Disordered system with n orbitals per site: $n = \infty$ limit

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A model of a randomly disordered system with n electronic states at each site of a d-dimensional lattice is introduced. It is a generalization of a model by Wigner to d dimensions and an extension of the usually considered model for disordered systems to n states per site. In the limit $n = \infty$, which is the limit of a dense system of weak scatterers, the one- and two-particle Green's function can be calculated exactly. The eigenstates are extended and the residual conductivity is finite, provided the Fermi energy is inside the band. Two special cases are considered more closely: (i) In the case of mere site-diagonal disorder the $n = \infty$ solution agrees with the $n = 1$ coherent-potential approximation for a semicircle distribution of the site-diagonal elements. (ii) In a "local gauge invariant model," where the phases at different sites are completely uncorrelated, the Green's functions vanish unless the points coincide pairwise in local space. Except for a special case of the gauge-invariant model, the systems (i) and (ii) show the same long-range correlation between eigenstates over a length L which diverges like $|\omega|^{-1/2}$ as the energy difference ω vanishes.

I. INTRODUCTION

In this paper a model of a randomly disordered system with n electronic states at each site of a d-dimensional lattice is introduced and its properties in the $n=\infty$ limit are determined.

This model is a generalization of two extensively discussed models. (i) Wigner[1] and subsequently others[2,3] have considered the zero-dimensional case in the limit $n=\infty$ where the interaction is given by an $n\times n$ symmetric matric with $\frac{1}{2}n(n+1)$ independent matrix elements $f/\sqrt{n}$. The f's obey a probability distribution $p(f)$ with vanishing $\langle f\rangle_{\rm av}$ and finite $\langle f^2\rangle_{\rm av}$. (ii) The case of one orbital at each site of a d-dimensional lattice has gained much interest[4] since Anderson's paper[5] in 1958.

In the $n=\infty$ limit, which is the limit of a dense system of weak scatterers, the Green's functions can be calculated exactly following essentially the arguments by Wigner[1] and Arnold.[3] The $n=\infty$ solution serves as a starting point for an expansion in powers of $1/n$ which will be considered in a forthcoming paper.[6] In all cases the leading term in order n is determined but it is not discussed here whether and how this limit is approached as n tends to infinity. The solution for $n=\infty$ has properties of the coherent-potential approximation[4,7,8] (CPA). This is not unexpected in view of the result by Schwartz and Siggia[9] that the CPA is exact up to second order in an expansion in the inverse coordination number. In particular the $n=\infty$ model with site-diagonal disorder is equivalent to the CPA for the $n=1$ model provided the site-diagonal elements obey a semicircle distribution. This distribution plays a similar role for the locator expansion in the CPA as the Gaussian distribution for a cumulant expansion since both terminate after the second term.

Off-diagonal disorder can be included in the model. A special case is the "local gauge invariant" model in which the phases of the eigenfunctions at different orbitals are completely independent from each other. Such an ensemble is obtained by choosing the sign of the off-diagonal elements at random. Consequently, the averaged one-particle Green's function vanishes except for the diagonal part, and the two-particle Green's function vanishes unless the four points coincide pairwise.

The long-range behavior of the two-particle Green's function for the site-diagonal disordered model and for the gauge-invariant model are very similar. Eigenstates separated by an energy difference ω are correlated over a length L which diverges like $|\omega|^{-1/2}$ for $\omega\to 0$, which indicates that eigenstates which are close in energy undergo the same phase fluctuations.[10] The two-particle Green's function in local space for energies in opposite halves of the complex plane differing by ω approaches a constant for $d>2$, diverges logarithmically as a function of ω for $d=2$ and like $|\omega|^{d/2-1}$ for $0\leq d<2$, repsectively, for $\omega\to 0$, which implies that the eigenstates are extended[11] for $d>0$. Both models exhibit a finite residual dc conductivity for the Fermi energy inside the band.

In Sec. II the model and special cases thereof are defined. The one-particle and two-particle Green's functions are determined in Secs. III and IV. A discussion of the long-range behavior of the eigenstates and the dc conductivity are given in Sec. V.

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II. MODEL

The ensemble consists of systems on simple d-dimensional lattices. At each lattice site r there are n electronic levels $|r\alpha\rangle$ numbered by $\alpha = 1, 2, \ldots, n$. The interaction is governed by a one-particle Hamiltonian of the form

$$H = \sum_{rr'\alpha\beta} \left(v_{rr'}\delta_{\alpha\beta} + \frac{1}{\sqrt{n}} f_{r\alpha,r'\beta} \right) |r\alpha\rangle\langle r'\beta| . \quad (2.1)$$

The matrix elements $v_{rr'}$ are identical for all systems of the ensemble and translational invariant

$$v_{rr'} = v_{r-r',0} . \quad (2.2)$$

Thus for vanishing f the Hamiltonian decomposes into a sum of n translational-invariant Hamiltonians

$$H_\alpha = \sum_{rr'} v_{rr'} |r\alpha\rangle\langle r'\alpha| \quad (2.3)$$

which allow the electrons to propagate in the decoupled systems labeled by α.

The matrix elements f are random variables. We require that the expectation values of these matrix elements vanish

$$\langle f_{r\alpha,r'\beta}\rangle_{\text{av}} = 0 \quad (2.4)$$

(the brackets $\langle \cdots \rangle_{\text{av}}$ indicate an ensemble average) and that the probability distribution of the submatrices $f_{\alpha\beta}$ (they contain all matrix elements $f_{r\alpha,r'\beta}$ for given α and β) are independent from each other apart from Hermiticity,

$$f_{\alpha\beta} = f^{\dagger}_{\beta\alpha} . \quad (2.5)$$

Moreover the probability distributions of all submatrices $f_{\alpha\beta}$ with $\alpha \neq \beta$ should be equal, as well as the distribution of the diagonal submatrices $f_{\alpha\alpha}$ so that the probability distribution can be written

$$\prod_{\alpha,\beta>\alpha} [P(f_{\alpha\beta}) d\{f_{\alpha\beta}\}] \prod_{\alpha} [Q(f_{\alpha\alpha}) d\{f_{\alpha\alpha}\}] . \quad (2.6)$$

Here $d\{f_{\alpha\beta}\}$ is a measure in the space of the submatrices $f_{\alpha\beta}$. It may be written as the product of the $n^2(2-\delta_{\alpha\beta})$ independent differentials $d\mathrm{Re} f_{r\alpha,r'\beta}$ and $d\mathrm{Im} f_{r\alpha,r'\beta}$.

Due to these restrictions, the second moments read

$$\langle f_{r\alpha,r'\beta} f_{r''\gamma,r'''\delta}\rangle_{\text{av}} = \delta_{\alpha\delta}\delta_{\beta\gamma} M_{rr'r''r'''} + \delta_{\alpha\gamma}\delta_{\beta\delta} M'_{rr'r''r'''} + \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta} M''_{rr'r''r'''} , \quad (2.7)$$

where M and M' are determined from P and $M + M' + M''$ from Q. Interchanging both factors f in (2.7) and using the fact that f is Hermitian yields

$$M_{rr'r''r'''} = M_{r''r'''rr'} = M^*_{r'rr'''r''} = M^*_{r'''r''r'r} \quad (2.8)$$

and similarly for M' and M''.

For the special choice $P = Q$ one obtains

$$M = M' = -M'' . \quad (2.9)$$

For real matrices f one obtains (real ensemble)

$$M_{rr'r''r'''} = M'_{rr'r'''r''} . \quad (2.10)$$

If the matrices f are complex and the ensemble is invariant against arbitrary phase transformations (phase-invariant ensemble)

$$|r\alpha\rangle \to \exp(i\varphi_\alpha)|r\alpha\rangle \quad (\varphi_\alpha \text{ real}) , \quad (2.11)$$

then one has

$$M' = 0 . \quad (2.12)$$

Finally we require that the ensemble is translational invariant, that is

$$M_{rr'r''r'''} = M_{r+R,r'+R,r''+R,r'''+R} \quad (2.13)$$

and similarly for M' and M''.

We assume that the higher-order moments exist to the extent required (compare Arnold[3]). Although we will derive the equations for the general case (2.7), we will particularly consider two special cases:

(i) *Site diagonal disorder.* In the Anderson model[5] only the site-diagonal elements are random variables. They are independent from site to site. Thus (2.7) reduces to

$$\langle f_{r\alpha,r'\beta} f_{r''\gamma,r'''\delta}\rangle_{\text{av}} = \delta_{rr'}\delta_{rr''}\delta_{rr'''}(\delta_{\alpha\delta}\delta_{\beta\gamma} M + \delta_{\alpha\gamma}\delta_{\beta\delta} M' + \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta} M'') . \quad (2.14)$$

(ii) *Local gauge-invariant model.* In a disordered system the averaged one-particle correlation function between two points decays rapidly with increasing distance due to phase fluctuations. Similarly, the two-particle correlation becomes small unless the four points of this function are pairwise close to each other. Thus, on a scale large in comparison to the phase coherence length the correlation functions contain practically δ functions between pairs of points. In order to investigate the long-range behavior it might be useful to consider an ensemble in which the phases are totally uncorrelated from site to site. Thus, we restrict to ensembles which are invariant against the local gauge transformations

$$|r\alpha\rangle \to \sigma_{r\alpha}|r\alpha\rangle , \quad \sigma_{r\alpha} = \pm 1 \quad (2.15)$$

for real matrices and

$$|r\alpha\rangle \to \exp(i\varphi_{r\alpha})|r\alpha\rangle \quad (\varphi_{r\alpha} \text{ real}) \quad (2.16)$$

for complex matrices. This implies

$$v_{rr'} = \delta_{rr'} v \quad (2.17)$$

and

$$\langle f_{r\alpha,r'\beta} f_{r''\gamma,r'''\delta}\rangle_{\mathrm{av}} = \delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{rr'''}\delta_{r'r''}M_{rr'} + \delta_{\alpha\gamma}\delta_{\beta\delta}\delta_{rr''}\delta_{r'r'''}M'_{rr'} + \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta}(\delta_{rr'''}\delta_{r'r''}M''_{rr'} + \delta_{rr''}\delta_{r'r'''}M'''_{rr'} + \delta_{rr'}\delta_{r''r'''}M''''_{rr''}). \tag{2.18}$$

For real matrices one has

$$M = M', \quad M'' = M'''. \tag{2.19}$$

If the invariance (2.16) holds, then

$$M' = M''' = 0. \tag{2.20}$$

Translational invariance yields

$$M_{rr'} = M_{r-r',0} \tag{2.21}$$

and similarly for M', M'', M''', M''''. In this gauge-invariant model the term $v_{rr'} = \delta_{rr'}v$, Eq. (2.17), can be eliminated by a shift of the energy scale by v. Thus the electrons propagate only due to the random off-diagonal terms f.

III. ONE-PARTICLE GREEN'S FUNCTION

In this section the averaged one-particle Green's function

$$G_{\alpha\beta}(r, r', z) = \left\langle\!\!\left\langle r\alpha \left| \frac{1}{z-H} \right| r'\beta \right\rangle\!\!\right\rangle_{\mathrm{av}} \tag{3.1}$$

is evaluated in lowest order in $1/n$ along the lines[12] by Wigner[1] and Arnold[3] for the zero-dimensional case. For this purpose $(z-H)^{-1}$ is expanded in powers of f yielding

$$\left\langle\!\!\left\langle r\alpha \left| \frac{1}{z-H} \right| r'\beta \right\rangle\!\!\right\rangle_{\mathrm{av}} = \langle r|G^0(z)|r'\rangle\delta_{\alpha\beta} + \frac{1}{\sqrt{n}}\langle r|G^0\langle f_{\alpha\beta}\rangle_{\mathrm{av}}G^0|r'\rangle + \frac{1}{n}\sum_{\alpha_1}\langle r|G^0\langle f_{\alpha\alpha_1}G^0 f_{\alpha_1\beta}\rangle_{\mathrm{av}}G^0|r'\rangle + \cdots \tag{3.2}$$

with the general term

$$n^{-k/2}\sum_{\alpha_1\cdots\alpha_{k-1}}\langle r|G^0\langle f_{\alpha\alpha_1}G^0 f_{\alpha_1\alpha_2}G^0\cdots f_{\alpha_{k-1}\beta}\rangle_{\mathrm{av}}G^0|r'\rangle \tag{3.3}$$

and

$$G^0(z) = (z-v)^{-1}. \tag{3.4}$$

In terms of the Fourier components

$$v(q) = \sum_r v_{r,0}e^{iqr}, \tag{3.5}$$

one has

$$\langle r|G^0(z)|r'\rangle = \int_q G^0(q,z)e^{iq(r'-r)} \tag{3.6}$$

with

$$\int_q = \frac{\mathcal{V}}{(2\pi)^d}\int d^dq, \tag{3.7}$$

$$G^0(q,z) = [z - v(q)]^{-1}, \tag{3.8}$$

and $\mathcal{V}$ being the volume of the primitive cell.

To determine the leading contributions of $G_{\alpha\alpha}$ we consider the partitions of the indices $\alpha, \alpha_1, \ldots, \alpha_{k-1}$ into all possible distinct sets. For example, $\alpha, \alpha_1, \alpha_2, \alpha_3$ can be divided into the three sets (α, α_2), (α_1), (α_3) or into the sets (α), (α_1, α_3), (α_2) or into the set $(\alpha, \alpha_1, \alpha_2, \alpha_3)$ or into the sets (α), (α_1), (α_2), (α_3) or others. Now the summation for a partition is performed with the restriction that all α's in the same set are equal, but the α's in different sets differ from each other. This summation yields $(n-1)(n-2)\cdots(n-l)$ equal contributions for a partition into $l+1$ sets.

Thus, a contribution of such a partition is of the order $n^{l-k/2}$. To obtain the leading behavior of G one has to find the partitions with maximum l for given k which yield nonvanishing contributions. For this purpose consider the sequence $\alpha, \alpha_1, \alpha_2, \ldots \alpha_{k-1}, \alpha$ as a walk of k steps from α to α_1 to α_2, etc., to α connecting $l+1$ different points α, respectively, α_i. Here a point is attributed to each set. If the step between α_{i-1} and α_i (including its reverse) is performed only once, then $\langle f_{\alpha_{i-1}\alpha_i}\rangle_{\mathrm{av}} = 0$ factors out of the expression (3.3). Thus each step of the walk has to be performed at least twice to yield a nonvanishing contribution. An example for such a walk is $\alpha, \alpha_1, \alpha_2, \ldots \alpha_{l-1}, \alpha_l, \alpha_{l-1}, \ldots, \alpha$ (with $k = 2l$) contributing in order n^0. Thus, for the leading contribution only walks with $k \leq 2l$ have to be considered. This implies that at least one of the indices $\alpha_i \neq \alpha$ is in a set of one member, since otherwise all of the $k-1$ labels $\alpha_1, \ldots, \alpha_{k-1}$ would be in sets of at least two members which would imply $k - 1 \geq 2l$ (we allow α to be in a set of one member) in contradiction to $k \leq 2l$. Since this α_i is connected to the other α's only by the steps from α_{i-1} to α_i and from α_i to α_{i+1} both steps have to be identical and $\alpha_{i-1} = \alpha_{i+1}$. Now let us skip the steps α_{i-1}, α_i, α_{i+1} and consider the reduced walk $\alpha, \alpha_1, \ldots, \alpha_{i-1}, \alpha_{i+2}, \ldots, \alpha$ with $k' = k-2$ steps and $l' = l-1$ different points. Again we have $k' \leq 2l'$. We reduce this walk again and

again until k and l are zero. Since k changes by 2 and l by 1 at each reduction, no walk with $k \leq 2l$ yields a contribution and $k = 2l$ yields the leading contribution.

At one step of the reduction α_1 will be the label (point) which occurs only once and the walk has been reduced to α, α_1, α or $\alpha, \alpha_1, \alpha, \ldots, \alpha$. The only exception is the zero-step walk. Thus, all the walks which contribute in leading order can be determined recursively as follows: Either perform no step [which corresponds to the term $G^0\delta_{\alpha\beta}$ in Eq. (3.2)] or perform the step from α to α_1, then a walk in leading order from α_1 to α_1, then a step from α_1 to α and then again a walk in leading order. Thus, we may write in leading order

$$G_{\alpha\alpha}(z) = G^0(z) + n^{-1} \sum_{\alpha_1} G^0(z) \langle f_{\alpha\alpha_1} G_{\alpha_1\alpha_1}(z) f_{\alpha_1\alpha} \rangle_{\mathrm{av}} \times G_{\alpha\alpha}(z) . \tag{3.9}$$

We have not yet considered $G_{\alpha\beta}(z)$ for $\alpha \neq \beta$. These off-diagonal contributions are of the order $n^{-3/2}$. This can be seen as follows: Since each step has to be performed at least twice, α and β have to be in sets of at least two members. If each set contains at least two labels, then $k+1 \geq 2(l+2)$ for $l+2$ different sets. Such a partition yields a contribution of order $n^{-3/2}$. If there are α_i's which are single members of their set then we perform the reduction until no more α_i is in a set of its own. For the reduced walk we have $k' \geq 2l'+3$ and thus $k \geq 2l+3$ for the original walk. An example for a walk which contributes in order $n^{-3/2}$ is $\alpha, \beta, \alpha, \beta$. We do not pursue the discussion of these off-diagonal elements of G.

Using Eq. (2.7) we may write Eq. (3.9) for the diagonal term $G_{\alpha\alpha} = G$ in leading order

$$G(r, r', z) = G^0(r, r', z) + \sum_{r_1, r_2} G^0(r, r_1, z) \Sigma(r_1, r_2, z) G(r_2, r', z) \tag{3.10}$$

with the self-energy

$$\Sigma(r_1, r_2, z) = \sum_{r_3, r_4} M_{r_1 r_3 r_4 r_2} G(r_3, r_4, z) . \tag{3.11}$$

Since M and G are translational invariant, Eqs. (3.10) and (3.11) reduce to

$$G(q, z) = G^0(q, z) + G^0(q, z) \Sigma(q, z) G(q, z) \tag{3.12}$$

with

$$G_{\alpha\alpha}(r, r', z) = \int_q G(q, z) e^{iq(r'-r)} , \tag{3.13}$$

$$\Sigma(q, z) = \int_{q'} M(q, q') G(q', z) , \tag{3.14}$$

$$M(q, q') = \sum_{r_1 r_3 r_4} M_{r_1 r_3 r_4 0} e^{iqr_1 + iq'(r_4 - r_3)} . \tag{3.15}$$

For the special case of *site-diagonal disorder* the self-energy, Eq. (3.11), becomes diagonal

$$\Sigma(r_1, r_2, z) = \delta_{r_1 r_2} \Sigma(z) \tag{3.16}$$

with

$$\Sigma(z) = M G_d(z) , \tag{3.17}$$

where $G_d(z)$ is a diagonal element of G

$$G_d(z) = G(r, r, z) , \tag{3.18}$$

thus

$$G(q, z) = G^0(q, z) + G^0(q, z) \Sigma(z) G(q, z) = [z - v(q) - \Sigma(z)]^{-1} \tag{3.19}$$

This equation has the form of the CPA equation[4,7] for the one-particle correlation for $n = 1$ provided the self-energy obeys Eq. (3.17). If we choose the semicircle distribution for the diagonal elements ϵ

$$p(\epsilon) = \begin{cases} (4M - \epsilon^2)^{1/2} / 2\pi M , & \epsilon^2 \leq 4M \\ 0 , & \epsilon^2 \geq 4M \end{cases} \tag{3.20}$$

then the average t matrix[4,7] vanishes

$$\left\langle \frac{\epsilon - \Sigma}{1 - (\epsilon - \Sigma) G_d} \right\rangle_{\mathrm{av}} = 0 \tag{3.21}$$

for Σ given by Eq. (3.17) which can be easily seen by evaluating the left-hand side of Eq. (3.21) with the probability distribution (3.20). Thus, the $n = \infty$ limit of the site-diagonal disorder model yields the CPA solution for the $n = 1$ model with semicircle distribution.

Coherent-potential approximations for systems with off-diagonal disorder governed by $n = 1$ Hamiltonians

$$H = H_0 + \sum_i \lambda_i H_i ,$$

where the λ_i assume independently one of two values have been considered by Takeno[13] and by Schwartz *et al.*[14] One can show that for a semicircle distribution of the λ's one obtains Eqs. (3.10) and (3.11).

For the *gauge-invariant model* Eq. (3.10) reduces to

$$G(r, r', z) = \delta_{rr'} z^{-1} + z^{-1} \sum_{r_1} M_{rr_1} G(r_1, r_1, z) G(r, r', z) . \tag{3.22}$$

G vanishes unless $r = r'$ because of the phase fluctuations

$$G(r, r', z) = G_1(z) \delta_{rr'} \tag{3.23}$$

and Eq. (3.22) reduces to

$$zG_1(z) = 1 + \tfrac{1}{4}E_0^2 G_1^2(z) \tag{3.24}$$

with

$$\sum_{r_1} M_{rr_1} = \frac{E_0^2}{4} . \tag{3.25}$$

For large z, $G_1(z)$ has to vanish like z^{-1} and $G_1(z)$ has to be analytic except for real z. This and Eq. (3.24) determine uniquely $G_1(z)$

$$G_1(z) = \frac{2}{E_0^2}[z - (z^2 - E_0^2)^{1/2}] = \frac{2}{z + (z^2 - E_0^2)^{1/2}} , \tag{3.26}$$

where the sign of $(z^2 - E_0^2)^{1/2}$ has to be chosen so that

$$\begin{aligned} &\operatorname{sgn} \operatorname{Im}(z^2 - E_0^2)^{1/2} = \operatorname{sgn} \operatorname{Im} z \quad \text{for complex } z , \\ &(z^2 - E_0^2)^{1/2} > 0 \quad \text{for real } z > E_0 , \\ &(z^2 - E_0^2)^{1/2} < 0 \quad \text{for real } z < -E_0 . \end{aligned} \tag{3.27}$$

$G_1(z)$ has a branch cut along the real axis in the interval

$$-E_0 < z < E_0 . \tag{3.28}$$

In this interval we may write

$$\begin{aligned} &G_1(z) = 2E_0^{-1} e^{-is\varphi} \quad \text{for } z = E_0 \cos\varphi + is0 , \\ &s = \pm 1, \quad 0 \leq \varphi \leq \pi . \end{aligned} \tag{3.29}$$

We note that

$$|G_1(z)| \leq 2/E_0 , \tag{3.30}$$

where the equal sign holds only along the branch cut (3.28). The density of states is given by the semicircle law

$$\rho(E) = \pi^{-1} \operatorname{Im} G_1(E - i0) = \begin{cases} 2(E_0^2 - E^2)^{1/2}/\pi E_0^2, & E^2 \leq E_0^2 \\ 0, & E^2 \geq E_0^2 \end{cases} \tag{3.31}$$

as in the zero-dimensional case.[1,3]

IV. TWO-PARTICLE GREEN'S FUNCTION

In this section the averaged two-particle Green's function

$$K_{\alpha\beta\gamma\delta}(r_1, r_2, z, r_3, r_4, z') = \left\langle \left\langle r_1\alpha \left| \frac{1}{z - H} \right| r_2\beta \right\rangle \left\langle r_3\gamma \left| \frac{1}{z' - H} \right| r_4\delta \right\rangle \right\rangle_{\text{av}} \tag{4.1}$$

will be considered. It may be written as

$$K_{\alpha\beta\gamma\delta}(r_1, r_2, z, r_3, r_4, z') = G_{\alpha\beta}(r_1, r_2, z) G_{\gamma\delta}(r_3, r_4, z') + \text{cumulant} . \tag{4.2}$$

The leading order in n of the cumulant depends on the labels $\alpha, \beta, \gamma, \delta$. The highest-order contribution n^{-1} is obtained for $\alpha = \delta$, $\beta = \gamma$ and $\alpha = \gamma$, $\beta = \delta$, respectively. Only these two cases will be discussed here.

To calculate $K_{\alpha\beta\beta\alpha}$ the right-hand side of Eq. (4.1) will be expanded in powers of G^0 and the contributions will be summed in which pairs of submatrices $f_{\alpha\beta}$ and/or $f_{\beta\alpha}$ occur. Such pairs of factors come either (i) both from $(z - H)^{-1}$, or (ii) both from $(z' - H)^{-1}$, or (iii) one from each resolvent. Consider for the moment only those pairs of factors f under (iii). In leading order they contribute

$$\begin{aligned} K_{\alpha\beta\beta\alpha} = {} & G^0(z) G^0(z') \delta_{\alpha\beta} + n^{-1} G^0 G^0 \langle f_{\alpha\beta} f_{\beta\alpha} \rangle_{\text{av}} G^0 G^0 \\ & + n^{-2} \sum_{\alpha_1} G^0 G^0 \langle f_{\alpha\alpha_1} f_{\alpha_1\alpha} \rangle_{\text{av}} G^0 G^0 \langle f_{\alpha_1\beta} f_{\beta\alpha_1} \rangle_{\text{av}} \\ & \times G^0 G^0 + \cdots \end{aligned}$$

which yields

$$K_{\alpha\beta\beta\alpha} = G^0 G^0 \delta_{\alpha\beta} + n^{-1} \sum_{\alpha_1} G^0 G^0 \langle f_{\alpha\alpha_1} f_{\alpha_1\alpha} \rangle_{\text{av}} K_{\alpha_1\beta\beta\alpha_1} .$$

If one now includes all contributions for which pairs of factors come from either $(z - H)^{-1}$ or $(z' - H)^{-1}$ then G^0 has to be replaced by G everywhere in the equations which yields

$$K_{\alpha\beta\beta\alpha} = GG\delta_{\alpha\beta} + n^{-1} \sum_{\alpha_1} GGMK_{\alpha_1\beta\beta\alpha_1} . \tag{4.3}$$

For the cumulant C

$$K_{\alpha\beta\beta\alpha} = GG\delta_{\alpha\beta} + C , \tag{4.4}$$

one obtains

$$C = GGMC + n^{-1} GGMGG . \tag{4.5}$$

Introducing the T matrix by

$$T = M + MGGT \tag{4.6}$$

and multiplying this equation from both sides by GG one obtains by comparison with Eq. (4.5)

$$C = n^{-1} GGTGG . \tag{4.7}$$

With full arguments the symbolic equations (4.4), (4.6), and (4.7) read

$$K_{\alpha\beta\beta\alpha}(r_1, r_2, z, r_3, r_4, z') = G(r_1, r_2, z) G(r_3, r_4, z') \delta_{\alpha\beta} + C(r_1, r_2, z, r_3, r_4, z') , \tag{4.4'}$$

$$T(r_1, r_2, z, r_3, r_4, z') = M(r_1, r_2, r_3, r_4) + \sum M(r_1, r_1', r_4', r_4) G(r_1', r_2', z) G(r_3', r_4', z') \, T(r_2', r_2, z, r_3, r_3', z') , \tag{4.6'}$$

$$C(r_1, r_2, z, r_3, r_4, z') = n^{-1} \sum G(r_1, r_1', z) G(r_4', r_4, z') T(r_1', r_2', z, r_3', r_4', z') \times G(r_2', r_2, z) G(r_3, r_3', z), \tag{4.7'}$$

where the sums run over all primed sites r'.

Similarly one obtains

$$K_{\alpha\beta\alpha\beta} = GG\delta_{\alpha\beta} + C' \tag{4.8}$$

and

$$C' = n^{-1} GGT'GG \tag{4.9}$$

with the same arguments as in (4.4') and (4.7'), however

$$T' = M' + M'GGT' \tag{4.10}$$

reads

$$T'(r_1, r_2, z, r_3, r_4, z') = M'(r_1, r_2, r_3, r_4) + \sum M'(r_1, r_1', r_3, r_3') G(r_1', r_2', z) \times G(r_3', r_4', z') T'(r_2', r_2, z, r_4', r_4, z'). \tag{4.10'}$$

Note that for $K_{\alpha\alpha\alpha\alpha}$ Eqs. (4.4) and (4.8) are only correct in order n^0. In order n^{-1} one has

$$K_{\alpha\alpha\alpha\alpha} = GG + C + C' + O(n^{-2}) \tag{4.11}$$

provided G is calculated to n^{-1}.

For real matrices one has

$$T'(r_1, r_2, z, r_3, r_4, z') = T(r_1, r_2, z, r_4, r_3, z') \tag{4.12}$$

which can be obtained from Eqs. (2.10) (4.6'), (4.10'), and $G(r, r', z) = G(r', r, z)$. For the phase-invariant ensemble (2.11) one has

$$T' = 0. \tag{4.13}$$

Sum rule. Starting from the equality

$$(z - z') \sum_{r'\beta} \left\langle\!\!\left\langle r\alpha \left| \frac{1}{z - H} \right| r'\beta \right\rangle \left\langle r'\beta \left| \frac{1}{z' - H} \right| r''\gamma \right\rangle\!\!\right\rangle_{\text{av}} = \left\langle\!\!\left\langle r\alpha \left| \frac{z - z'}{(z - H)(z' - H)} \right| r''\gamma \right\rangle\!\!\right\rangle_{\text{av}} = G_{\alpha\gamma}(r, r'', z') - G_{\alpha\gamma}(r, r'', z), \tag{4.14}$$

one obtains the sum rule[8]

$$(z - z') \sum_{r'\beta} K_{\alpha\beta\beta\gamma}(r, r', z, r', r'', z') = G_{\alpha\gamma}(r, r'', z') - G_{\alpha\gamma}(r, r'', z). \tag{4.15}$$

This sum rule is fulfilled in the leading order calculated. To see this introduce the notation

$$[MG(z)]_{r_1 r_2} = \sum_{r_3 r_4} M_{r_1 r_3 r_4 r_2} G(r_3, r_4, z) \tag{4.16}$$

in Eq. (3.11). Then Eq. (3.10) reads as a matrix equation

$$G(z) = G^0(z) + G^0(z)[MG(z)]G(z) \tag{4.17}$$

from which one obtains

$$G(z') = G(z)(G^0(z))^{-1} G(z') - G(z)[MG(z)]G(z') \tag{4.18a}$$

and similarly

$$G(z) = G(z)(G^0(z'))^{-1} G(z') - G(z)[MG(z')]G(z'). \tag{4.18b}$$

Subtraction of these two equations and the use of

$$(G^0(z))^{-1} - (G^0(z'))^{-1} = z - z' \tag{4.19}$$

yields

$$P = G(z)G(z') + G(z)[MP]G(z') \tag{4.20}$$

for

$$P = (G(z') - G(z))/(z - z'). \tag{4.21}$$

Comparison of Eq. (4.20) with Eq. (4.3) shows that

$$P(r, r'') = \sum_{r'\beta} K_{\alpha\beta\beta\alpha}(r, r', z, r', r'', z'). \tag{4.22}$$

From Eq. (4.21) one sees that the sum rule (4.15) is fulfilled for $\alpha = \gamma$ ($\alpha \neq \gamma$ does not contribute in leading order).

In the special case of *site-diagonal disorder* T reduces to

$$T(r_1, r_2, z, r_3, r_4, z') = \delta_{r_1 r_4} \delta_{r_2 r_3} \tilde{T}(r_1, r_2, z, z') \tag{4.23}$$

with

$$\tilde{T}(r_1, r_2, z, z') = M\delta_{r_1 r_2} + \sum_{r'} MG(r_1, r', z) G(r', r_1, z') \times \tilde{T}(r', r_2, z, z'). \tag{4.24}$$

To compare with the CPA[4,8] this equation can be rewritten in the form

$$\tilde{T}(r_1, r_2, z, z') = \Lambda(z, z')\delta_{r_1 r_2} + \sum_{r' \neq r_1} \Lambda(z, z') G(r_1, r', z) \times G(r', r_1, z') \tilde{T}(r', r_2, z, z') \tag{4.25}$$

where $\Lambda(z, z')$ contains all contributions from repeated scattering at the same site

$$\Lambda(z, z') = M/(1 - M G_d G_d'), \tag{4.26}$$

where here and in the following the abbreviations $G_d = G_d(z)$, $G_d' = G_d(z')$, $\Sigma = \Sigma(z)$, $\Sigma' = \Sigma(z')$ are used. Equation (4.25) is the CPA equation for the two-particle correlation function for $n=1$ where Λ is the average of the product of the single-site t matrices

$$\Lambda(z, z') = \left\langle \frac{\epsilon - \Sigma}{1 - (\epsilon - \Sigma) G_d} \frac{\epsilon - \Sigma'}{1 - (\epsilon - \Sigma') G_d'} \right\rangle_{\text{av}}. \tag{4.27}$$

The average can be evaluated using Eq. (3.21)

$$\Lambda = \frac{\Sigma - \Sigma'}{G_d - G_d' + G_d G_d' (\Sigma' - \Sigma)} \tag{4.28}$$

which reduces with Eq. (3.17) to Eq. (4.26). Therefore, the $n=\infty$ limit of the site-diagonal disorder model yields apart from the factor n^{-1} [in Eq. (4.9)] the CPA for the cumulant of the $n=1$ model with semicircle distribution.

To discuss the long-range behavior of the two-particle correlation let us determine the cumulant

$$\tilde{C}(r_1, r_2, z, z') = C(r_1, r_2, z, r_2, r_1, z'). \tag{4.29}$$

In terms of the Fourier transforms

$$\tilde{C}(q, z, z') = \sum_r e^{iqr} \tilde{C}(0, r, z, z'), \tag{4.30}$$

$$\tilde{T}(q, z, z') = \sum_r e^{iqr} \tilde{T}(0, r, z, z'), \tag{4.31}$$

one obtains from Eqs. (4.7) and (4.24)

$$\tilde{C}(q, z, z') = G_2^2(q, z, z') \tilde{T}(q, z, z') \tag{4.32}$$

and

$$\tilde{T}(q, z, z') = M/[1 - M G_2(q, z, z')] \tag{4.33}$$

with

$$G_2(q, z, z') = \sum_r G(r, 0, z) G(0, r, z) e^{iqr} = \int_{q'} G(q', z) G(q' - q, z'). \tag{4.34}$$

This quantity G_2 can be easily evaluated for $q=0$ either via the sum rule or by means of the partial fraction decomposition

$$G(q', z) G(q', z') = \frac{1}{z - M G_d - z' + M G_d'} [G(q', z') - G(q', z)] \tag{4.35}$$

which yields

$$G_2(0, z, z') = \frac{1}{M} + \frac{z' - z}{M(z - z') + M^2 (G_d' - G_d)}. \tag{4.36}$$

The denominator of Eq. (4.33) vanishes for $q=0$ if the second term on the right-hand side of Eq. (4.36) vanishes, that is for

$$\lim z = z', \quad \lim G_d(z') \neq G_d(z) \tag{4.37}$$

Thus, $\tilde{T}$ diverges for $q=0$ if z and z' approach the same energy E from different halves of the complex plane along the branch cut of G, that is for $\rho(E) \neq 0$. For

$$z = E + \tfrac{1}{2}\omega, \quad z' = E - \tfrac{1}{2}\omega, \tag{4.38}$$

where E is real and ω has an imaginary part of sign s one obtains for small ω

$$G_2(0, z, z') = \frac{1}{M} - \frac{\omega}{2\pi i s M^2 \rho(E)} \tag{4.39}$$

which yields for small ω and q^2 (here and in the following we assume cubic symmetry)

$$n\tilde{C}(q, z, z') = \left(- \frac{i\omega s}{2\pi\rho(E)} + A q^2 \right)^{-1} \tag{4.40}$$

with

$$A = -M^2 \frac{\partial G_2(q)}{\partial q^2}\bigg|_{q=0} = \frac{M^2}{2d} \sum_r r^2 G(0, r, z) G(r, 0, z'). \tag{4.41}$$

The vanishing denominator in Eq. (4.40) indicates a long-range behavior of $\tilde{C}$ which will be discussed in Sec. V.

Next, we determine $\tilde{C}$ for the *gauge-invariant model*. From Eq. (4.6) one obtains for $\tilde{T}$, Eq. (4.23)

$$\tilde{T}(r_1, r_2, z, z') = M_{r_1 r_2} + \sum_{r'} M_{r r'} G_1(z) G_1(z') \times \tilde{T}(r', r_2, z, z') \tag{4.42}$$

which yields

$$\tilde{T}(q, z, z') = \frac{M(q)}{1 - G_1(z) G_1(z') M(q)} \tag{4.43}$$

with

$$M(q) = \sum_r M_{r0} e^{iqr}. \tag{4.44}$$

The cumulant obeys

$$C(r_1, r_2, z, r_3, r_4, z') = \delta_{r_1 r_4}\delta_{r_2 r_3}\tilde{C}(r_1, r_2, z, z') \tag{4.45}$$

with

$$n\tilde{C}(r_1, r_2, z, z') = G_1^2(z)G_1^2(z')\tilde{T}(r_1, r_2, z, z') . \tag{4.46}$$

Thus, one has

$$n\tilde{C}(q, z, z') = \frac{G_1(z)G_1(z')M(q)}{G_1^{-1}(z)G_1^{-1}(z') - M(q)} . \tag{4.47}$$

In order to discuss the singularities first consider $M(q)$, Eq. (4.44). Since $M_{rr'}$ is the average of an absolute value, it is not negative and $M(q)$ is real and obeys

$$|M(q)| \leq M(0) = \tfrac{1}{4}E_0^2 . \tag{4.48}$$

Now turn to $G_1^{-1}(z)G_1^{-1}(z')$. According to Eq. (3.30) the absolute value of this product cannot be less than $\frac{1}{4}E_0^2$. This minimum value can be obtained only along the branch cuts. For the parametrization

$$z = E_0\cos\varphi + is0, \quad z' = E_0\cos\varphi' + is'0, \tag{4.49}$$

one obtains along the branch cut

$$n\tilde{C}(q, z, z') = \frac{4e^{-i(s\varphi + s'\varphi')}M(q)/E_0^2}{\frac{1}{4}e^{i(s\varphi + s'\varphi')}E_0^2 - M(q)} . \tag{4.50}$$

For the moment assume $|M(q)| = M(0)$ holds only for $q = 0$. Then $\tilde{C}$ becomes singular only for $s = -s'$, $z = -z'$ at $q = 0$. In this hydrodynamic limit one obtains with (4.38) the same long-range behavior (4.40) as for the site-diagonal disorder model with

$$A = -\left.\frac{\partial M(q)}{\partial q^2}\right|_{q=0} = \frac{1}{2d}\sum_r r^2 M_{o,r} . \tag{4.51}$$

This result is in agreement with our assumption that for the discussion of the long-range behavior one may substitute the gauge-invariant model.

There is an important exception to this. It is not always true that $|M(q)| = M(0)$ implies $q = 0$ (apart from reciprocal-lattice vectors). This assumption fails in the trivial case when the system consists of several sublattices with no interaction between different sublattices. It also fails in the case where the system consists of two sublattices A and B so that f connects both sublattices but vanishes between sites of the same sublattices. One-dimensional models for $n = 1$ of this type have been considered by Theodorou and Cohen,[15] and Eggarter and Riedinger.[16] They show a singularity of the density of states at zero energy and have the property that an eigenstate $\psi(r)$ of energy E implies an eigenstate $\psi'(r) = e^{iq_0 r}\psi(r)$ with energy $-E$, where

$$e^{iq_0 r} = \begin{cases} +1 & \text{for one sublattice} \\ -1 & \text{for the other sublattice} . \end{cases} \tag{4.52}$$

Thus, eigenstates of energy E and $-E$ are strongly correlated. Indeed, for such a system with $n = \infty$ one has

$$M(q_0 + q) = \sum_r M_{0r}e^{i(q_0+q)r} = -\sum_r M_{0r}e^{iqr} = -M(q) . \tag{4.53}$$

Thus, $\tilde{C}(k)$, Eq. (4.50), diverges for $k = q_0$, $s = s'$, $\varphi + \varphi' = \pi$, that is for energies $z = E + is0$, $z' = -E + is0$ which implies a long-range behavior with oscillations of wave vector q_o. More precisely for

$$z = E + \tfrac{1}{2}\omega, \quad z' = -E + \tfrac{1}{2}\omega, \tag{4.54}$$

where E is real and ω has an imaginary part of sign s one obtains

$$n\tilde{C}(q_0 + q) = (i\omega s/2\pi\rho(E) - Aq^2)^{-1} . \tag{4.55}$$

V. LONG-RANGE BEHAVIOR AND ELECTRIC CONDUCTIVITY

The long-range behavior can be best discussed in terms of the spectral function

$$S(r, r', E_1, E_2) = \left\langle \sum_\beta \langle r\alpha|\delta(H - E_1)|r'\beta\rangle \times \langle r'\beta|\delta(H - E_2)|r\alpha\rangle \right\rangle_{\text{av}} = \left\langle \sum_{\beta ij} \psi_i(r\alpha)\psi_i^*(r'\beta)\psi_j(r'\beta)\psi_j^*(r\alpha) \times \delta(E_i - E_1)\delta(E_j - E_2) \right\rangle_{\text{av}} , \tag{5.1}$$

where the indices i and j number the eigenstates of the system. The spectral function is the product of the density of states at energies E_1 and E_2 multiplied by the averaged correlation function of the electrons at these energies. Since

$$\delta(H - E) = \frac{i}{2\pi}\sum_s \frac{s}{E - H + is0}, \quad s = \pm 1 , \tag{5.2}$$

S is expressed in terms of the Green's functions

$$S(r, r', E_1, E_2) = -(4\pi^2)^{-1}\sum_{ss'\beta} ss' K_{\alpha\beta\beta\alpha}(r, r', E_1 + is0, r', r, E_2 + is'0) . \tag{5.3}$$

The product in Eq. (4.3) yields only a short-range contribution. Thus, one may neglect GG and obtains

$$S(r, r', E_1, E_2) = -(4\pi^2)^{-1} \sum_{ss'} ss' n\tilde{C}(r, r', E_1 + is0, r', r, E_2 + is'0) . \tag{5.4}$$

For $E_1 = E + \frac{1}{2}\omega$ and $E_2 = E - \frac{1}{2}\omega$, Eq. (4.40) yields the long-range contribution

$$S(0, r) = (4\pi^2)^{-1} \sum_s \int e^{-i\sigma r} \left(-\frac{i\omega s}{2\pi\rho(E)} + Aq^2 \right)^{-1} , \tag{5.5}$$

where the short-range contributions for $s = s'$ have been neglected.

Introducing the wave vector

$$\kappa = \left(\frac{-i\omega s}{2\pi A\rho(E)} \right)^{1/2} , \quad \mathrm{Re}\kappa > 0 \tag{5.6}$$

one obtains for $|r| \gg |\kappa|^{-1}$

$$S(0, r) = \mathrm{Re} \frac{\upsilon}{4\pi^2 \kappa A} \left(\frac{\kappa}{2\pi r} \right)^{(d-1)/2} e^{-\kappa r} \tag{5.7}$$

which indicates that the correlation between wave functions separated by an energy difference ω decays on the length

$$L = |\kappa|^{-1} = [2\pi A\rho(E)/|\omega|]^{1/2} \tag{5.8}$$

which diverges like $|\omega|^{-1/2}$. We may interpret this length as the length over which the wave functions lose phase coherence.

For the gauge-invariant model with the special property (4.53) one shows similarly that for $E_1 = E + \frac{1}{2}\omega$ and $E_2 = -E + \frac{1}{2}\omega$ one obtains the long-range behavior (5.7) with an addition factor $e^{iq_0 r}$.

For $|r| \ll L$ however $S(0, r)$ approaches a finite value for fixed r and $\omega \to 0$ provided $d > 2$, since the integral (5.5) exists for $\omega = 0$. For $d = 2$ S diverges logarithmically and for $d < 2$ it diverges like $|\omega|^{d/2-1}$. The same behavior is observed for $\tilde{C}$ and complex ω. Following Economou and Cohen[11] this indicates that for $d > 0$ the eigenstates are extended since $\tilde{C}$ does not diverge as fast as $|\omega|^{-1}$.

Conductivity. According to Kubo[17] and Greenwood[18] the conductivity $\sigma_T(\omega)$ can be expressed in terms of the current-current or density-density spectral function

$$\sigma_T(\omega) = \omega^{-1} \int \sigma(\omega, E) \left[\tilde{f}_T\left(E - \frac{\omega}{2}\right) - \tilde{f}_T\left(E + \frac{\omega}{2}\right) \right] dE \tag{5.9}$$

with the Fermi distribution function

$$\tilde{f}_T(E) = \{\exp[(E - \mu)/kT] + 1\}^{-1} \tag{5.10}$$

and

$$\sigma(\omega, E) = -\frac{e^2\pi n}{2d\upsilon} \omega^2 \sum_r r^2 S\left(0, r, E + \frac{\omega}{2}, E - \frac{\omega}{2}\right) . \tag{5.11}$$

In the dc limit $\omega = 0$ only the long-range contribution of $\tilde{C}$ will survive. Thus, one obtains

$$\sigma(\omega, E) = -\frac{e^2 n}{8\pi^2 d\upsilon} \omega^2 \sum_{rs} r^2 n\tilde{C}\left(0, r, E + \frac{\omega}{2} + is0, E - \frac{\omega}{2} - is\right)$$

$$= \frac{e^2 n}{4\pi^2 \upsilon} \omega^2 \sum_s \frac{\partial}{\partial q^2} \tilde{C}(q, \cdots, \cdots) = \frac{2\pi e^2 n A\rho^2(E)}{\upsilon} . \tag{5.12}$$

The conductivity is finite everywhere inside the band.

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