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# Coarse-Grained Quantities and Local Environment Effects in Disordered Systems*)

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It is proved that the effective "distance" $\bar{m}(\varepsilon+i\Gamma)$, proposed first by Matsuda for a linear chain model with nearest-neighbour interaction, exists in any dimensional disordered systems described by a bounded Hamiltonian with short-range interaction. Thus the local situation or short-range order plays an essential role in determining various physical quantities in the sense that the Green function $G_{l,l'}(\varepsilon+i\Gamma)$ is almost determined by the local situation of the system at and around the sites $l$ and $l'$.

## § 1. Introduction

Since the pioneering works of Dyson,[2] Broadbent and Hammersley,[3] Anderson,[4] Dean,[5] Edwards[6] and Ziman,[7] the study of systems without periodicity has become an important theme in solid state physics.

For periodic systems, tremendous progress has been made in the last half century on the basis of Bloch's theorem[8] and the band picture has become one of the most important concepts for understanding the characteristics of the solid states. On the other hand, a widely accepted concept in the molecular field[9),10] suggests strongly that the local situation of the system also affects many physical quantities. In fact, many workers have succeeded in obtaining reasonable results, using the molecular field approximation or molecular field-like approximations.

Roughly speaking, there are three types of physical phenomena. One is characterized by the existence of long-range order of the system such as those due to the van Hove singularities of the density of states. Another is characterized by the local properties of the system as discussed in recent works of Ioffe and Regel,[11] Weaire and Thorpe,[12] Ziman,[13] and Haydock et al.[14] The other is of the intermediate type which is characterized by the local situation in a wider range. The last is regarded as one of the difficulties in the detailed study of amorphous solids and of alloys.[15]

As for the latter two types of phenomena it is essential to disregard Bloch's theorem and to find new fundamental principles or theorems from another point of view such as the local picture. This has been the author's principal aim in

*) An essential part of this paper has been reported in Int. Conf.; Lattice Dynamics (Paris, 1977) (Ref. 1)).

carrying out some work in the field.[16)~19)]

The concept of effective "distance", which will be generally proved in this paper is important in discussing the effect of the local situation or short-range order of the systems. This concept was first proposed by Matsuda[20),*)] for a linear chain model with nearest-neighbour interaction. He succeeded in proving for the model that its local character almost determines various coarse-grained physical quantities. In this paper more general conclusions are obtained for general disordered systems of any dimension with arbitrary short-range interaction.

In § 2, a model is introduced and a short remark is given on the term coarse-graining. In § 3, Matsuda's approach is applied to the recursion method.[21),22)] Fundamental theorems on general disordered systems are given in § 4. The final section is devoted to conclusions and discussion.

## § 2. Model Hamiltonian and coarse-grained quantities

Let us consider the following type of Hamiltonian described in a site representation as

$$H=\sum_{l}|l\rangle a_l\langle l|+\sum_{l\neq l'}|l\rangle t_{l,l'}\langle l'|\,, \tag{2·1}$$

where $\{|l\rangle\}$ is a set of orthonormalized bases characterised by $N_0$ sites $\{l\}$. Two following restrictions are assumed on (2·1). One is that $H$ is bounded, that is,

$$\|H\|\equiv\sup_{|f\rangle\neq 0}\sqrt{\frac{\langle f|H^2|f\rangle}{\langle f|f\rangle}}\Rightarrow E_M<\infty\,. \tag{2·2}$$

The other is that the interaction is of short-range, that is, there exists a value $l_0$ representing the range of interaction such that

$$t_{l,l'}=0 \qquad \text{for } \{l,\, l'\|l-l'|>l_0\}, \tag{2·3}$$

where $|l-l'|$ is some distance between sites $l$ and $l'$. The Hamiltonian (2·1) with conditions (2·2) and (2·3) can describe a wide range of disordered systems including topologically disordered one such as the Weaire-Thorpe model.[12)]

The Green function $G(E)$ is defined by

$$(H-E)G(E)=1\,, \tag{2·4}$$

$$E=\varepsilon+i\Gamma\,, \qquad \Gamma>0\,. \tag{2·5}$$

The following relation exists for the Green function (see M)

*) Reference 20) is referred to as M hereafter in this paper.

$$\text{Im } G_{l,l'}(E)=\frac{1}{\pi}\int_{-\infty}^{\infty}G''_{l,l'}(\varepsilon')\frac{\Gamma}{(\varepsilon'-\varepsilon)^2+\Gamma^2}d\varepsilon' ,$$

$$G''_{l,l'}(\varepsilon)\equiv\lim_{\Gamma'\to 0_+}\text{Im } G_{l,l'}(\varepsilon+i\Gamma'), \tag{2·6}$$

and accordingly various physical quantities derived from the Green function are coarse-grained by $\Gamma$.

## § 3. Matsuda's approach applied to recursion method

Let us construct a set of orthonormalized bases starting from an arbitrary state $|1)$,[21),22)]

$$|1), \qquad (1|1)=1 ,$$

$$|n)=\{(1-\sum_{n'=1}^{n-1}|n')(n'|)H|n-1)\}\Big/\sqrt{(n-1|H(1-\sum_{n'=1}^{n-1}|n')(n'|)H|n-1)} ,$$

$$(n=2, 3, \cdots, N). \tag{3·1}$$

The integer $N$ is equal to or smaller than $N_0$ in (2·1), because in some case a state $|n')$ can vanish for $n'\leqq N_0$ owing to the symmetries of $H$ and $|1)$. The Hamiltonian $H$ is closed and real tri-diagonal in the subspace on the sequence of bases $\{|n);\ n=1, 2, \cdots, N\}$. Let us denote its non-vanishing matrix elements as

$$\beta_n^-\equiv(n|H|n-1)=(n-1|H|n)\equiv\beta_{n-1}^+$$

$$=\sqrt{(n-1|H(1-\sum_{n'=1}^{n-1}|n')(n'|)H|n-1)} , \quad (n=2, \cdots, N)$$

$$a_n\equiv(n|H|n). \qquad (n=1, \cdots, N) \tag{3·2}$$

Some examples of the set of bases on an ordered square lattice with nearest-neighbour interaction are shown in Fig. 1.

In this subspace with the $\{|n)\}$ representation the Green function satisfies

$$\beta_n^- G_{n-1,n'}(E)+(a_n-E)G_{n,n'}(E)+\beta_n^+ G_{n+1,n'}(E)=\delta_{n,n'} ,$$

$$(n, n'=1, \cdots, N) \tag{3·3}$$

with the condition

$$\beta_1^-=\beta_N^+=0 . \tag{3·4}$$

The subscripts $n$, $n'$ ($n''$, $m$, 1 and $N$) are used throughout this paper when a new set of bases $\{|n)\}$ is used to describe the Green function, while the subscripts $l$, $l'$ ($l''$ and $l'''$) are used when the site representation with $\{|l\rangle\}$ is adopted.

Equation (3·3) with the condition (3·4) is just Eq. (3·4) in M and hence we

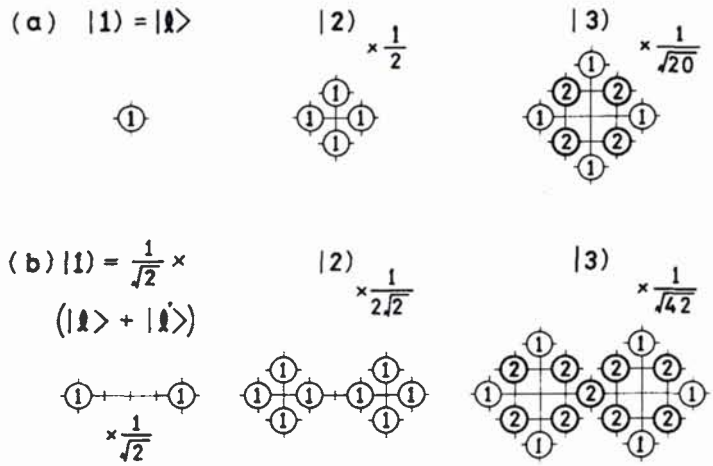


Fig. 1. Some examples of the wave functions of the bases $\{|n)\}$ on the ordered square lattice with nearest-neighbour interaction and with one-component on each site.

can obtain immediately the following results.

There exists an effective distance $\bar{m}=\bar{m}(E)$ corresponding to each $E$ ($\mathrm{Im}\,E>0$) such that

(i) $|G_{n,n'}(E)|<\sqrt{\bar{m}}\,\mathrm{Min}\{|G_{n,n}(E)|, |G_{n',n'}(E)|\}\exp\{-|n-n'|/2\bar{m}\}$.

(ii) The value of $G_{n,n'}(E)$, ($|n-n'|<\bar{m}$) is almost determined by the set of values $\{\alpha_{n''}\}$ and $\{\beta^{\pm}_{n''}\}$ with $|n''-n|\leqq\bar{m}$ or $|n''-n'|\leqq\bar{m}$ in the sense that its dependence on the values $\{\alpha_{n''}\}$ and $\{\beta^{\pm}_{n''}\}$ with $|n''-n|>m$ and $|n''-n'|>m$ decreases with increasing $m$ by a factor of $\exp\{-m/\bar{m}\}$.

(iii) $\bar{m}(E)\leqq\sup(1+(\beta^{-}_{n})^2/\Gamma^2)\leqq m_0$.

(iv) $m_0\equiv 1+(E_M/\Gamma)^2$.

In the last inequality in (iii) the following inequality has been used:

$$|\beta^{\pm}_{n}|\leqq E_M\,. \tag{3·5}$$

## § 4. Upper bound and convergence property of the Green function

Let us define the "distance" $m(l, l')$ between sites $l$ and $l'$ by

$$m(l, l')\equiv\mathrm{Min}\{k|\langle l'|H|k-1\rangle\cdots\cdots\langle l_2|H|l_1\rangle\langle l_1|H|l\rangle\neq 0 \quad \text{for some}(l_1, l_2, \cdots, l_{k-1})\}, \qquad \text{for } l\neq l'$$

and by

$$m(l, l)\equiv 0\,, \tag{4·1}$$

which has the following properties:

$$m(l, l')\geqq 0\,, \quad (m(l, l')=0 \text{ if and only if } l=l')$$

$$m(l, l')=m(l', l),$$
$$m(l, l')\leqq m(l, l'')+m(l'', l'). \tag{4·2}$$

The distance $m(l, l')$ corresponds to the path of minimum length between the sites $l$ and $l'$, providing that the lengths between sites $l''$ and $l'''(\neq l'')$ for $\langle l''|H|l'''\rangle \neq 0$ are 1. A simple example of the distance is seen in Fig. 1(a) for the ordered square lattice with nearest-neighbour interaction. In this case the distance between the sites on which the base $|2\rangle$ ($|3\rangle$ or $|4\rangle$) has nonzero values and the site $|1\rangle=|l\rangle$ is 1(2 or 3). Roughly speaking, we can find the sites, at a distance $m$ from a site $l$, by seeing the "wave front" of the base $|m+1\rangle$ providing $|1\rangle=|l\rangle$.

Now we can consider the upper bound and the convergence property of the matrix element $G_{l,l'}(E)$ of the Green function in the site representation. In the case when $|1\rangle=|l\rangle$ for a fixed site $l$, we obtain from (i) in § 3

$$|G_{1,m+1}(E)|\equiv|\langle l|G(E)|m+1\rangle|<\mathrm{Min}\{|G_{l,l}(E)|, |G_{m+1,m+1}(E)|\}\sqrt{m_0}$$
$$\times\exp\{-m/2m_0\}\ni f^l(m). \tag{4·3}$$

If a site $l'$ is at a distance $m(l, l')$ from $l$, then the state $|l'\rangle$ is a linear combination of the states $\{|n'\rangle, (n'\geqq m+1)\}$ and a state $|\sigma\rangle$ which is orthogonal to the states $\{|n\rangle, n=1, \cdots, N\}$, that is,

$$|l'\rangle=\sum_{n'\geqq m+1}^{N} C^l_{n'}|n'\rangle+|\sigma, l\rangle,$$
$$\sum_{n'\geqq m+1}^{N}|C^l_{n'}|^2+\langle\sigma, l|\sigma, l\rangle=1. \tag{4·4}$$

Accordingly we have

$$|G_{l,l'}|=|\langle l|G|l'\rangle|=|\sum_{n'\geqq m+1}^{N} C^l_{n'}\langle l|G|n'\rangle|$$
$$\leqq\sqrt{\sum_{n'\geqq m+1}^{N}|C^l_{n'}|^2\cdot\sum_{n'\geqq m+1}^{N}|\langle l|G|n'\rangle|^2}$$
$$\leqq f^l(m)/\sqrt{1-\exp\{-1/m_0\}}. \tag{4·5}$$

Recalling that

$$|G_{l,l'}(E)|=|G_{l',l}(E)|, \tag{4·6}$$

we have a final expression

$$|G_{l,l'}(E)|<\mathrm{Min}\{|G_{l,l}(E)|, |G_{l',l'}(E)|\}\sqrt{m_0/(1-\exp\{-1/m_0\})}$$
$$\times\exp\{-m(l, l')/2m_0\}. \tag{4·7}$$

The convergence property of the Green function $G_{l,l'}$ can be proved as

follows. First, supposing $|1\rangle=|l\rangle$ we see from the convergence results in § 3 that the value of $G_{l,l}=\langle l|G|l\rangle=(1|G|1)$ is almost determined by the set of values $\{a_{l''}\}$ and $\{t_{l'',l'''}\}$ in the region $m(l'', l)$, $m(l''', l)\leqq m_0$ in the sense that its dependence on the set of values $\{a_{l''}\}$ and $\{t_{l'',l'''}\}$ in the region $m(l'', l)>m$ decreases with increasing $m$ by factor of $\exp\{-m/m_0\}$. Next, supposing $|1\rangle=(1/2)(|l\rangle+|l'\rangle)$ and $|1\rangle=(1/2)(|l\rangle+i|l'\rangle)$ we see the convergence results for

$$(1|G|1)=\frac{1}{2}(G_{l,l}+G_{l',l'})+\mathrm{Re}\ G_{l,l'} \tag{4·8a}$$

and

$$(1|G|1)=\frac{1}{2}(G_{l,l}+G_{l',l'})-\mathrm{Im}\ G_{l,l'}, \tag{4·8b}$$

respectively. This implies that the same is true for $G_{l,l'}(E)$.

## § 5. Conclusions and discussion

The first conclusion is that the effective "distance", $\bar{m}(\varepsilon+i\Gamma)$ proposed first by Matsuda for a linear chain model with nearest-neighbour interaction, exists in general in disordered systems described by the bounded Hamiltonian (2·1) with the short-range interaction. The concept of "distance" was introduced for the first time in this paper as a metric naturally induced by the Hamiltonian.

The effective distance $\bar{m}(E)$ guarantees the properties (1) and (2) in the following and its existence is guaranteed by the inequality (3).

(1) $|G_{l,l'}(E)|\leqq \mathrm{Min}\{|G_{l,l}(E)|, |G_{l',l'}(E)|\}\sqrt{\bar{m}(E)/(1-\exp\{-1/\bar{m}(E)\})}$
$\times\exp\{-m(l, l')/2\bar{m}(E)\}$.

(2) The Green function $G_{l,l'}(E)$ is essentially determined by the local situation within the effective "distance" $\bar{m}(E)$ from the sites $l$ and $l'$ in the sense that the dependence of $G_{l,l'}(E)$ on the matrix elements $\{a_{l''}\}$ and $\{t_{l'',l'''}\}$ in the region $m(l'', l)$, $m(l'', l')>m$ decreases by increasing $m$ by a factor of $\exp\{-m/\bar{m}(E)\}$.

(3) $\bar{m}(E)\leqq m_0\equiv(1+(E_M/\Gamma)^2)$.

The first conclusion mentioned above has been obtained for any finite system (2·1) ($N_0<\infty$) with the conditions (2·2) and (2·3). We have seen that the proof and hence the results do not depend on the size of the system $N_0$ or $N$.

We have thus come to the second conclusion that the first conclusion is valid also for infinite systems which have the properties (2·2) and (2·3) and which are constructed by the limit from the finite systems.

We have shown an upper bound of the $\mathrm{Max}|\beta_n^-|$ as $E_M$ and hence an upper

bound of the effective distance. However, as has been shown in M, the effective distance can be much smaller than the estimated upper bound. It is thus important to study the effective distance quantitatively. This problem is open for the future study.

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