forth. We have to associate with this diagram the cumulant factor $P_s(c) P_t(c)$ with $s = s_1 + s_2$ and $t = t_1 + t_2$, and sum up over all possible combinations of the non-vanishing integers s_1, s_2, t_1 and t_2. Let $B_{s,p}$ be the number of the partitions of s into p groups, then the contribution from the first diagram in Fig. 2(b) is calculated as

$$\delta(k-k') N \sum_R \exp(-ik\cdot R) f(E, R) |f(E, R)|^2$$

$$\times \sum_{s=2}^{\infty} P_s(c) B_{s,2}(-V_0)^s [f(E, 0)]^{s-2} \sum_{t=2}^{\infty} P_t(c) B_{t,2}(-V_0)^t [f(E, 0)]^{t-2}.$$

Quite similarly, the second diagram in Fig. 2(b) is the infinite sum of diagrams such as Fig. 3(b) and contributes

$$\delta(k-k') N \sum_R |f(E, R)|^4 \sum_{s=3}^{\infty} P_s(c) B_{s,3}(-V_0)^s [f(E, 0)]^{s-3}$$

$$\times \sum_{t=2}^{\infty} P_t(c) B_{t,2}(-V_0)^t [f(E, 0)]^{t-2}.$$

Fig. 3.

(a)   A typical diagram included in the first diagram in Fig. 2(b).

(b)   A typical diagram included in the second diagram in Fig. 2(b).

On inspection of the above results, it is concluded that the contribution from the $(2p-3)$rd diagram in Fig. 2(b) is generally given by

$$S_{kk'}^{(2p-3)} = \delta(k-k') N \sum_R \exp(-ik\cdot R) f(E, R) |f(E, R)|^{2(p-1)} [f(E, 0)]^{-2p}$$

$$\times \sum_{s=p}^{\infty} P_s(c) B_{s,p} [f(E, 0)]^s (-V_0)^s \cdot \sum_{t=p}^{\infty} P_t(c) B_{t,p} [f(E,0)]^t (-V_0)^t$$

$$(p \geq 2) \qquad\qquad (3\cdot4)$$

while the $(2p-2)$nd diagram contributes to the self-energy part

$$S_{kk'}^{(2p-2)} = \delta(\boldsymbol{k}-\boldsymbol{k}')N\sum_{\boldsymbol{R}}|f(E,\boldsymbol{R})|^{2p}[f(E,0)]^{-(2p+1)}$$

$$\times \sum_{s=p+1}^{\infty}P_s(c)B_{s,p+1}[-V_0f(E,0)]^s \cdot \sum_{t=p}^{\infty}P_t(c)B_{t,p}[-V_0f(E,0)]^t.$$

$$(p\geq 2) \qquad (3\cdot 5)$$

The quantity $B_{s,p}$ is related to the generating function $h(x)=x/1-x$ by

$$[h(x)]^p = (x/1-x)^p = \sum_{s=p}^{\infty}B_{s,p}x^s, \qquad (3\cdot 6)$$

so that the general expression of $B_{s,p}$ is determined as

$$B_{s,p} = \frac{1}{s!}\frac{d^s}{dx^s}[h(x)]^p\Big|_{x=0} = \frac{(s-1)!}{(p-1)!(s-p)!}. \qquad (3\cdot 7)$$

There are two ways of performing the summation of Eqs. $(3\cdot 4)$ and $(3\cdot 5)$ over all p larger than 2; one is by means of the generating function of $P_s(c)$ and other is by making use of the generating function of $B_{s,p}$. We shall present here only the first method. As has been proved in II, $P_s(c)$ is the coefficient of $x^s/s!$ in the expansion of the generating function

$$g(x:c) = \log(1-c+c\exp[x]), \qquad (3\cdot 8)$$

that is,

$$P_s(c) = \frac{d^s}{dx^s}g(x:c)\Big|_{x=0} = D_x^s g(x:c)\Big|_{x=0}. \qquad (3\cdot 9)$$

Therefore, in Eqs. $(3\cdot 4)$ and $(3\cdot 5)$, $P_s(c)$ or $P_t(c)$ can be replaced by the differential operator D_x^s or D_y^t which is to operate on the generating function $g(x:c)$ or $g(y:c)$. Thus Eq. $(3\cdot 4)$ results in

$$S_{kk'}^{(2p-3)} = \delta(\boldsymbol{k}-\boldsymbol{k}')N\sum_{\boldsymbol{R}}\exp(-i\boldsymbol{k}\cdot\boldsymbol{R})f(E,\boldsymbol{R})|f(E,\boldsymbol{R})|^{2(p-1)}[f(E,0)]^{-2p}$$

$$\times \sum_{s=p}^{\infty}B_{s,p}[-V_0f(E,0)D_x]^s g(x:c)\Big|_{x=0}\sum_{t=p}^{\infty}B_{t,p}[-V_0f(E,0)D_y]^t g(y:c)\Big|_{y=0}$$

$$= \delta(\boldsymbol{k}-\boldsymbol{k}')N\sum_{\boldsymbol{R}}\exp(-i\boldsymbol{k}\cdot\boldsymbol{R})f(E,\boldsymbol{R})|f(E,\boldsymbol{R})|^{2(p-1)}[f(E,0)]^{-2p}$$

$$\times [h(-V_0f(E,0)D_x)h(-V_0f(E,0)D_y)]^p g(x:c)g(y:c)\Big|_{x=0,y=0} \qquad (3\cdot 4\text{a})$$

and similarly

$$S_{kk'}^{(2p-2)} = \delta(\boldsymbol{k}-\boldsymbol{k}')N\sum_{\boldsymbol{R}}|f(E,\boldsymbol{R})|^{2p}[f(E,0)]^{-(2p+1)}h(-V_0f(E,0)D_x)$$

$$\times [h(-V_0f(E,0)D_x)h(-V_0f(E,0)D_y)]^p g(x:c)g(y:c)\Big|_{x=0,y=0}, \qquad (3\cdot 5\text{a})$$

where use has been made of the relation (3·6). Now we are ready to sum up (3·4a) and (3·5a) over p to obtain the expression for the second-order self-energy part:

$$\sum_{kk'}^{(b)}(2) = \sum_{p=2}^{\infty}\{S_{kk'}^{(2p-3)} + S_{kk'}^{(2p-2)}\}$$

$$= \delta(k-k')\frac{NV_0^4}{[1+V_0f(E,0)D_x]^2[1+V_0f(E,0)D_y]}$$

$$\times \sum_{R}\frac{\{|f(E,R)|^2 f(E,R)[1+V_0f(E,0)D_x]\exp(-ik\cdot R)-V_0|f(E,R)|^4 D_y\}D_x^2 D_y^2}{[1+V_0f(E,0)D_x][1+V_0f(E,0)D_y]-V_0^2|f(E,R)|^2 D_x D_y}$$

$$\times g(x:c)g(y:c)|_{x=0,y=0}.   \tag{3·10}$$

Incidentally, in the same notation the first-order self-energy part can be written as

$$\sum_{kk'}^{(b)}(1) = \frac{-V_0 D_x}{[1+V_0f(E,0)D_x]}g(x:c)\Big|_{x=0}.   \tag{3·11}$$

It is possible to express the final result for the self-energy part in a form which does not contain the differential operator D_x or D_y. For this purpose, it is more convenient to use, instead of $g(x:c)$, its derivative

$$g'(x:c) = \frac{c\exp(x)}{1-c+c\exp(x)} = \sum_{s=0}^{\infty}P_{s+1}(c)x^s/s!,   \tag{3·12}$$

so that $P_s(c)$ may be expressed as

$$P_s(c) = \frac{1}{2\pi i}\oint dx\int_0^{\infty} dt\, t^{s-1}\exp(-t)\frac{g'(x:c)}{x^s},   \tag{3·13}$$

where $\oint$ is the Cauchy integral in the complex x-plane. It is not difficult to sum (3·4) and (3·5) over p by making use of Eq. (3·13). As a result, the self-energy part with corrections up to the second order is given by

$$\Sigma_0(1) + \Sigma_0(2) = \frac{1}{2\pi i}\oint dx\int_0^{\infty} dt\, \frac{\exp(-t)}{x+V_0f(E,0)t}\frac{-NcV_0\exp(x)}{1-c+c\exp(x)}$$

$$+ \frac{1}{(2\pi i)^2}\oint\oint dx\,dy\int_0^{\infty} dt\int_0^{\infty} ds\, \frac{Nc^2 st\exp(-t-s+x+y)}{[1-c+c\exp(x)][1-c+c\exp(y)]}$$

$$\times \frac{V_0^4}{[x+V_0f(E,0)t]^2[y+V_0f(E,0)s]}$$

$$\times \sum_{R}\frac{|f(E,R)|^2 f(E,R)[x+V_0f(E,0)t]\exp(-ik\cdot R)-V_0|f(E,R)|^4 s}{[x+V_0f(E,0)t][y+V_0f(E,0)s]-V_0^2|f(E,R)|^2 ts}.$$

$$\tag{3·14}$$

It is interesting to note that if we adopted the approximation $P_s(c) = c$, Eq. (3·14) would be reduced to

$$\Sigma_0(1) + \Sigma_0(2) = \frac{-NcV_0}{1 + V_0 f(E, 0)} + \frac{Nc^2 V_0^4}{[1 + V_0 f(E, 0)]^5}$$

$$\times \sum_{\boldsymbol{R}} \frac{|f(E, \boldsymbol{R})|^2 f(E, \boldsymbol{R}) [1 + V_0 f(E, 0)] \exp(-i\boldsymbol{k} \cdot \boldsymbol{R}) - V_0 |f(E, \boldsymbol{R})|^4}{[1 + V_0 f(E, 0)]^2 - V_0^2 |f(E, \boldsymbol{R})|^2}.$$

$$(3·15)$$

In this approximation, $\Sigma_0(1)$ has a pole at the energy corresponding to the discrete level for a single impurity determined from Eq. (2·15), whereas $\Sigma_0(2)$ has poles at the energies determined from Eq. (2·13) which correspond to the isolated levels associated with the clusters of two impurity atoms with variable separation $\boldsymbol{R}$.

Obviously, some of the lower-order diagrams are excluded from $\Sigma_0(1) + \Sigma_0(2)$ given by Eq. (3·14). As discussed in detail at the end of §4 in II, these diagrams come to be included on changing the Green's function appearing in the self-energy part into the true Green's function. This can be achieved by replacing all $f(E, \boldsymbol{R})$ in Eq. (3·14) with $F(E, \boldsymbol{R})$ defined by

$$F(E, \boldsymbol{R}) = \sum_{\boldsymbol{k}} G(\boldsymbol{k}) \exp(-i\boldsymbol{k} \cdot \boldsymbol{R}) \qquad (3·16)$$

where $G(\boldsymbol{k})$ is the true Green's function which, on the other hand, is self-consistently determined from the new self-energy part by the relation

$$G(\boldsymbol{k}) = [G_0^{-1}(\boldsymbol{k}) - \Sigma(1) - \Sigma(2)]^{-1}. \qquad (3·17)$$

Here we denote the new self-energy part by $\Sigma(1) + \Sigma(2)$, the explicit expression is obtained by putting $F(E, \boldsymbol{R})$ in place of $f(E, \boldsymbol{R})$ in Eq. (3·14).

It is easy to check that the change of description in the sense introduced in §5 of II does not bring about any change in $\Sigma(2)$. In other words, the second-order self-energy part fulfils the requirement of dual invariance. Actually, however, this proves to be obvious if we consider the problem carefully. As we have seen in the discussion of §5 in II, the only term which causes a shift in the self-energy is one with $P_1(c)$, while higher-order terms do not suffer any change under the change of description because the dual relation of $P_s(c)$ (for $s \geq 2$) given by Eq. (5·12) just cancels the change of sign which comes from the potential V. This consideration suggests that all higher-order self-energy parts have the property of dual invariance since they do not retain $P_1(c)$.

§4. An alternative method

——*The M-T method*——

In §3, the second-order self-energy part has been evaluated through Edwards' method, while in this section we try to obtain the same result by means of an

alternative method (the *M-T* method) in order to see the correspondence between the two methods. As has been examined in I, the criterion for choosing one method or the other depends on the properties of the approximations used, on the nature of the required quantities or on the aim of the calculation, so that it is meaningful to formulate problems through both methods.

Since a detailed discussion of the application of the *M-T* method to the present problem is given in I, only a brief review of it will be presented here. We start with Eq. (3·1) which is written as

$$G_{kk'}(E) = \delta_{kk'} G_0(k) - G_0(k) V_0 \sum_{k''} \sum_{[n]} \exp\left[-i(k-k'') \cdot R_n\right] G_{k''k'}(E). \quad (4\cdot1)$$

To facilitate the formulation, we introduce a function $F_n(k)$ defined by

$$F_n(k) = \sum_{k'} \exp\left[-i(k-k') \cdot R_n\right] G_{k'k}(E), \quad (4\cdot2)$$

which together with Eq. (4·1) leads to

$$G(k) = G_0(k) - G_0(k) V_0 \sum_{[n]} F_n(k), \quad (4\cdot3)$$

$$F_n(k) = G_0(k) - V_0 \sum_{k'} \sum_{[m]} G_0(k') \exp\left[-i(k-k') \cdot (R_n - R_m)\right] F_m(k). \quad (4\cdot4)$$

On taking the term with $R_n = R_m$ out of the summation, Eq. (4·4) is put in the form :

$$F_n(k) = \frac{G_0(k)}{1 + V_0 f(E, 0)} - \frac{V_0}{1 + V_0 f(E, 0)} \sum_{[m \neq n]} W_k(n-m) F_m(k), \quad (4\cdot5)$$
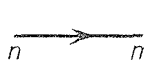
where

$$W_k(n-m) = \sum_{k'} G_0(k') \exp\left[-i(k-k') \cdot (R_n - R_m)\right] \quad (4\cdot6)$$

and use has been made of Eq. (2·12). To simplify the notation, we shall put

$$\frac{V_0}{1 + V_0 f(E, 0)} = V \quad \text{and} \quad \frac{G_0(k)}{1 + V_0 f(E, 0)} = G_0'(k).$$

(a)   O   : $\dfrac{G_0(k)}{1 + V_0 f(E, 0)} = G_0'(k)$

(b) $\xrightarrow[n \quad\quad m]{}$: $\dfrac{-V_0}{1 + V_0 f(E, 0)} W_k(n-m) = -V W_k(n-m)$

(c)   ⊛   : $\sum_{[n]}$

Fig. 4. Rules for calculating $F_n(k)$ with diagrams.

    To solve Eq. (4·5) by the iteration procedure, it is convenient to derive help from the diagrams, the rules for calculating with which are given in Fig. 4. It is easy to see that the first few terms of the expansion of Eq. (4·5) correspond to the diagrams shown in Fig. 5(a). A complete investigation has been given in I so far as the first-order correction is concerned and we have seen that the optical model—the simplest of all—is the approximation that only those diagrams in Fig. 5(b) are summed up to give $F_n(k)$. The prescriptions in Fig. 4 yield

$$F_n^{op}(k) = G_0'(k)\sum_{\nu=0}^{\infty}(-V)^{\nu}\sum_{[R_1]}\cdots\sum_{[R_\nu]}W_k(R_n-R_1)\,W_k(R_1-R_2)\cdots W_k(R_{\nu-1}-R_\nu).$$

$$(4\cdot7)$$

Hereupon, it is necessary to average over the random distribution of the impurity sites. In I, coincidence of the impurity sites has not been considered but we have supposed that the average over various sites can be carried out independently, which is in effect equivalent to assuming that $P_s(c)$ is regarded as c for all values of s. Of course, it is possible to take account of the coincidence of the impurity sites and obtain an exact cumulant average in the M-T method as well, but in order to avoid the complexity associated with the accurate treatment of the averaging process, we shall adopt the above mentioned approximation and leave the exact discussion for a later chance.
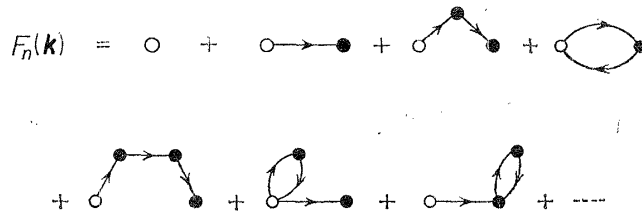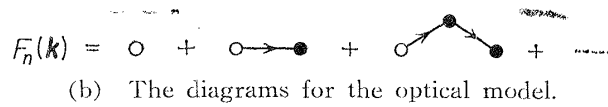

Fig. 5.   (a) The diagrammatical representation of $F_n(k)$.

(b)   The diagrams for the optical model.

    With the replacement $\sum_{[n]}\to c\sum_{n}$ and the definition of $W_k(R)$ given by Eq. (4·6), we have

$$\sum_{[n]}W_k(R_n) = \sum_{k'}G_0(k')\sum_{[n]}\exp[-i(k-k')\cdot R_n]$$

$$= c\sum_{k'}G_0(k')\sum_{n}\exp[-i(k-k')\cdot R_n]$$

$$= Nc\,G_0(k).$$

$$(4\cdot8)$$

Thus, Eq. (4·7) becomes

$$F_n^{op}(k) = G_0'(k)\sum_{\nu=0}^{\infty}[-NcVG_0(k)]^{\nu}$$

$$= \frac{G_0'(k)}{1 + NcVG_0(k)} = \frac{G_0(k)}{1 + V_0 f(E, 0) + NcV_0 G_0(k)}, \qquad (4\cdot9)$$

which together with Eq. (4·3) gives the Green's function for the optical model

$$G^{op}(k) = [G_0^{-1}(k) - \Sigma^{op}(1)]^{-1} \qquad (4\cdot10a)$$

where

$$\Sigma^{op}(1) = -NcV = \frac{-NcV_0}{1 + V_0 f(E, 0)}. \qquad (4\cdot10b)$$

This is exactly the same as Eq. (4·4) in II if $P_s(c)$ is taken to be c for all s. This fact suggests that the Edwards' diagrams drawn in Fig. 4 of II correspond to the M-T diagrams given in Fig. 5(b).

Now, we have to prove that, when $F_n(k)$ is approximated by the sum of the diagrams in Fig. 6(a) with such a vertex renormalization as in Fig. 6(b), the resulting second-order self-energy part is equal to $\Sigma_0(1) + \Sigma_0(2)$ in Eq. (3·15). On referring to the rules given in Fig. 4, $W_k^{(3)}(R)$ defined by a sum of the diagrams in Fig. 6(b) is shown to be

$$W_k^{(3)}(R) = W_k(R) |W_k(R)|^2 (-V)^3 \sum_{\nu=0}^{\infty} [-V|W_k(R)|]^{2\nu}$$

$$= \frac{W_k(R) |W_k(R)|^2 (-V)^3}{1 - V^2 |W_k(R)|^2}.$$
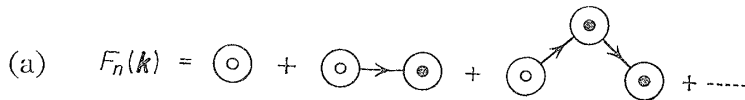
Fig. 6. The second-order approximation in the M-T method.
(a) The diagrams of $F_n(k)$ which give $\Sigma_0(1) + \Sigma_0(2)$.
(b) Renormalization of vertex.

As is easily seen, $W_k(R)$ is rewritten by using Eqs. (2·12) and (4·6) as

$$W_k(R) = \exp(-ik \cdot R) f(E, R), \qquad (4\cdot11)$$

so that $W_k^{(3)}(R)$ finally takes the form:

$$W_k^{(3)}(R) = \frac{(-V)^3 |f(E, R)|^2 f(E, R) \exp(-ik \cdot R)}{1 - V^2 |f(E, R)|^2}, \qquad (4\cdot12)$$

from which the expression for the vertex renormalization $\hat{\xi}_A$ immediately follows:

$$\hat{\xi}_A = 1 + \sum_{[R]} W_k^{(3)}(R) + \sum_{[R]} (-V) W_k^{(3)}(R) W_k^*(R)$$

$$= 1 + c \sum_R \frac{(-V)^3 |f(E, R)|^2 f(E, R) \exp(-i\boldsymbol{k} \cdot \boldsymbol{R}) + (-V)^4 |f(E, R)|^4}{1 - V^2 |f(E, R)|^2}$$

$$= 1 + \frac{-cV_0^3}{[1 + V_0 f(E, 0)]^2}$$

$$\times \sum_R \frac{|f(E, R)|^2 f(E, R)[1 + V_0 f(E, 0)] \exp(-i\boldsymbol{k} \cdot \boldsymbol{R}) - V_0 |f(E, R)|^4}{[1 + V_0 f(E, 0)]^2 - V_0^2 |f(E, R)|^2}$$

$$(4 \cdot 13)$$

with the help of the replacement $\sum_{[R]} \to c \sum_R$. The infinite sum of the diagrams in Fig. 6(a) then gives

$$F_n(\boldsymbol{k}) = \hat{\xi}_A G_0'(\boldsymbol{k}) \sum_{\nu=0}^{\infty} [-V \hat{\xi}_A N c G_0(\boldsymbol{k})]^{\nu}$$

$$= \frac{\hat{\xi}_A G_0'(\boldsymbol{k})}{1 + N c \hat{\xi}_A V G_0(\boldsymbol{k})} = \frac{\hat{\xi}_A G_0(\boldsymbol{k})}{1 + V_0 f(E, 0) + N c \hat{\xi}_A V_0 G_0(\boldsymbol{k})} \qquad (4 \cdot 14)$$

so that the Green's function is obtained, by virtue of Eq. (4·3), as

$$G(\boldsymbol{k}) = G_0(\boldsymbol{k}) [1 - V_0 \sum_{[n]} F_n(\boldsymbol{k})]$$

$$= \left[G_0^{-1}(\boldsymbol{k}) + \frac{N c \hat{\xi}_A V_0}{1 + V_0 f(E, 0)} \right]^{-1}, \qquad (4 \cdot 15)$$

where again $\sum_{[n]}$ has been replaced with $c \sum_n = Nc$. In this approximation the self-energy part is obviously given by

$$\Sigma_A = -N c V \hat{\xi}_A = \frac{-N c V_0}{1 + V_0 f(E, 0)} \hat{\xi}_A \qquad (4 \cdot 16)$$

and on inserting (4·13) for $\hat{\xi}_A$ in the above equation, we can readily verify that Σ_A is precisely the same as $\Sigma_0(1) + \Sigma_0(2)$ in Eq. (3·15) under the restriction that $P_s(c) = c$.

As the next stage, let us try and find what kinds of *M-T* diagrams correspond to the self-energy part $\Sigma(1) + \Sigma(2)$ in Eq. (3·17) which is actually derived from Eq. (3·15) on changing $f(E, \boldsymbol{k})$ into $F(E, \boldsymbol{R})$. In the *M-T* method, this result is attained by improving the vertex renormalization $(\hat{\xi}_A \to \hat{\xi}_B)$ in the way described in Figs. 7(a) to (*g*). To be more precise, we first define a renormalized *W*-function $\widetilde{W}_k(n-m)$ by a sum of the diagrams in Fig. 7(a).

$$\widetilde{W}_k(n-m) = \sum_{\nu=0}^{\infty} (-V)^{\nu+1} \hat{\xi}_B^{\nu} \sum_{[n_1]} \cdots \sum_{[n_\nu]} W_k(n-n_1) \cdots W_k(n_\nu - m), \qquad (4 \cdot 17)$$

where $\hat{\xi}_B$ is the vertex renormalization constant which is to be determined self-

consistently. The definition (4·5) together with the replacement $\sum_{[n]} \to c\sum_{n}$ gives rise to

$$\sum_{[n_1]} \cdots \sum_{[n\nu]} W_k(n-n_1) \cdots W_k(n_\nu - m)$$

$$= (Nc)^\nu \exp\left[-i\boldsymbol{k}\cdot(\boldsymbol{R}_n - \boldsymbol{R}_m)\right] \sum_{k'} G_0^{\nu+1}(k') \exp\left[-i\boldsymbol{k}'\cdot(\boldsymbol{R}_n - \boldsymbol{R}_m)\right]$$

and hence $\widetilde{W}_k(\boldsymbol{R})$ can be easily summed up to give

$$\widetilde{W}_k(\boldsymbol{R}) = (-V)\exp(-i\boldsymbol{k}\cdot\boldsymbol{R})\sum_{k'}\frac{G_0(k')\exp(i\boldsymbol{k}'\cdot\boldsymbol{R})}{1+Nc\xi_B VG_0(k')} \ . \qquad (4\cdot18)$$

Let us put

$$F(E, \boldsymbol{R}) = \sum_{k}\frac{G_0(k)\exp(i\boldsymbol{k}\cdot\boldsymbol{R})}{1+Nc\xi_B VG_0(k)} \qquad (4\cdot19)$$

and put (4·18) in a compact form

$$\widetilde{W}_k(\boldsymbol{R}) = (-V)\exp\left[-i\boldsymbol{k}\cdot\boldsymbol{R}\right]F(E, \boldsymbol{R}). \qquad (4\cdot20)$$
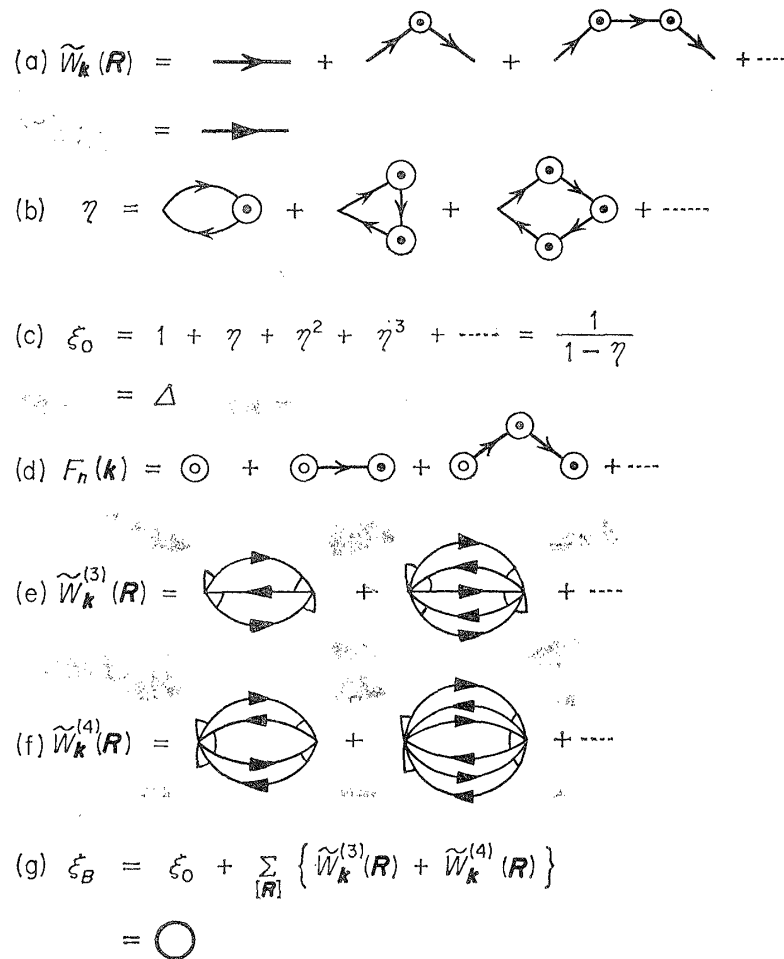

Fig. 7. The second-order self-consistent approximation in the M-T method.

As will be shortly proved, $F(E, \mathbf{R})$ defined in Eq. (4·19) is exactly the same function as that obtained from $f(E, \mathbf{R})$ by changing $G_0(\mathbf{k})$ to $G(\mathbf{k})$.

In the next place, we perform the first-order renormalization of the vertex by introducing η in Fig. 7 (b) and ξ_0 in Fig. 7 (c). η is a sum over all the ring diagrams obtained through connecting both ends of $W_k(n-m)$:

$$\eta = \sum_{\nu=1}^{\infty} (-V)^{\nu+1} \xi_B^{\nu} \sum_{[n_1]} \cdots \sum_{[n_\nu]} W_k(n-n_1) W_k(n_1-n_2) \cdots W_k(n_\nu-n)$$

$$= \sum_{k} \frac{Nc\xi_B V^2 G_0^2(\mathbf{k})}{1 + Nc\xi_B V G_0(\mathbf{k})}, \tag{4·21}$$

while ξ_0 is given by

$$\xi_0 = 1 + \eta + \eta^2 + \eta^3 + \cdots = \frac{1}{1-\eta}$$

$$= \frac{1 + V_0 f(E, 0)}{1 + V_0 f(E, 0) - V_0 \sum_{k} \dfrac{Nc\xi_B V G_0^2(\mathbf{k})}{1 + Nc\xi_B V G_0(\mathbf{k})}}$$

$$= \frac{1 + V_0 f(E, 0)}{1 + V_0 F(E, 0)}. \tag{4·22}$$

The last result follows from the definition (4·19) and the relation

$$f(E, 0) = \sum_{k} G_0(\mathbf{k}).$$

We call ξ_0 the first-order vertex renormalization constant because it modifies the self-energy part of the optical model $\Sigma^{op}(1)$ into the true first-order self-energy part $\Sigma(1)$:

$$\Sigma^{op}(1) \to \xi_0 \Sigma^{op}(1) = \frac{-Nc\xi_0 V_0}{1 + V_0 f(E, 0)}$$

$$= \frac{-NcV_0}{1 + V_0 F(E, 0)} = \Sigma(1). \tag{4·23}$$

Now, we assume that $F_n(\mathbf{k})$ is given by a sum of diagrams in Fig. 7 (d) with renormalization constant ξ_B. Since this is the same as Fig. 6 (a), the expression for $F_n(\mathbf{k})$ is also the same as (4·14) except that ξ_A should be replaced by ξ_B. Thus we have

$$F_n(\mathbf{k}) = \frac{\xi_B G_0'(\mathbf{k})}{1 + Nc\xi_B V G_0(\mathbf{k})} = \frac{\xi_B G_0(\mathbf{k})}{1 + V_0 f(E, 0) + Nc\xi_B V_0 G_0(\mathbf{k})} \tag{4·24}$$

and, on using Eq. (4·3),

$$G(\mathbf{k}) = \frac{G_0(\mathbf{k})}{1 + Nc\xi_B V G_0(\mathbf{k})}. \tag{4·25}$$

This result proves two facts: First, comparison between (4·25) and (4·19) yields

$$F(E, R) = \sum_k G(k) \exp(ik \cdot R) \tag{4·26}$$

and secondly the self-energy part is now given by

$$\Sigma_B = - NcV\xi_B = \frac{-NcV_0}{1 + V_0 f(E, 0)} \xi_B. \tag{4·27}$$

In the last place, we have to determine ξ_B. We have seen above that ξ_0 gives rise to a correct first-order self-energy part, but to be consistent and include the second-order self-energy part, we must add some correction to ξ_0. This can be easily achieved if we generalize ξ_A by carrying out the first-order renormalization at each vertex and replacing every $W_k(R)$ with $\widetilde{W}_k(R)$. That is, of the three terms in ξ_A, Eq. (4·13) or Fig. 6(b), 1 should be replaced with ξ_0, $W_k^{(3)}(R)$ with $\widetilde{W}_k^{(3)}(R)$ as in Fig. 7(e) and $W_k^{(4)}(R) = (-V)W_k^{(3)}(R) \times W_k^*(R)$ with $\widetilde{W}_k^{(4)}(R)$ as in Fig. 7(f). With (4·20) and (4·22), $\widetilde{W}_k^{(3)}(R)$ and $\widetilde{W}_k^{(4)}(R)$ are constructed in the form

$$\widetilde{W}_k^{(3)}(R) = \frac{\xi_0^4 |\widetilde{W}_k(R)|^2 \widetilde{W}_k(R)}{1 - \xi_0^2 |\widetilde{W}_k(R)|^2}$$

$$= \frac{\xi_0}{1 + V_0 F(E, 0)} \frac{V_0^3 |F(E, R)|^2 F(E, R) \exp(-ik \cdot R)}{[1 + V_0 F(E, 0)]^2 - V_0^2 |F(E, R)|^2} \tag{4·28}$$

and

$$\widetilde{W}_k^{(4)}(R) = \frac{\xi_0^5 |\widetilde{W}_k(R)|^4}{1 - \xi_0^2 |\widetilde{W}_k(R)|^2}$$

$$= \frac{\xi_0}{[1 + V_0 F(E, 0)]^2} \frac{V_0^4 |F(E, R)|^4}{[1 + V_0 F(E, 0)]^2 - V_0^2 |F(E, R)|^2}. \tag{4·29}$$

Collecting these results into ξ_B given in Fig. 7(g), we have

$$\xi_B = \xi_0 + \sum_{[k]} \{\widetilde{W}_k^{(3)}(R) + \widetilde{W}_k^{(4)}(R)\}$$

$$= \xi_0 \left\{ 1 - \frac{cV_0^3}{[1 + V_0 F(E, 0)]^2} \right.$$

$$\left. \times \sum_k \frac{|F(E, R)|^2 F(E, R)[1 + V_0 F(E, 0)] \exp(-ik \cdot R) - V_0 |F(E, R)|^4}{[1 + V_0 F(E, 0)]^2 - V_0^2 |F(E, R)|^2} \right\}. \tag{4·30}$$

It is an easy task to check that the self-energy part (4·27) together with (4·30) satisfies the relation

$$\Sigma_B = \Sigma(1) + \Sigma(2) \tag{4·31}$$

when $P_s(c) = c$. Thus our original purpose has been accomplished.

§ 5. Discussion and summary

Let us first consider the relation between the local modes of one impurity and of the cluster of two impurities and the fine spikes of a random system which appear in the band gap of the regular lattice. The level density including the first-order correction $\Sigma(1)$ has been calculated with the approximation that electrons in the main band are taken to be free and that the concentration c of impurities is so small that $P_s(c)$ is regarded as c. The result of the computation is pictured in Fig. 15 of I. It is obvious from this figure that an impurity band arises around the local mode of an impurity—the smallest of the solutions given by Eq. (2·6). The level density including the second-order correction given by Eq. (3·14) is examined and leads to the similar conclusion that, for the very small values of c, the impurity levels are found at the eigenenergies which are derived from Eq. (2·14). In this way, the correspondence between the local modes caused by the islands of impurity atoms and the many spikes in the energy spectrum of a disordered system may be seen through the Green's function method as well.

On the other hand, the existence of the special frequencies is not so easily seen. For instance, Fig. 15 of I shows that, when c deviates from zero, the band gap is rapidly smeared up irrespective of the magnitude of V_0, so that the band gap does not persist. This breakdown actually comes from the fact that taking $P_s(c)$ as c is a terribly bad approximation except for extremely small values of c. Therefore, we require a numerical result or a general proof based on a formulation which treats $P_s(c)$ without any approximation. The results of the calculation will be reported shortly.

From Eq. (2·17) of II written as

$$D(E) = -\lim_{\delta \to 0+} \mathrm{Im} \left[\frac{1}{\pi} \, \mathrm{tr} \, G(E+i\delta) \right]$$

which relates the Green's function with the state density, it is concluded that the special frequencies are determined by those energy values E which give real values to $G(E)$, since the state density vanishes for such E.

In the next place, we consider how the approximation for the self-energy part is improved. From a mathematical point of view, it may be supposed to be adequate to sum up all the third-order diagrams in which three impurities are involved; the diagram in Fig. 8(a) is one of them. But, as a matter of fact, it will be seen that the diagrams in Fig. 8(b) play a more important role; the summation in this case is carried out by using the criterion that only one or two impurities are concerned with the scattering of an electron at any arbitrary instance. By way of example, let us consider the point A on the electron line in Fig. 8(a). At this moment, all the three impurities are in the process of interaction with the electron. If we take the point B on the electron line in
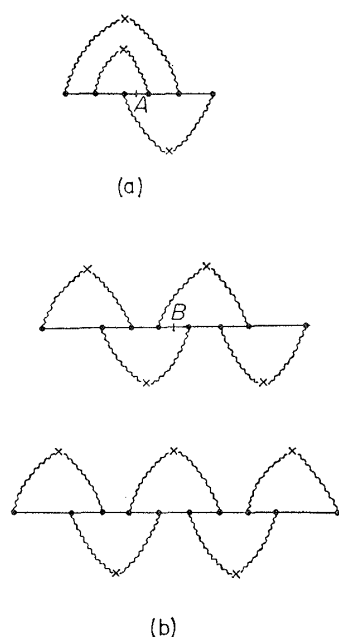
(a)

(b)

Fig. 8. Higher order diagrams.

Fig. 8(b), it is apparent that the interaction of the electron with the first impurity has already been completed and the interaction with the last one has not yet set in, so that only the second and third impurities are interacting with the electron.

The physical picture of the former approximation is that the effective ranges of two or three impurities overlap and are isolated from the effective ranges of the rest of the impurities. This is the opposite of the assumption that the two kinds of atoms are mixed up completely at random; that is, the probability for several impurities to gather in the host lattice is very small. In the latter case, the diagrams are summed on the ground that the effective ranges of all the impurities are distributed almost uniformly and that there is only a poor chance for the formation of islands. This is expected to be more realistic for the problem under consideration.

In § 3 and § 4, the formulation of $\Sigma(2)$ has been demonstrated by means of two different methods. It can be shown that the M-T method is more useful in dealing with the latter of the two approximations described in the above, because this method gives a more visual insight into the problem. The detailed discussion will be given elsewhere.

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