Renormalization group and critical localization*

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The renormalization-group (RG) method is applied to the problem of formation of a localized state of a particle moving in a given potential. It is shown that RG transformation on the particle's Green's function can be performed exactly. The fixed-point equations yield information on the critical binding strength, while the transformation equations near the fixed points give scaling laws and critical exponents, e.g., for the dependence of the localization radius on the energy and the potential strength. The general theory is illustrated by considering the simplest case of the Slater-Koster problem in detail. We find that it is possible to take all the irrelevant variables into account and thus obtain the exact result for the critical binding point. Critical exponents and scaling laws are, however, universal in character. The method is then extended to the case of motion in random potentials, and some applications are pointed out. In particular it is shown that the RG properties of the averaged absolute value squared ($\langle |G|^2 \rangle$) of the Green's function do not correspond to a simple second-order phase transition. The analysis illustrates certain features of RG methods which have not heretofore been encountered in other problems and which are likely to be found in treatments of disordered materials. In particular, the runaway behavior observed in the RG transformation of $\langle G \rangle$ and $\langle |G|^2 \rangle$ as well as in many random-spin systems, might be associated with the formation of bound states in the band tail for any amount of randomness.

I. INTRODUCTION

Since its introduction by Wilson into the field of critical phenomena,[1] renormalization-group (RG) theory has been extensively studied.[2,3] Most of the work to date has been focused on using the theory to treat various problems in phase transitions and critical phenomena, though some applications in the theory of polymers (excluded volume problem)[4] and percolation theory[5] have been published. The close connection of both the excluded volume problem[6,7] and percolation theory[7,8] with the quantum theory of motion in a random potential[9] suggests that RG theory may be useful also for this last problem, and an attempt in this direction has been made.[10]

In this paper we study a new application of RG theory—to the problem of critical binding. We consider a particle moving on an infinite lattice under the influence of a given potential. If the strength of the potential is characterized by a given parameter, it is of interest to determine the critical value of the parameter that gives rise to a bound state. The applicability of RG theory to this problem is related to the fact that this is actually a question about the behavior of the wave functions at large distances from the binding center: A potential which does not give rise to a bound state does not affect the long-distance behavior of the (free-particle) wave functions, while a potential which leads to at least one bound state

does. We therefore expect that under conditions where no bound state exists, the potential is an irrelevant variable of the RG transformation with respect to the free-particle fixed point, and that averaging out short-wavelength information leads to a free-particle Hamiltonian. At the critical value of the binding-strength parameter, the potential should become a relevant variable. The RG equations around the corresponding fixed point then contain information about the critical binding region (such as the way in which the localization radius becomes infinite when the binding strength approaches its critical value from above).

The Hamiltonian for the problem is taken to be (in the lattice-site representation)

$$H = \sum_{\vec{n}\vec{m}} J_{\vec{n}\vec{m}} a_{\vec{n}}^{\dagger} a_{\vec{m}} + \sum_{\vec{n}} \vec{V}_{\vec{n}} a_{\vec{n}}^{\dagger} a_{\vec{n}}, \tag{1.1}$$

where $a_{\vec{n}}^{\dagger}$ and $a_{\vec{n}}$ are creation and annihilation operators for the particle on site $\vec{n}$ and where $J_{\vec{n}\vec{m}} = J$ for nearest neighbors and is zero otherwise. It is possible to include non-nearest-neighbor terms at the cost of more tedious algebra. The first term in (1.1) corresponds to a single-band model for the motion of a particle on a pure (periodic) lattice (or, in the continuous limit, to the kinetic energy of a free particle), while the second part is the imposed local potential. A matrix element of the corresponding Green's function can be represented as a correlation function of a classical field by employing the identity for multivariate Gaussian variables:

$$G_{\bar{i}\bar{j}}=\left(\frac{1}{\bar{E}-H}\right)_{\bar{i}\bar{j}}=\frac{\alpha}{Z}\int d\vec{X}\,\vec{X}_{\bar{i}}\vec{X}_{\bar{j}}e^{-\alpha U[\vec{X}]}, \qquad (1.2)$$

$$Z=\int d\mathbf{X}\,e^{-\alpha U[\vec{X}]}, \qquad (1.3)$$

$$U[\mathbf{X}]=\frac{1}{2}\sum_{\bar{n}}(\bar{E}-\bar{V}_{\bar{n}})X_{\bar{n}}^{2}-\frac{1}{2}\sum_{\bar{m}}\sum_{\bar{n}}J_{\bar{m}\bar{n}}X_{\bar{m}}X_{\bar{n}}$$

$$=\frac{1}{2}\sum_{\bar{n}}(\bar{E}-2dJ-\bar{V}_{\bar{n}})X_{\bar{n}}^{2}+\frac{1}{2}J\sum_{\bar{n}}\sum_{\bar{i}}(X_{\bar{n}}-X_{\bar{n}+\bar{i}})^{2}. \qquad (1.4)$$

In Eq. (1.4) d is the dimensionality and $\sum_{i}$ corresponds to the sum over nearest neighbors. α is a free parameter which can be chosen so that the integrals in Eqs. (1.3) and (1.4) converge wherever G is analytic. This feature of the theory is important in treating disordered systems, since, without α, averages of G, etc., over the random potentials are undefined. For simplicity we have specialized here to a d-dimensional generalization of a simple cubic lattice. In q space $U[X]$ takes the form

$$U[X]=\frac{1}{2}\int_{\bar{q}}\left[\bar{E}-2dJ+2J\left(d-\sum_{i}\cos(2\pi q_{i})\right)\right]X_{\bar{q}}X_{-\bar{q}}$$

$$-\frac{1}{2}\int_{\bar{q}}\int_{\bar{q}'}\bar{V}_{-(\bar{q}+\bar{q}')}X_{\bar{q}}X_{\bar{q}'}, \qquad (1.5)$$

where $\int_{\bar{q}}=\int_{0}^{1}d^{d}q$ and where the transformation is

$$X_{\bar{n}}=\int_{\bar{q}}X_{\bar{q}}e^{2\pi i\bar{n}\cdot\bar{q}},$$

$$X_{\bar{q}}=\sum_{\bar{n}}X_{\bar{n}}e^{-2\pi i\bar{n}\cdot\bar{q}}. \qquad (1.6)$$

The normalization is chosen so $\bar{q}$ is dimensionless, and the lattice spacing is 2π. q_{i} is the component of the vector q along the ith axis. Defining E and V to be

$$E=(\bar{E}+2dJ)/(2\pi)^{2}J,$$

$$V=\bar{V}/2(2\pi)^{2}J, \qquad (1.7)$$

and making the effective-mass approximation about the lower band edge we obtain

$$U=\frac{1}{2}\int_{\bar{q}}(E-q^{2})X_{\bar{q}}X_{-\bar{q}}-\int_{q}\int_{q'}V_{-(\bar{q}+\bar{q}')}X_{\bar{q}}X_{\bar{q}'}. \qquad (1.8)$$

The neglected terms are of higher order in q^{2} and are irrelevant under the RG transformation. They are not expected to affect any universal feature of the critical-binding problem, but are important (and are reintroduced) in determining the exact value of the critical-binding strength. Equation (1.8) can also be viewed as the starting point for the critical-binding problem in the continuous limit.

In the language of the theory of critical phenomena, Eqs. (1.2)–(1.5) and (1.8) constitute a generalized Gaussian model with a nonisotropic Hamiltonian. Recently, Wegner[11] has discussed the influence of adding such nonisotropic terms to an otherwise isotropic Hamiltonian and showed that this leads to renormalization of the scaling fields, namely, to a change in the critical temperature. In the model discussed here, however, expanding the parameter space on which H is defined by including the new anisotropic term leads to a new fixed point which plays a crucial role in the critical-binding problem.

The analysis described above is the starting point for the use of RG methods in problems involving single-particle Hamiltonians in contrast to problems involving Ising-like models arising in applications to critical phenomena. This generalization of RG methods is a prerequisite to attempts at applying it to disordered quantum-mechanical systems. In this paper we first study the nonrandom case with special attention given to the single-impurity problem. This simple application serves to illustrate a number of novel features of the RG method as applied to single-particle quantum-mechanical Hamiltonians. First, it represents one of the very few cases in which a nontrivial solution to the RG transformations is obtained exactly, thereby generating a means for testing various hypotheses concerning approximations in general cases and providing a useful example of the rather involved theory. Second, the calculation shows how a "critical phenomenon," the occurrence of a bound state, is associated with unstable fixed points of the RG transformation, rather than the usual cases where the saddle-point-type fixed points are associated with the physical phenomena. Third, it is demonstrated that all the irrelevant variables must be included to obtain the critical-binding criterion correctly.

The present approach can be easily extended to include the case where V is a random potential. In this case we study the transformation properties of the moments of this random potential rather than the potential itself. To discuss the localization problem the RG transformation is applied to $\langle|G|\rangle^{2}$—the average of the absolute value squared of the Green's function. In contrast to the single-impurity problem, a runaway behavior is obtained which may possibly indicate that the transition to localization as the randomness increases is either smeared or of the first-order type.

The RG method can also be applied to the calculation of density of states in disordered systems. Some comments on this possibility are made at the end of Sec. V (A).

In the following sections we give a detailed discussion of the critical-localization problem within the context of RG theory. A general treatment, which is applicable for arbitrary short-range potentials, is provided in Sec. II. In Sec. III we specialize the general theory to the simplest case of the single-impurity problem, and in Sec. IV we study the role of the irrelevant variables and obtain the exact solution for the Slater-Koster problem[12] (localization of an impurity state in a periodic lattice). Finally, in Sec. V we outline the extension of this method to motion in a random potential and discuss the behavior of the averaged quantities $\langle G \rangle$ and $\langle |G|^2 \rangle$ under the RG transformation.

II. RG TRANSFORMATION

Let the q-space Green's function be written

$$G_{\vec{q}\vec{q}'} = \frac{1}{Z} \int d\vec{X} X_{\vec{q}} X_{\vec{q}'} e^{-U[\vec{X}]}, \qquad (2.1)$$

$$U[\vec{X}] = \frac{1}{2} \int_{\vec{q}} u_2(q) X_{\vec{q}} X_{-\vec{q}} - \int_q \int_{q'} V_{-(\vec{q}+\vec{q}')} X_{\vec{q}} X_{\vec{q}'}, \qquad (2.2)$$

$$u_2(q) = E - q^2 .$$

Strictly speaking the parameter α should be retained here as in (1.2) and (1.3) to insure convergence, but this parameter can be shown to cancel at the end of the calculations that are presented herein. Focusing attention on the "partition function,"

$$Z = \int d\vec{X} \exp\left(-\frac{1}{2}\int_q u_2(q) X_{\vec{q}} X_{-\vec{q}} + \int_{\vec{q}} \int_{\vec{q}'} V_{-(\vec{q}+\vec{q}')} X_{\vec{q}} X_{\vec{q}}\right) , \qquad (2.3)$$

the RG transformation is performed with the by now conventional steps: (a) Integrate over all X_q with $1/s < q \le 1(s > 1)$. (b) Redefine new momentum variables $q' = sq$ which have the same cutoff 1 as the old variable q in the original Hamiltonian. (c) Redefine the field variables X_q to make the q^2 term in $u_2(q)$ invariant under the transformation. As in the simple Gaussian model, no anomalous dimensions appear in this model, and $X'_{q'} = s^{-(d+2)/2} X_q$.

In carrying out step (a) we encounter a simple perturbation expansion which can easily be resummed to all orders. Let us rewrite Eq. (2.3)

FIG. 1. Typical diagram in the expansion Eq. (2.5).

as

$$Z = I'_0 \int^{''} d\vec{X} \exp\left(-\frac{1}{2}\int_{\vec{q}}^{''} u_2(q) X_{\vec{q}} X_{-\vec{q}}\right) I , \qquad (2.4a)$$

$$I = \frac{1}{I'_0} \int^{'} d\vec{X} \exp\left(-\frac{1}{2}\int_{\vec{q}}^{'} u_2(q) X_{\vec{q}} X_{-\vec{q}}\right.$$

$$\left. + \int_{\vec{q}} \int_{\vec{q}} V_{-\vec{q},\vec{q}'} X_{\vec{q}} X_{\vec{q}'}\right) , \qquad (2.4b)$$

$$I'_0 = \int^{'} d\vec{X} \exp\left(-\frac{1}{2}\int_{\vec{q}}^{'} u_2(q) X_{\vec{q}} X_{-\vec{q}}\right) , \qquad (2.4c)$$

where the general notation $V_{-\vec{q},\vec{q}'}$ is used instead of $V_{-(q+q')}$ as the latter is appropriate only for local operators in n space. The general definition is

$$\langle \vec{P}_i | V | \vec{P}_j \rangle = V_{\vec{P}_i, \vec{P}_j} = \sum_{\vec{n}} \sum_{\vec{n}'} e^{-i\vec{P}_i \cdot \vec{n}} V_{\vec{n}\vec{n}'} e^{i\vec{P}_i \cdot \vec{n}} . \qquad (2.5)$$

For local operators $V_{\vec{n}\vec{n}'} = V_{\vec{n}} \delta_{\vec{n}\vec{n}'}$ and

$$V_{-(\vec{q}+\vec{q}')} = V_{-\vec{q},\vec{q}'} = \langle -\vec{q} | V | \vec{q}' \rangle . \qquad (2.6)$$

Also in Eqs. (2.4) $\int^{''}$ denotes integration over variables $0 < q \le 1/s$, while $\int^{'}$ denotes integration over variables $1/s < q \le 1$. The I'_0 terms in Eq. (2.4a) can be disregarded when RG transformation on $G_{qq'}$ is being considered. I can be expanded in powers of V in the form

$$I = \exp\left(\sum_n \frac{1}{n!} W_n\right), \qquad (2.7)$$

where W_n stands for the contribution of all linked diagrams of order n. A typical such diagram is shown in Fig. 1. A straight line carrying momentum $\vec{P}$ stands for $u_2(P)^{-1}$. A dotted line, between q and P stands for $V_{-\vec{q},-\vec{p}}$. Internal momenta are integrated from s^{-1} to 1. External momenta are integrated from 0 to s^{-1}. Thus the diagram in Fig. 1 is given by

$$\int_{\vec{q}}^{''} \int_{\vec{q}'}^{''} \left(\int_{\vec{P}_1}^{'} \int_{\vec{P}_2}^{'} \cdots \int_{\vec{P}_{n-1}}^{'}\right) \frac{V_{-\vec{q}_1, -\vec{P}_1} V_{-\vec{P}_1, -\vec{P}_2} V_{-\vec{P}_2, -\vec{P}_3} \cdots V_{-\vec{P}_{n-2}, -\vec{P}_{n-1}} V_{-\vec{P}_{n-1}, \vec{q}'}}{u_2(P_1) u_2(P_2) \cdots u_2(P_{n-1})} \; X_{\vec{q}} X_{\vec{q}'} . \qquad (2.8)$$

Now define the projected propagator

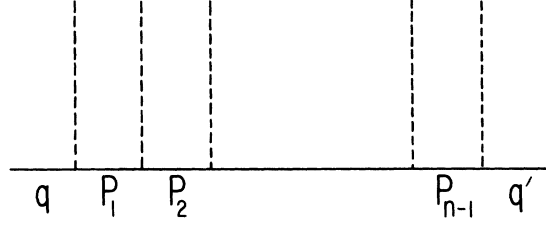$$A_0 = \int_{\vec{p}}^{'} |\vec{P}\rangle u_2(p)^{-1} \langle \vec{P} | . \qquad (2.9)$$

With this notation, the expression (2.8) takes the compact form

$$\int_{\vec{q}}^{''} \int_{\vec{q}'}^{''} \langle -\vec{q} | (VA_0)^{n-1} V | \vec{q}' \rangle X_{\vec{q}} X_{\vec{q}'} . \qquad (2.10)$$

It is easy to realize that all the diagrams in order n are equivalent and that there are $2^{n-1} n!$ such equivalent diagrams. Equation (2.7) therefore becomes

$$I = \exp\left(\sum_{n=1}^{\infty} 2^{n-1} \int_{\vec{q}} \int_{\vec{q}'} \langle -\vec{q} | (VA_0)^{n-1} V | \vec{q}' \rangle X_{\vec{q}} X_{\vec{q}'} \right)$$

$$= \exp\left(\int_{\vec{q}}^{''} \int_{\vec{q}'}^{''} \langle -\vec{q} | \bar{V} | \vec{q}' \rangle X_{\vec{q}} X_{\vec{q}'} \right) , \qquad (2.11)$$

where

$$\bar{V} = (1 - 2VA_0)^{-1} V . \qquad (2.12)$$

This completes step (a) of the RG transformation. After this step the "partition function" takes the form

$$Z = \int^{''} d\vec{X} \exp\left(-\frac{1}{2} \int_{\vec{q}} u_2(q) X_{\vec{q}} X_{-\vec{q}} \right.$$

$$\left. + \int_{\vec{q}}^{''} \int_{\vec{q}'}^{''} \bar{V}_{-\vec{q},\vec{q}'} X_{\vec{q}} X_{\vec{q}'} \right) . \qquad (2.13)$$

Here the factor I_0', which appears in (2.4a), has been disregarded as discussed above. Steps (b) and (c) can now be easily performed. The final form of the transformed "partition function" is idential to (2.3) with $u_2'(q)$ replacing $u_2(q)$ and $V_{-\vec{q},\vec{q}'}'$ replacing $V_{-\vec{q},\vec{q}'}$, where

$$u_2'(q) = s^2 u_2(q/s) \qquad (2.14a)$$

and

$$V' = s^{2-d} (1 - 2VA_0)^{-1} V . \qquad (2.14b)$$

These are the RG equations for a transformation which involves scaling by a factor s. It is convenient to rewrite these equations for an infinitesimal transformation $s = 1 + \delta t$. Recalling that $u_2(q)$ is of the form $E - q^2 + O(q^4)$, it is evident that the $O(q^4)$ terms are irrelevant in Wilson's sense. Equation (2.14a) then leads to the differential equation for E:

$$\frac{dE}{dt} = 2E , \qquad (2.15)$$

which is the usual Gaussian equation. We see that $E = 0$ must be satisfied at any fixed point. To obtain a differential equation from Eq. (2.14b) we note that A_0, Eq. (2.9), takes the form

$$A_0 = \delta t (E - 1)^{-1} Q , \qquad (2.16)$$

where Q is the projection operator

$$Q = \int d\Omega | \vec{1} \rangle \langle \vec{1} | , \qquad (2.17)$$

in which $\vec{1}$ is a unit vector and the integration is over all the $d - 1$ angular coordinates. The differential RG equation for V then becomes (in an operator form)

$$\frac{dV}{dt} = (2 - d)V + \frac{2}{E - 1} VQV . \qquad (2.18)$$

The following points should be noted:

(a) Equations (2.15) and (2.18) are the *exact* RG equations for the relevant variables, and these equations are valid for arbitrary short-ranged potentials V.

(b) In addition to the Gaussian fixed point $V = E = 0$, there may be other fixed points as is evident from Eq. (2.18).

(c) $d = 2$ emerges, as expected, as the critical dimensionality. For $d > 2$ the Gaussian fixed point, $E = V = 0$, is stable in the V direction, while for $d < 2$ it is unstable. This is related to the fact that small perturbations on a free particle Hamiltonian cannot cause localization in dimensionality $d > 2$ but they can for $d < 2$. This statement is clarified in Sec. III.

(d) Though the initial interaction V is local in n space, it is obvious from Eq. (2.18) that nonlocal terms may be generated by the transformation. The fixed-point equation is a matrix equation

$$(2 - d) \langle \vec{q} | V^* | \vec{q}' \rangle = 2 \int d\Omega \langle \vec{q} | V^* | \vec{1} \rangle \langle \vec{1} | V^* | \vec{q}' \rangle , \qquad (2.19)$$

and in general is difficult to solve. The single-impurity case is treated in Sec. III to illustrate the new features of the RG transformation (2.15) and (2.18). This case is simple because Eq. (2.19) then becomes a single algebraic equation. In fact, the single-impurity problem is a useful example because the RG equations for the irrelevant variables can likewise be exactly solved for this case (Sec. IV).

III. SINGLE-IMPURITY PROBLEM

In this section we consider the implications of the RG equations (2.15) and (2.18) for the case of a single impurity in an otherwise homogeneous cubic lattice. If the impurity is located at the point $\vec{m}$ we have

$$V_{\vec{n}} = V \delta_{\vec{n}\vec{m}} , \qquad (3.1)$$

$$\langle \vec{q} | V | \vec{q}' \rangle = V \exp[i(\vec{q}' - \vec{q}) \cdot \vec{m}] , \qquad (3.2)$$

$$\int d\Omega \langle \vec{q} | V | \vec{1} \rangle \langle \vec{1} | V | \vec{q}' \rangle = V^2 K_d \exp[i(\vec{q}' - \vec{q}) \cdot \vec{m}] , \qquad (3.3)$$

where K_d is the surface area of a unit d-dimen-

sional sphere. The fixed-point equation (2.19) then becomes a simple algebraic equation for the parameter V whose solutions are $V^* = 0$ and

$$V^* = (2 - d)/2K_d. \qquad (3.4)$$

In terms of the physical parameters $\bar{E}$ and $\bar{V}$ we then have the fixed points: $\bar{E}^* = -2dJ, \bar{V}^* = 0$ (Gaussian or free-particle-like) and $\bar{E}^* = -2dJ, \bar{V}^* = (2\pi)^2 J(2 - d)/K_d$. We denote these points by F_1 and F_2, respectively. Obviously, if we define our momentum variable to correspond to the effective-mass approximation about the upper band edge, we get similar results with both $\bar{E}^*$ and $\bar{V}^*$ changing their signs.

The interpretation of these results is readily made by referring to the flow diagram given in Fig. 2. From Fig. 2(a) we see that for $d < 2$ a negative perturbation V of any size is sufficient to change drastically the long-distance behavior of the free-particle state, while Fig. 2(b) shows that for $d > 2$ a small negative impurity potential is not sufficient to change what is effectively (at long distances) a free-particle state. This corresponds to the fact that for $d < 2$ any binding perturbation on a free-particle Hamiltonian is sufficient to create at least one bound state, while for $d > 2$ the impurity potential must be less than a negative critical value for a local state to emerge from the bottom of the band.[13] It is tempting to associate the point F_2 for $d > 2$ with this critical potential. We show below that this interpretation is essentially correct.

From the linearized forms of the RG equations we can find scaling relations for the Green's function and for the characteristic length. This length plays the role of the correlation length of statistical mechanics and has the same meaning; it describes the effective range of the impurity potential. In the case of localization, this is the localization radius and it diverges at the critical-binding point. To see this, consider again the RG equations,

$$\frac{dE}{dt} = 2E,$$
$$\frac{dV}{dt} = (2 - d)V - \frac{2K_d}{1 - E}V^2, \qquad (3.5)$$

and their linearized form (for $d \neq 2$)

$$\frac{d}{dt}\begin{pmatrix} \delta E \\ \delta V \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ B & C \end{pmatrix}\begin{pmatrix} \delta E \\ \delta V \end{pmatrix}, \qquad (3.6)$$

with

$$B = -2K_d V^{*2} \qquad (3.7a)$$

and

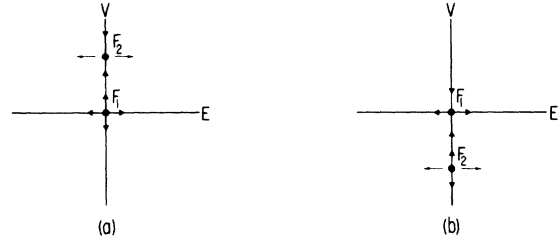$$C = 2 - d - 4K_d V^*. \qquad (3.7b)$$

FIG. 2. Flow diagrams for the solutions of Eq. (3.5). (a) $d < 2$; (b) $d > 2$.

Near $F_1, V^*_{F_1} = 0$ and the solutions of the linearized equations are

$$\delta E = \delta E_0 e^{2t} \qquad (3.8)$$

and

$$\delta V = \delta V_0 e^{(2-d)t}. \qquad (3.9)$$

Near $F_2, V^*_{F_2} = (2 - d)/2K_d$, and

$$\delta E = \delta E_0 e^{2t}, \qquad (3.10)$$

while

$$\delta V = \{\delta V_0 + [(2 - d)^2/2K_d(4 - d)]\delta E_0\} e^{-(2-d)t}$$
$$\quad - [(2 - d)^2/2K_d(4 - d)]\delta E_0 e^{2t} \quad \text{for } d \neq 4, \qquad (3.11a)$$

$$\delta V = \delta V_0 e^{2t} - (4/K_d)\delta E_0 t e^{2t} \quad \text{for } d = 4. \qquad (3.11b)$$

For $d \neq 4$ it is convenient to define the scaling variable

$$W = V + [(2 - d)^2/2K_d(4 - d)]E, \qquad (3.12)$$

which scales near F_2 like $\delta W = \delta W_0 e^{-(2-d)t}$. From these results we can derive the following scaling relations for the Green's function (for $d \neq 2$):

Near F_1,

$$G(k; E; \delta V) = e^{(2-d)t}G(e^t k; e^{2t}E; e^{(2-d)t}V), \qquad (3.13)$$

where k stands for both the k and k' indices.

Near F_2, $d \neq 4$,

$$G(k; E; \delta W) = e^{(2-d)t}G(e^t k; e^{2t}E; e^{-(2-d)t}\delta W) \qquad (3.14)$$

(where $\delta W = W - W^*_{F_2}$), while near F_2, for $d = 4$,

$$G(k; E; \delta V) = e^{(2-d)t}G(e^t k; e^{2t}E; e^{(d-2)t}\delta V)$$
$$\quad - te^{2t}[(2 - d)^2/2K_d]E). \qquad (3.15)$$

All these relations are, of course, special approximate cases of the result

$$G(k; E_0; V_0; J_n^0) = e^{(2-d)t}G(e^t k; e^{2t}E_0; V(t); J_n(t)), \qquad (3.16)$$

where $V(t)$ is the solution of (3.5) with the initial value V_0 and with $E = E_0 e^{2t}$ (see Sec. IV for a discussion of the solution of a general equation of this kind), and similarly $J_n(t)$ are the scaled irrelevant variables with J_n^0 their initial values.

To obtain information about the characteristic length ξ we use the general scaling rule for length variables

$$\xi(t) = e^{-t}\xi(0) \tag{3.17}$$

to obtain

$$\xi(E_0, V_0) = e^t \xi(E_0 e^{2t}, V(t)). \tag{3.18}$$

Focusing attention on the band edge $E_0 = 0$, we get in the linear region

$$\xi(V^* - V_0) = e^t \xi[(V^* - V_0)e^{\gamma t}], \quad d \neq 2, \tag{3.19}$$

where for $d < 2$ the fixed point relevant to critical binding is F_1 and

$$\gamma = 2 - d, \tag{3.20}$$

while for $d > 2$ it is F_2 and

$$\gamma = d - 2. \tag{3.21}$$

Equations (3.19)–(3.21) lead to a relation for the way ξ diverges when $V^* - V_0 \to 0+$,

$$\xi(V^* - V_0) \propto (V^* - V_0)^{-|d-2|}, \quad d \neq 2. \tag{3.22}$$

The case $d = 2$ is similar to the case $d = 4$ in the S^4 model for the theory of critical phenomena. Here the linear approximation cannot be used. Equation (3.5) takes the form (for $E = 0$)

$$\frac{dV}{dt} = -2K_d V^2, \tag{3.23}$$

with the solution

$$V(t) = (1/V_0 + 2K_d t)^{-1}. \tag{3.24}$$

The scaling relation

$$\xi(V_0) = e^t \xi[(1/V_0 + 2K_d t)^{-1}] \tag{3.25}$$

then leads to

$$\xi(V_0) \propto e^{-1/4\pi V_0}. \tag{3.26}$$

Other scaling relations are also easily obtained. Most trivially, since the energy scales like e^{2t} while distances scale like e^{-t}, it follows that $\xi \sim |E_I|^{-1/2}$, where E_I is the energy of the local state below the band edge. Similarly, the fact that $\delta V = V^* - V_0$ scales for $d \neq 2$ like $e^{|d-2|t}$ and E scales like e^{2t} leads to the relation $\delta V \sim |E|^{|d-2|/2}$ between the binding potential (measured from its critical value) and the energy of the local impurity state (measured from the band edge). Similar arguments for $d = 2$ lead to $(\delta V)^{-1} \sim \ln|E|$. All these relations are in agreement with the results obtained by utilizing the relation

$$\frac{1}{V} = P \int \frac{\rho(E')}{E - E'} dE' \tag{3.27}$$

between the energy of the local state $E < 0$ and the impurity potential $V[\rho(E)$ is the density of states of the pure material and P denotes the Cauchy principal value]. It is interesting to note that this information is obtained by considering a totally unstable fixed point rather than the saddle-point-type fixed point as is usually the case in the theory of phase transitions.

To conclude this section we note that for one-dimensional motion there is a fixed point, stable in the V direction, with a positive (repulsive) V, and that the Gaussian fixed point is unstable in this case. This reflects the fact that the effect of (even infinitesimally small) repulsive potential can, in one dimension, be carried to infinity (e.g., for any V there are some energies giving rise to total transmission).

IV. ROLE OF IRRELEVANT VARIABLES

While the scaling results presented in Sec. III do not depend on the nature of irrelevant variables, the actual magnitude of the critical binding strength cannot be calculated exactly without taking these variables into account. Their role is similar here to the role they play in determining the exact critical temperature in statistical mechanics. In this section we discuss this point within the context of calculating (for $d > 2$) the exact critical impurity potential, for which a bound state just emerges at the band edge.

Substitute

$$d - \sum_i \cos(2\pi q_i) = 2d - \tfrac{1}{2}(2\pi)^2 q^2$$

$$+ \sum_{n=2}^{\infty} (-1)^n \frac{(2\pi)^{2n}}{(2n)!} \sum_i q_i^{2n} \tag{4.1}$$

into Eq. (1.5), and define

$$2(-1)^n (2\pi)^{n-2}/(2n)! = J_n, \tag{4.2}$$

to obtain

$$U = \frac{1}{2} \int_q \left(E - q^2 + \sum_{n=2}^{\infty} J_n \sum_{i=1}^{d} q_i^{2n} \right) X_q X_{-q}$$

$$- \int_q \int_{q'} V_{-(q+q')} X_q X_{q'}, \tag{4.3}$$

where V is defined by Eqs. (3.1) and (3.2).

The RG equations for the variables E and J_n are obtained simply as before

$$\frac{dE}{dt} = 2E, \tag{4.4}$$

$$\frac{dJ_n}{dt} = -2(n-1)J_n, \quad n = 2, 3, \ldots . \tag{4.5}$$

We should be more careful in deriving the corresponding equation for V, because we are now interested in the exact position of the fixed point. In particular we note that the initial Hamiltonian is defined with a cutoff given in a Cartesian coordinate system. We therefore perform the RG transformation by integrating out field variables with momenta in the range $s^{-1} < q_i \leq 1; i = 1, 2, \ldots, d$. The RG equation is the same as (2.14b), only again V is a parameter rather than an operator and

$$A_0 = \int_P' \left(E - P^2 + \sum_{n=2}^{\infty} J_n \sum_i P_i^{2n} \right)^{-1}, \tag{4.6}$$

where $\int_P'$ denotes now an integration over this rectangular shell. A_0 can be written explicitly in the form (for $s = 1 + \delta t$)

$$A_0 = \sum_{i=1}^{d} \int_{i-\delta t}' dP_i \left(\prod_{j \neq i} \int_0^1 dP_j \right) R_i + O(\delta t^2), \tag{4.7}$$

where

$$R_i = \left[E - 1 - \sum_{j \neq i}^{d} P_j^2 + \sum_{n=2}^{\infty} J_n \left(1 + \sum_{j \neq i}^{d} P_j^{2n} \right) \right]^{-1}. \tag{4.8}$$

The symmetry of this expression implies that the term inside the summation sign in Eq. (4.7) does not depend on i. Therefore (4.7) yields

$$A_0 = d \delta t A_1, \tag{4.9}$$

where

$$A_1 = \left(\prod_{j \neq i}^{d} \int_0^1 dP_j \right) R_i \tag{4.10}$$

is independent of i. The RG equation for V is finally obtained in the form

$$\frac{dV}{dt} = (2 - d)V - M(E, J_n)V^2, \tag{4.11}$$

with

$$M(E, J_n) = -2dA_1. \tag{4.12}$$

Combining Eqs. (4.8)–(4.12) with (4.4) and (4.5) we can write the RG equation for the parameter V in the form

$$\frac{dV}{dt} = (2 - d)V - M(t)V^2, \tag{4.13}$$

$$M(t) = M(E(t), J_n(t)) = -2d \left(\prod_{j=1}^{d-1} \int_0^1 dP_j \right) \left[E_0 e^{2t} - 1 - \sum_{j=1}^{d-1} P_j^2 + \sum_{n=2}^{\infty} J_n^0 e^{-2(n-1)t} \left(1 + \sum_{j=1}^{d-1} P_j^{2n} \right) \right]^{-1}. \tag{4.14}$$

Recalling the definition of J_n, Eq. (4.2), $M(t)$ can be recast in the somewhat simpler form

$$M(t) = d(2\pi e^{-t})^2 \left(\prod_{j=1}^{d-1} \int_0^1 dP_j \right) \left(-E_0 e^{2t} + d - \cos(2\pi e^{-t}) - \sum_{j=1}^{d-1} \cos(2\pi e^{-t} P_j) \right)^{-1}. \tag{4.15}$$

The solution of Eq. (4.13) is given by

$$V(t) = V_0 e^{-(d-2)t} \left(1 + V_0 \int_0^t e^{-(d-2)t} M(t) dt \right)^{-1}. \tag{4.16}$$

We are interested in the asymptotic behavior of $V(t)$ for $t \to \infty$. As long as $|V_0|$ is small enough, $V(t) \to 0$, when $t \to \infty$. The vanishing of the term in brackets in Eq. (4.16) signals the departure from this behavior. This sets the condition for criticality

$$V_0 = - \left(\int_0^{\infty} e^{-(d-2)t} M(t) dt \right)^{-1}. \tag{4.17}$$

Equations (4.6) and (4.14) or (4.15) constitute the exact solution of the RG equation. The desired critical value of V_0 is obtained by taking $E_0 = 0$ in these equations. Equations (4.15) and (4.17) then yield

$$V_0 = - \left[d(2\pi)^2 \int_0^{\infty} dt \, e^{-dt} \left(\prod_{j=1}^{d-1} \int_0^1 dP_j \right) \left(d - \cos(2\pi e^{-t}) - \sum_{j=1}^{d-1} \cos(2\pi e^{-t} P_j) \right)^{-1} \right]^{-1}, \tag{4.18}$$

which can be transformed into

$$V_0 = - (2\pi)^{d-2} \left[\left(\prod_{j=1}^{d} \int_0^{2\pi} dP_j \right) \left(d - \sum_{j=1}^{d} \cos(P_j) \right)^{-1} \right]^{-1}. \tag{4.19}$$

Using Eq. (1.7) we obtain for the physical impurity potential

$$\tilde{V}_0 = - 2(2\pi)^d J \left[\left(\prod_{j=1}^{d} \int_0^{2\pi} dP_j \right) \left(d - \sum_{j=1}^{d} \cos(P_j) \right)^{-1} \right]^{-1}. \tag{4.20}$$

This is the critical value of the impurity potential necessary for an impurity state to just emerge at the bottom of the band. For $d = 3$ this is identical to the known result obtained originally by Slater

and Koster.[12] The method described here may be the most complicated one ever used to solve this problem. The importance of the result obtained lies, of course, not in the result itself but in demonstrating the validity of our interpretation of the RG transformation results as discussed in Sec. III, and in providing an illustration of the use and new features of the RG for single-particle Hamiltonians.

V. MOTION IN A RANDOM POTENTIAL

A. Averaged Green's function

In this section we extend the method described before to the problem of localization of a particle moving in a random potential. It is shown that the onset of localization, as randomness increases, is different in nature than the onset of binding in an attractive potential field. Typical runaway behavior similar to this, known in some random spin systems, is found in the RG transformation. A discussion of the possible meaning of this behavior is given at the end of this section.

We start again with the integral representation of the Green's function for a particle moving in a given potential [Eqs. (2.1)–(2.3)]

$$G_{\vec{q}\vec{q}'} = \frac{a}{z} \int d\vec{X} X_{\vec{q}} X_{\vec{q}'} e^{-aU[X]} , \tag{5.1}$$

$$U[X] = \frac{1}{2} \int_{\vec{q}} u_2(q) X_{\vec{q}} X_{-\vec{q}} - \int_{\vec{q}} \int_{\vec{q}'} V_{(-q+q')} X_{\vec{q}} X_{\vec{q}'} ,$$

$$u_2(q) = E - q^2 , \tag{5.2}$$

$$Z = \int d\vec{X} e^{-aU[X]} . \tag{5.3}$$

Now let $V_{\vec{n}}$ be a random function of space. Let

$$\langle V_{\vec{n}} \rangle = 0 , \tag{5.4a}$$

$$\langle V_{\vec{n}} V_{\vec{n}'} \rangle = M_{\vec{n}-\vec{n}'} , \tag{5.4b}$$

with higher-order cumulants being zero. Then

$$\langle V_{\vec{q}} \rangle = 0 \tag{5.5a}$$

and

$$\langle V_{\vec{q}} V_{\vec{q}'} \rangle = M_{\vec{q}} \delta(\vec{q} + \vec{q}') , \tag{5.5b}$$

again with vanishing higher-order cumulants.

For the sake of simplicity, we shall restrict the treatment to the case where $V_{\vec{n}}$ (and $V_{\vec{q}}$) is a Gaussian random function of the lattice site, $\vec{n}$, so that cumulants higher than the second are disregarded.

Next we consider the average $\langle G_{\vec{q}\vec{q}'} \rangle$. In order to obtain a useful expression for this average it is convenient to rewrite $G_{\vec{q}\vec{q}'}$ in the form

$$G_{\vec{q}\vec{q}'} = a \lim_{n \to 0} \int d(\vec{X}_\alpha) X_{\alpha\vec{q}} X_{\alpha\vec{q}'} \exp\left(-a \sum_{\alpha=1}^n U[X_\alpha]\right) . \tag{5.6}$$

Here we have replaced the field variable $X_{\vec{q}}$ by a n-vector $X_{\alpha\vec{q}}$, $\alpha = 1, 2, \ldots, n$. $\int d(\vec{X}_\alpha)$ stands for

$$\prod_{\alpha=1}^n \int dX_\alpha$$

and $U[X_\alpha]$ is given by Eq. (5.2) with $X_{\vec{q}}$ replaced by $X_{\alpha\vec{q}}$ everywhere. Equation (5.6) is verified by noting that it can be written also in the form

$$G_{\vec{q}\vec{q}'} = a \lim_{n \to 0} \left(\int d\vec{X}_\alpha X_{\alpha\vec{q}} X_{\alpha\vec{q}'} e^{-aU[X_\alpha]} Z^{n-1} \right) . \tag{5.7}$$

The form [Eq. (56)] enables us to take the average of $G_{\vec{q}\vec{q}'}$ over the random distribution of V in a simple form. A cumulant average yields

$$\langle G_{\vec{q}\vec{q}'} \rangle = a \lim_{n \to 0} \int d(\vec{X}_\alpha) X_{\alpha\vec{q}} X_{\alpha\vec{q}'} \exp\left(-\frac{1}{2} a \int_q u_2(q) \sum_\alpha X_{\alpha q} X_{\alpha, -q}\right.$$

$$\left. + a^2 \int_{\vec{q}_1, \ldots, \vec{q}_4} \int u_4(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4) \delta(\vec{q}_1 + \vec{q}_2 + \vec{q}_3 + \vec{q}_4) \sum_{\alpha\beta} X_{\alpha\vec{q}_1} X_{\alpha\vec{q}_2} X_{\beta\vec{q}_3} X_{\beta\vec{q}_4}\right), \tag{5.8}$$

where

$$u_4(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4) = \frac{1}{2} M_{-(q_1 + q_2)} . \tag{5.9}$$

Equation (5.8) is a representation of the averaged single-particle Green's function for a particle moving in a Gaussian random potential, given in the form of a two-point correlation function on a classical vector field of n components, in the limit $n \to 0$. Note that a in this equation is an arbitrary constant which can be chosen at will. It is chosen here to make the functional integral in Eq. (5.8) convergent wherever $\langle G \rangle$ is analytic.

Other than that it has no role in our discussion. As in the case treated in Sec. II, a can be shown to cancel in the RG equations.

A representation similar to Eq. (5.8) has formerly been suggested by Ma,[10] who has obtained it by comparing graph expansions of this expression to the conventional graph expansion for the average Green's function. Ma's contribution was withdrawn because it did not contain the parameter a appearing in Eq. (5.8), (i.e., $a = 1$), and, therefore, it was argued that the representation [Eqs. (5.8) and (5.9)] was not convergent (since

$M > 0$). As we see now this is a rather trivial point.

A similar approach, based on the $n \to 0$ limit of a correlation function on a n-vector field, has been introduced by DeGennes[4] for the excluded-volume problem. Also Emery[14] has simplified and extended DeGennes's approach. The relation between the random walk with excluded-volume problem and between particle motion in a random potential is best demonstrated by utilizing the fact[6,7] that the Green's function for both cases corresponds to formally the same form of equation of motion (written for the continuous limit)

$$\frac{\partial \psi}{\partial t} = D\nabla^2 \psi - iV(r)\psi, \tag{5.10}$$

where V is the Gaussian random potential satisfying $\langle V(r) \rangle = 0$ and $\langle V(r)V(r') \rangle = M(r - r')$. D is a positive constant for the excluded volume problem while $D = i\hbar^2/2m$ (m is the mass) for the particle motion (Schrödinger equation) case. Therefore, Eq. (5.8) is appropriate also for the random walk problem if we replace $u_2(q) = E - q^2$ by $E - iq^2$. Most generally we can write the corresponding partition function in the form

$$Z = \int d(\vec{X}_\alpha) \exp\left(-\frac{a}{2} \int_q (E + cq^2) \sum_\alpha X_{\alpha\vec{q}} X_{\alpha,-\vec{q}}\right.$$

$$\left. + a^2 b \int \cdots \int_{\vec{q}_1,\ldots,\vec{q}_2} \int \delta(\vec{q}_1 + \vec{q}_2 + \vec{q}_3 + \vec{q}_4) u_4(\vec{q}_1\vec{q}_2\vec{q}_3\vec{q}_4) \sum_{\alpha\beta} X_{\alpha\vec{q}_1} X_{\alpha\vec{q}_2} X_{\beta\vec{q}_3} X_{\beta\vec{q}_4}\right), \tag{5.11}$$

where for the particle motion case $c = -1$ and $b = 1$, while for the excluded volume problem $c = -i$ and $b = 1$.

The partition function [Eq. (5.11)] is formally identical to the one treated by Wilson and co-workers[2] for the critical properties of a classical n-component spin system. The appropriate choice for b and c for this case is $c = -b = 1$. We note again that for any choice of b we can make the integral defining Z convergent by a proper choice of the constant a. (In the current localization problem, Z is analytic for all values of E if an imaginary part $\text{Im} E$ is appended and if a is chosen to be pure imaginary with $a\,\text{Im}\,E < 0$. The limit $\text{Im}\,E \to 0$ is then applied at the end of the calculation in the usual fashion.)

The RG equations for the parameters appearing in Eq. (5.11) have been obtained by Wilson and co-workers in the $\epsilon = 4 - \delta$ expansion. To the first order in ϵ these are

$$\frac{dE}{dt} = 2E - (4n + 8)bK_d\frac{u_4}{E + c},$$

$$\frac{du}{dt} = \epsilon u + (4n + 32)bK_d\left(\frac{u_4}{E + c}\right)^2, \tag{5.12}$$

where u_4 is $\vec{q}$ independent in this order. The corresponding fixed points are

$$E^* = -c[(n + 2)/2(n + 8)]\epsilon,$$

$$u^* = -(c^2/bK_d)[4(n + 8)]^{-1}\epsilon, \tag{5.13}$$

and the Gaussian point $E^* = u^* = 0$. For all three (Wilson's, excluded volume, and particle motion) cases these results can be written in the form

$$\frac{dz}{dt} = 2z + (4n + 8)K_d\frac{u}{z + 1},$$

$$\frac{du}{dt} = \epsilon u - 4(n + 8)K_d\left(\frac{u}{z + 1}\right)^2, \tag{5.14a}$$

with the nontrivial fixed point

$$z^* = -\frac{n + 2}{2(n + 8)}\epsilon,$$

$$u^* = \frac{1}{K_d}\frac{1}{4(n + 8)}\epsilon, \tag{5.14b}$$

where $z = E$, $u = u_4$ in Wilson's case, $z = iE$, $u = u_4$ for the excluded-volume problem, and where $z = -E$, $u = -u_4$ for the particle motion in a Gaussian random potential. The crucial difference between the first two problems and the last one is that the physical initial value of u is positive for the Wilson's and the excluded-volume problems, while it is negative for the motion in a random-potential case. It is seen by inspection and has been confirmed by us numerically that while physical trajectories may, for appropriate initial conditions, converge to the non-Gaussian fixed point in the first two cases, they cannot do so for our problem. Wilson analysis of the critical behavior of the Hamiltonian defining the partition function (5.11) is thus useful also (in the $n \to 0$ limit) for the excluded-volume problem, as has been shown first by DeGennes and extensively studied since. However, no implication of this critical behavior exists for the averaged Green's function in the problem of motion in a random potential.

The following points should now be mentioned:

(a) This result is in accord with our knowledge that the averaged Green's function should not

contain information about localization of a quantum-mechanical particle in a random potential field.

(b) Our conclusions here have been reached on the basis of an ϵ expansion, for z and u of order ϵ, and for a Gaussian-type randomness. There are several indications however that this result is more general. Aharony, Imry, and Ma[15] have recently studied the problem of critical behavior of a random spin system, where the randomness is described by a binary distribution. In our notation this is given by the following distribution for the potential V:

$$P(V_n) = (1 - C)\delta_{V_n, 0} + C\delta_{V_n, V}, \qquad (5.15a)$$

$$P(\{V_i, i = 1, 2, 3, \ldots\}) = \prod_i P(V_i), \qquad (5.15b)$$

which corresponds to a random-binary-alloy model with local randomness. The free energy of the random m-component spin system is calculated as the $n \to 0$ limit of a nonrandom nm-spin system. The averaged Green's function for the binary-alloy problem corresponds to the $m = 1$ limit of the Aharony-Imry-Ma[15] study with the nonrandom fourth-order spin interaction term taken to be zero. For a small amount of randomness [small ϵ or small V in Eq. (5.15a)], these authors also conclude that the corresponding fixed point is unattainable. They also argue that this conclusion remains valid as well for large c and V. Furthermore, calculations based on the Wilson's approximate recursion relation seem to sustain this result.[16]

(c) It is interesting to note that there exist random models where the averaged Green's function does have singularities which express themselves as attainable fixed points of the RG equations. For example, a model in which the random potential has a nonvanishing second and third cumulants with the higher cumulants being zero is mathematically equivalent to a model which has been used in the theory of critical phenomena to discuss tricritical behavior.[17] We have not studied the implications of this analogy on the form of the

averaged Green's function or the density of states in this model. It is clear from our previous discussion that this has nothing to do with the localization problem.

(d) Even though, as was expected, no critical behavior of the averaged Green's function of a particle moving in a random (Gaussian or binary-alloy type) potential is found, the RG method may still be useful in studying the properties of $\langle G \rangle$. It is well known, within the context of the theory of critical phenomena, that the RG method can be applied to obtain scaling laws as well as for a direct calculation of the free energy or the correlation function near the critical point. The idea is to use the RG recursion relations to relate the free energy far from the critical point (which is amenable to theoretical calculation) to the free energy near the critical point. Similarly, it is possible to use the RG recursion relations to find scaling laws for $\langle G \rangle$ and for the density of states, and possibly also for a direct calculation of these quantities in "difficult" regions (such as the band edges of the corresponding ordered system) given data from easier regions.

B. $\langle |G|^2 \rangle$ and the localization problem

It is now generally agreed that the averaged Green's function of a particle moving in a random potential field does not contain information about localization. Such information is contained however in the averaged absolute square, $\langle |G|^2 \rangle$, of the Green's function. It may be expected that the mobility edge corresponds to a critical point where $\langle |G|^2 \rangle$ develops in infinite range. In this case we might find a fixed point of the RG transformation on $\langle |G|^2 \rangle$ which corresponds to this transition.

In this section we show that the RG transformation on $\langle |G|^2 \rangle$ is characterized by the same runaway behavior that we saw in the $\langle G \rangle$ case. We have to conclude that the mobility edge does not correspond to a simple second-order phase transition.

The RG transformation of $\langle |G|^2 \rangle$ can be handled in a way similar to that we used for $\langle G \rangle$. We start with [cf. Eq. (5.8)]

$$G^1_{\vec{q}_1 \vec{q}_1'} G^2_{\vec{q}_2 \vec{q}_2'} = ab \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int d(\vec{X}_\alpha) d(\vec{Y}_\beta) X_{\alpha \vec{q}_1} X_{\alpha \vec{q}_1'} Y_{\beta \vec{q}_2} Y_{\beta \vec{q}_2'} \exp\left(-a \sum_{\alpha=1}^{n_1} U^1[X_\alpha] - b \sum_{\beta=1}^{n_2} U^2[Y_\beta]\right), \qquad (5.16)$$

where

$$U^i[z] = \tfrac{1}{2} \int_{\vec{q}} (E_i - q^2) Z_{\vec{q}} Z_{-\vec{q}} - \int_{\vec{q}} \int_{\vec{q}'} V_{-(\vec{q}+\vec{q}')} Z_{\vec{q}} Z_{\vec{q}'}, \qquad (5.17)$$

and where, for $|G|^2$, we have to take $E_1 = E_2^*$. Taking the average and assuming again the properties [(5.4) and (5.5)] for V, we obtain

$$\langle G^1_{\vec{q}_1 \vec{q}'_1} G^2_{\vec{q}_2 \vec{q}'_2} \rangle = ab \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int d(\vec{X}_\alpha) d(\vec{Y}_\alpha) X_{\alpha \vec{q}_1} X_{\alpha \vec{q}'_1} Y_{\beta \vec{q}_2} Y_{\beta \vec{q}'_2}$$

$$\times \exp\left[-\tfrac{1}{2} a \int_{\vec{q}} u_2^1(q) \sum_\alpha X_{\alpha \vec{q}} X_{\alpha, -\vec{q}} - \tfrac{1}{2} b \int_q u_2^2(q) \sum_\beta Y_{\beta \vec{q}} Y_{\beta, -\vec{q}} \right.$$

$$+ a^2 \int_{\vec{q}_1, \ldots, \vec{q}_4} \int u(\vec{q}_1, \ldots, \vec{q}_4) \delta\left(\sum \vec{q} \right) \sum_{\alpha_1 \alpha_2} X_{\alpha_1 \vec{q}_1} X_{\alpha_1 \vec{q}_2} X_{\alpha_2 \vec{q}_3} X_{\alpha_2 \vec{q}_4}$$

$$+ b^2 \int_{\vec{q}_1, \ldots, \vec{q}_4} \int v(\vec{q}_1, \ldots, \vec{q}_4) \delta\left(\sum \vec{q} \right) \sum_{\beta_1 \beta_2} Y_{\beta_1 \vec{q}_1} Y_{\beta_1 \vec{q}_2} Y_{\beta_2 \vec{q}_3} Y_{\beta_2 \vec{q}_4}$$

$$+ 2ab \int_{q_1, \ldots, q_4} \int w(\vec{q}_1, \ldots, \vec{q}_4) \delta\left(\sum \vec{q} \right) \sum_{\alpha \beta} X_{\alpha \vec{q}_1} X_{\alpha \vec{q}_2} Y_{\beta \vec{q}_3} Y_{\beta \vec{q}_4} \right] \tag{5.18}$$

Here $\sum \vec{q} = \vec{q}_1 + \vec{q}_2 + \vec{q}_3 + \vec{q}_4$, $u_2^i(q) = E_i - q^2$, and $u = v = w$ are identical to u_4 defined in Eq. (5.9). We use three different notations to account for the possibility of these parameters becoming different during the RG transformation. The parameters a and b can always be chosen to insure convergence of the representation [Eq. (5.18)] whenever $\langle |G|^2 \rangle$ exists. Thus if $E_1 = E_R + iE_I$, $E_2 = E_R - iE_I$, with $E_I > 0$, we should choose $a = -i$ and $b = i$ to insure this convergence. As was the case with $\langle G \rangle$, it can also be shown here that the parameters a and b cancel from the RG recursion relations in any order.

Consider now the RG equations on the Hamiltonian defining the averaged product [Eq. (5.18)]. The derivation for small u, v, and w follows the same perturbation approach used in the ϵ expansion, only now we have to consider two zero-order propagators

$$G_1^0(q) = (E_1 - q^2)^{-1}, \quad G_2^0(q) = (E_2 - q^2)^{-1}, \tag{5.19}$$

for the X and Y fields, respectively. The two fields are coupled to each other by the w form in Eq. (5.18). The result for small u, v, and w is ($\epsilon = 4 - d$)

$$\frac{dE_1}{dt} = 2E_1 - (8 + 4n_1) K_d \frac{u}{E_1 - 1} - 4n_2 K_d \frac{w}{E_2 - 1},$$

$$\frac{dE_2}{dt} = 2E_2 - (8 + 4n_2) K_d \frac{v}{E_2 - 1} - 4n_1 K_d \frac{w}{E_1 - 1},$$

$$\frac{du}{dt} = \epsilon u + (32 + 4n_1) K_d \left(\frac{u}{E_1 - 1} \right)^2 + 4n_2 K_d \left(\frac{w}{E_2 - 1} \right)^2,$$

$$\frac{dv}{dt} = \epsilon v + (32 + 4n_2) K_d \left(\frac{v}{E_2 - 1} \right)^2 + 4n_1 K_d \left(\frac{w}{E_1 - 1} \right)^2, \tag{5.20}$$

$$\frac{dw}{dt} = \epsilon w + (8 + 4n_1) K_d \frac{uw}{(E_1 - 1)^2}$$
$$+ (8 + 4n_2) K_d \frac{vw}{(E_2 - 1)^2} + 16 K_d \frac{w^2}{(E_1 - 1)(E_2 - 1)}.$$

Now, for $n_1, n_2 \to 0$ the pairs of equations for (E_1, u)

and (E_2, v) decouple from each other and from the w equation and become identical (by changing the sign of the variables) to Eq. (5.14). Therefore, the conclusion arrived at for the $\langle G \rangle$ case about the runaway behavior persists also in the present case.

This result, namely the decoupling of the fields X and Y in the $n_1, n_2 \to 0$ limit, which was demonstrated here for small coupling parameters u, v, and w, can be easily shown to be general for any order in these parameters and for any kind of randomness (see Appendix).

We thus see that any conclusion reached for the RG transformation on $\langle G \rangle$ remains valid also for $\langle |G|^2 \rangle$. In particular, the runaway behavior, which we found unsurprising in the $\langle G \rangle$ case, persists also for $\langle |G|^2 \rangle$.

There is one important difference between the RG transformation that we applied for $\langle G \rangle$ and the one we used for $\langle |G|^2 \rangle$. The difference is best seen by focusing on the spatial Green's functions. For these we have ($\vec{i}, \vec{j}$ are two lattice sites)

$$\langle G_{\vec{i} \vec{j}} \rangle = a \lim_{n \to 0} \int d(\vec{X}_\alpha) X_{\alpha \vec{i}} X_{\alpha \vec{j}} e^{-\mathcal{K}_1[X]}, \tag{5.21}$$

$$\langle |G_{\vec{i} \vec{j}}|^2 \rangle = ab \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int \int d(\vec{X}_\alpha) d(\vec{Y}_\alpha)$$

$$\times X_{\alpha \vec{i}} X_{\alpha \vec{j}} Y_{\beta \vec{i}} Y_{\beta \vec{j}} e^{-\mathcal{K}_2[X, Y]}. \tag{5.22}$$

Here $\mathcal{K}_1[X]$ is the Hamiltonian appearing in the exponential in Eq. (5.8) while $\mathcal{K}_2[X]$ is the Hamiltonian appearing in the exponential in Eq. (5.18), [and also in a more general form in Eq. (A1)]. Going now to q space we obtain for $\langle G \rangle$

$$\langle G_{\vec{q} \vec{q}'} \rangle = \delta(\vec{q} + \vec{q}') a \lim_{n \to 0} \int d(\vec{X}_\alpha) X_{\alpha \vec{q}} X_{\alpha, -\vec{q}} e^{-\mathcal{K}_1[X]}$$

$$= \delta(\vec{q} + \vec{q}') \langle G \rangle_{\vec{q}}, \tag{5.23}$$

such that

$$\langle G_{\vec{1}\,\vec{j}} \rangle = \langle G_{\vec{1}\,\vec{j}} \rangle = \int_{\vec{q}} \langle G \rangle_q e^{2\pi i \vec{q} \cdot (\vec{1}-\vec{j})}. \qquad (5.24)$$

On the other hand for $\langle |G|^2 \rangle$ we have

$$\langle |G_{\vec{1}\,\vec{j}}|^2 \rangle = \int_{\vec{q}} e^{2\pi i \vec{q} \cdot (\vec{1}-\vec{j})} \langle |G|^2 \rangle_{\vec{q}}, \qquad (5.25)$$

where

$$\langle |G|^2 \rangle_{\vec{q}} \equiv ab \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int \int d(\vec{X}) d(\vec{Y}) \, \rho_q \rho_{-q} e^{-\mathcal{K}_2[X, Y]}, \qquad (5.26)$$

and where

$$\rho_{\vec{q}} = \int_{\vec{q}'} X_{\vec{q}'} Y_{\vec{q}-\vec{q}'}. \qquad (5.27)$$

In the RG transformation on $\langle G \rangle$ we integrate over $X_{\vec{q}}$ variables with high-q values. Physically this means that we focus on values of $\langle G_{\vec{1}\,\vec{j}} \rangle$ for large $|\vec{1}-\vec{j}|$ distances, disregarding the short-range behavior of $\langle G_{\vec{1}\,\vec{j}} \rangle$. The equivalent thing for $\langle |G|^2 \rangle$ would be integrating Eq. (5.26) over variables ρ_q with large q values since, as we see in Eq. (5.25), it is q only which is related to the distance $\vec{1}-\vec{j}$. What we actually do to obtain RG recursion relations such as Eq. (5.20) is to integrate over all variables $X_{\vec{q}}$ and $Y_{\vec{q}}$ with high-q values.

Can this difference be of importance in the present context? We believe that the answer is no. The reason is best seen by focusing back on the critical-binding problem in a nonrandom potential field discussed in Sec. II. In this case space is not homogeneous and $G_{\vec{1}\,\vec{j}}$ or $G_{\vec{q}\,\vec{q}'}$ depends explicitly on the two space or momentum indices. By integrating out in Eq. (2.3) those variables $X_{\vec{q}}$ with large-q values, we have related $G_{\vec{q}\,\vec{q}'}$ to another matrix element of G between waves of smaller momenta. Such matrix elements of small q and q' values do not contain enough information to describe spatial matrix elements G_{ij} with large $|i-j|$. However, they contain enough information on matrix elements of G taken between wave packets which are concentrated around the sites i and j, for wide enough wave packets (which contain only low-q waves) and for $|i-j|$ large enough so that the wave packets do not overlap. In other words, the RG transformation in which we integrate over all variables of high-q indices provides a relation between Green's-function matrix elements taken with wave packets concentrated around given lattice sites, and between similar matrix elements with wider wave packets concentrated around more distant sites. It is this transformation which converges to a fixed point when the Green's function of a particle moving in a binding nonrandom potential

field develops an infinite range.

An exactly similar interpretation holds also for the RG transformation that we apply for $\langle |G|^2 \rangle$. We conclude that this transformation is sufficient to give indication of localization if it corresponds to a second-order phase transition like the case discussed in Sec. II.

The fact that no attainable fixed point is found to this RG transformation, suggests that the transition to localization in a random system is not a simple second-order phase transition. Usually in the theory of critical phenomena, runaway behavior in the RG transformation is associated with either a first-order or a smeared transition. It is interesting to note that very recently Licciardello and Thouless[18] have argued that there exists a minimum metallic conductivity (that is first order transition) with a universal value in two dimensions and sustained their arguments by numerical computations. However their numerical accuracy is insufficient to distinguish among first-order, second-order, and smeared transitions. On the other hand, Aharony, Imry, and Ma[15] have argued that at least in the random alloy case the runaway behavior cannot be associated with a first-order transition. None of these arguments can be classified as a rigorous proof. Furthermore, it should be kept in mind that while the existence of an attainable fixed point is a sufficient condition for the occurrence of an infinite range in the system, it is by no means a necessary one. An alternative way to account for the runaway behavior is provided by comparison to the Slater-Koster problem treated in Secs. III and IV. We have seen that no fixed point is attained if our initial impurity potential is larger than the critical value. In the one-dimensional case the critical potential is zero, and a runaway behavior is obtained for any initial finite binding potential. Now, in the random problem there exist in any dimensionality localized states for any amount of randomness [expressed by the size of M_q, Eq. (5.5b)]. By analogy, we may expect a runaway behavior following any initial finite positive M_q. If this contention is correct then the mobility edge cannot be obtained as a fixed point of the RG transformation described in this paper.

In summary, we have shown that the RG equations on $\langle |G|^2 \rangle$ decouple to yield recursion relations identical to those found in the RG transformation on $\langle G \rangle$. This result is exact, and since $\langle G \rangle$ is not expected to have any critical properties we have concluded that whatever the critical properties of $\langle |G|^2 \rangle$ are, they do not correspond to a simple second order phase transition. This in turn may mean either that the transition is really not a second order phase transition and/or

that $\langle |G|^2 \rangle$ is, for some reason, not the correct quantity to renormalize. Comparison to the non-random-binding-potential case suggests that the observed runaway behavior may be associated with the occurrence of localized states at the band tails.

VI. CONCLUSION

In this paper we have studied the critical localization problem within the context of RG theory. We have formulated generally the RG problem for a single particle moving on a lattice and subjected to an arbitrary given potential field, and described in particular the detailed solution for the Slater-Koster model. "Universal" properties like scaling laws and critical exponents have been obtained as well as the exact critical value for the binding potential in the Slater-Koster problem. Furthermore, we have shown how RG ideas can be used in the study of a particle motion in a random potential field and concluded that the observed properties of the RG transformation do not correspond to a simple second-order phase transition.

From the point of view of the RG theory, our study contributes to the understanding of this important method. The generalized Gaussian model treated here provides a simple and exactly soluble but nontrivial model for critical behavior. Of particular interest is the fact that the critical

point for binding in a nonrandom potential appears as an unstable fixed point of the RG transformation; such that in the absence of a localized state the transformation leads to the free-particle limit, while in the presence of a bound state it leads away from this limit.

Since no attainable fixed point has been found for the random localization problem, we cannot yet obtain any information about the nature of the transition beyond the observation that the RG properties of $\langle |G|^2 \rangle$ do not correspond to a simple second-order phase transition. It is hoped that, as our understanding of the RG theory increases, the methods described here could be used to shed more light on the true nature of this transition.

APPENDIX

Here we show that in the RG transformation on $\langle |G|^2 \rangle$, performed using the $n_1, n_2 \to 0$ limit of a four-point correlation function on two coupled fields, the equations for the renormalized pure vertices do not involve any coupling between the two fields. By pure vertices we mean those vertices which couple free propagators belonging to one field only.

The Hamiltonian which is used to represent $\langle G^1 G^2 \rangle$ as a correlation function in Eq. (5.18) can be written for a general model for the randomness in the form

$$\mathcal{H} = -\tfrac{1}{2}a \int_{\vec{q}} u_2^1(q) \sum_\alpha X_{\alpha\vec{q}} X_{\alpha,-\vec{q}} - \tfrac{1}{2}b \int_{\vec{q}} u_2^2(q) \sum_\beta Y_{\beta\vec{q}} Y_{\beta-\vec{q}}$$

$$+ \sum_{l=2}^{\infty} \int_{\vec{q}_1} \int_{\vec{q}_1'} \cdots_{\vec{q}_l} \int_{\vec{q}_l'} u_{2l}(\vec{q}_1\vec{q}_1', \ldots, \vec{q}_l\vec{q}_l') \delta\left(\sum q\right) \prod_{l=1}^{l}\left(\sum_\alpha X_{\alpha\vec{q}_l} X_{\alpha\vec{q}_l'} + \sum_\beta Y_{\beta\vec{q}_l} Y_{\beta\vec{q}_l'}\right) (\alpha = 1, \ldots, n_1; \quad \beta = 1, \ldots, n_2).$$

$$(A1)$$

A typical vertex has several pairs of type-1 and several pairs of type-2 propagator lines going out of it. A pure vertex has pairs only of one kind going out of it. Consider now a renormalized pure vertex of kind 1 which is obtained by linking together several vertices, some of which are not pure or pure of the other kind 2. It is obvious that, since all the propagator lines of kind 2 must terminate (so-called internal lines), there will

necessarily be closed loops of kind 2. Each such closed loop contributes an order n_2 to the renormalized vertex, which then must vanish when the limit $n_2 \to 0$ is taken.

Exactly the same arguments hold for the renormalized energy. We conclude that the RG transformation does not couple those parameters in the Hamiltonian which purely belong to one field.

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