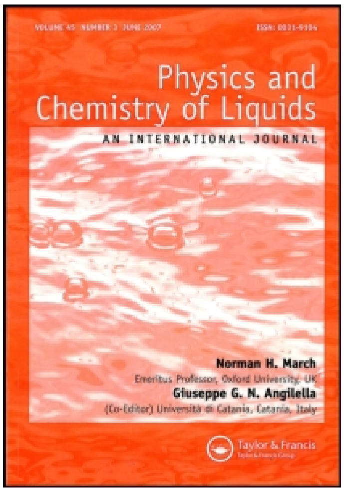

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Localization in Spatially Disordered Systems: Screening and Band Structure Effects at the EMA Level

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To cite this Article Winn, Martyn D. and Logan, David E.(1990) 'Localization in Spatially Disordered Systems: Screening and Band Structure Effects at the EMA Level', Physics and Chemistry of Liquids, 22: 1, 11 — 26
To link to this Article: DOI: 10.1080/00319109008036407
URL: http://dx.doi.org/10.1080/00319109008036407

Phys. Chem. Liq., 1990, Vol. 22, pp. 11–26
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LOCALIZATION IN SPATIALLY DISORDERED SYSTEMS: SCREENING AND BAND STRUCTURE EFFECTS AT THE EMA LEVEL

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(Received 11 January 1990)

An analysis is given of Anderson localization in a one-band tight-binding model with off-diagonal disorder characteristic of a quenched liquid-like structure. We extend a localization criterion due to Logan and Wolynes, based on a self-consistent determination of the most probable value of the imaginary part of the site self-energy, to include screening arising from many-body terms in the renormalized perturbation series. Liquid state methods are used to examine screening, as embodied in an effective energy and density dependent transfer matrix element, at the level of the effective medium approximation. It is shown that this effective transfer matrix element is screened in high energy regions and anti-screened in low energy regions, so that extended states tend to occur in the low energy low density of states regime. Theoretical predictions for the mobility edge trajectories are found to be in reasonable agreement with recent computer simulations. The effects of the short-ranged structure of the system are also examined.

KEY WORDS: Anderson localization, screening, effective medium approximation.

1 INTRODUCTION

A theoretical study of the electronic properties of liquids and amorphous solids is an area of active research. The disorder inherent in these systems must be taken seriously and, even at an idealized one-electron level of description, can lead to profound effects such as disorder-induced (Anderson) localization, a mechanism of possible relevance to metal-insulator transitions occurring for example in the impurity band of doped semiconductors and in both monovalent and divalent liquid metals. Modelled at the level of a tight-binding Hamiltonian, the disorder manifests itself in both the diagonal elements (site-diagonal disorder, SDD) and in the off-diagonal transfer matrix elements (off-diagonal disorder, ODD). Most work on the localization problem has focussed on spatially periodic systems with SDD alone. Consideration of the ODD characteristic of topologically disordered systems is a more recent area of concern.

Some of the simpler non-trivial quantities to analyze are the configurationally averaged Green functions of a spatially disordered tight-binding model, from which follow the density of states of the system and the electrical conductivity in a weak disorder (Boltzmann) regime. Anderson localization, however, which is the primary concern of this paper, requires a more subtle treatment and although the averaged Green functions do supply necessary input to a theory of localization, to infer localization itself one must study typical rather than average quantities. A probabilistic analysis is therefore required, and this centres usually on the renormalized perturbation series (RPS) for the site self-energy[1].

Recently Logan and Wolynes[2] have developed a simple mean field theory of localization in spatially disordered systems, in which self-consistency is enforced on the most probable value of the imaginary part of the self-energy, the vanishing of which at a certain critical number density of sites (and for a given energy E) is taken as the signature of a transition to localized states of energy E. The theory is formulated at the level of second order RPS and thereby omits contributions to the localization characteristics of the system arising from irreducible $m \geq 3$-body interactions embodied in the higher order RPS terms. Such contributions give rise to asymmetry in the mobility edge trajectories of the system, as predicted theoretically[3] and observed in computer simulations[4,5]. The effects of higher order RPS terms have been studied by Logan and Wolynes[3] within the framework of the self-consistent theory of localization due to Abou-Chacra *et al.*[6], and have been interpreted in terms of an energy-dependent screening of the interaction between a pair of atoms by the other atoms in the system, embodied in an energy and density-dependent renormalized or effective transfer matrix element.

In Section 2 of this paper we incorporate screening effects into the most probable value theory of localization, and describe the resultant localization criterion which depends on both the first moment of the renormalized transfer matrix element and the averaged density of states. In Section 3 we investigate the role of liquid-like structure in determining the localization characteristics of the system. It is known that the best single-site approximation to the density of states is the effective medium approximation[7] (EMA), which we have recently studied[8]. By exploiting parallels between the theory for the averaged Green functions and that for the renormalized transfer matrix element, we show in Section 3 how to formulate a description of the latter at the EMA level. Theoretical predictions for the mobility edge trajectories are then compared with a recent computer study by Gibbons *et al.*[5] with which they are found to be in reasonable agreement.

2 LOCALIZATION CRITERION

The excitation of interest moves in a quenched configuration of atoms with centre-of-mass positions $\{\mathbf{R}_i\}$; the atoms interact via an appropriately chosen classical potential which determines the weights of the possible spatial configurations. For a one-band system a single characteristic energy, the zero-order site energy ε_i, is associated with each atom/site. SDD is modelled by assuming the ε_i's to be independent random variables with a common probability distribution $P(\varepsilon_i)$. The excitation hops from site j to site i via a transfer matrix element $V_{ij} \equiv V(\mathbf{R}_i - \mathbf{R}_j)$; ODD thus arises from the spatial disorder inherent in the site centre of mass distribution.

The site Green functions for the random tight-binding model satisfy

$$(z - \varepsilon_i)G_{ij}(z) - \sum_k{}' V_{ik}G_{kj}(z) = \delta_{ij} \tag{1}$$

where the prime excludes $k = i$, and $z = E + i\eta$ ($\eta \to 0+$) where E is the energy. The site self-energy $S_i(z) = E_i(E) - i\Delta_i(E)$ is defined via the diagonal Green function by:

$$G_{ii}(z) = [z - \varepsilon_i - S_i(z)]^{-1} \tag{2}$$

For a given realization of the random system the nature of eigenstates of energy E is determined by the behaviour of $\Delta_i(E) = -\operatorname{Im} S_i(z)$ as $\eta \to 0+$: for localized states $\Delta_i(E) \propto \eta \to 0+$, whereas for extended states $\Delta_i(E)$ is finite in this limit[9]. For an ensemble of systems the question of whether states of a given energy are localized or extended is studied by examining probablistically the convergence characteristics of renormalized perturbation theory for the site self-energy. One considers the renormalized perturbation series[1] (RPS) for $S_i(E)$, given by

$$\begin{aligned} S_i(E) = {} & \sum_j{}' V_{ij}[z - \varepsilon_j - S_j^{(i)}]^{-1}V_{ji} \\ & + \sum_{j,k}{}' V_{ik}[z - \varepsilon_k - S_k^{(i,j)}]^{-1}V_{kj}[z - \varepsilon_j - S_j^{(i)}]^{-1}V_{ji} + \cdots \end{aligned} \tag{3}$$

where the primes restrict each summation to a self-avoiding path. Quantities such as $S_j^{(i)}(E)$ refer to the self-energy of site j with site i removed from the system, and are defined by a series analogous to (3) but with the relevant sites excluded from the sums; each term in the RPS can thus be iterated as a continued fraction. A divergence in the resultant renormalized perturbation expression for $S_i(E)$, which indicates the existence of extended eigenstates of energy E[9], can thus arise either from a divergence in the RPS or from a divergence in the iteration procedure. In practice, most approximate theories of localization focus on the convergence characteristics of either the RPS or the iteration procedure alone. In particular we mention the self consistent theory of Abou-Chacra *et al.*[6], which considers solely the convergence of the iteration procedure by truncating the RPS at the second order term—a procedure which is exact for a Cayley tree. Conflating $S_j^{(i)}$ with S_j, the resultant second order RPS reduces to

$$S_i(E) = \sum_j{}' \frac{|V_{ij}|^2}{E + i\eta - \varepsilon_j - S_j(E)} \tag{4}$$

which is analyzed self-consistently by assuming that the probability distributions for $\{S_j\}$ are independent, and demanding that they be identical.

The self-consistent theory has been extended to spatially disordered systems, and investigated by a number of authors[10–12]. A simple mean field method has also been developed[3] for incorporating higher order (irreducible $m \geq 3$-body) terms in the RPS, while retaining the underlying simplicity of the self-consistent theory of localization. A basic result of this approach is that, in a domain of localized states, the imaginary part of the site self-energy is given approximately by[3]:

$$\Delta_i(E) \simeq \sum_j{}' \frac{|\Phi_{ij}|^2(\eta + \Delta_j(E))}{(E - \varepsilon_j - E_j(E))^2} \tag{5}$$

This equation has the same form as that which results from the second order RPS, Eq. (4), except that the bare transfer matrix element is replaced by an energy- and density-dependent effective or renormalized transfer matrix element, $\Phi_{ij} \equiv \Phi(\mathbf{R}_i, \mathbf{R}_j; \rho, E)$, where ρ is the number density of sites. The effective transfer matrix element takes account of higher order RPS terms in a simple mean field sense and, physically, reflects the screening of the interaction between a pair of atoms by the other atoms in the system. The manner in which Φ_{ij} differs from V_{ij}, and thus the specific localization characteristics of the system, depends on details of the (quenched) liquid-like structure of the disordered material. These effects, which are implicit in the specification of Φ_{ij} as a sum of liquid-state interaction diagrams (see Reference 3), will be investigated in some detail in the following section. Here we simply note that the renormalized transfer matrix element does not depend explicitly on the random variables $\{E_j, \Delta_j\}$. The basic self-consistent theory of localization can thus be modified to include the effects of screening embodied in the effective transfer matrix element, as studied in Reference 3.

When dealing with the self-consistent theory, however, whether with the conventional second order RPS or at the higher-order level of Eq. (5), one is forced to analyze non-linear integral equations for the self-energy probability distributions; further, these are derived under the initial assumption that states of energy E are localized. In practice, therefore, the theories ultimately reduce to a stability analysis of localized states. To both simplify and go beyond a stability analysis of localized states, and to incorporate dephasing effects such as electron-phonon coupling into the problem, Logan and Wolynes[2] have recently developed a mean field theory of localization in which self-consistency is enforced solely on the most probable value, $\Delta_{\mathrm{mp}}(E)$, of the site self-energy. In this way the self-consistency conditions ultimately reduce to algebraic rather than integral equations, and the pure localization problem may be examined as the transition is approached from either the localized or extended domains. The basic idea of this approach is to consider a given realization of the system in which the imaginary parts of the site self-energies of all atoms other than a specific "tagged" atom, i, are constrained to their most probable values. Using liquid state methods an explicit functional form is derived for the probability distribution $f(\Delta_i)$ of the imaginary part of the self-energy for the tagged atom. Self-consistency is then enforced simply by requiring that the resultant most probable value $\Delta_{\mathrm{mp}}(E; \mu)$ of $f(\Delta_i)$ (where $\mu = \eta + \Delta_{\mathrm{mp}}(E)$) be equal to the assumed "input" most probable value $\Delta_{\mathrm{mp}}(E)$ for the other sites.

In practice, as described in Ref. 2, the behaviour of $\Delta_{\mathrm{mp}}(E; \mu)$ is examined explicitly in two limits, $\mu \to 0+$ and $\mu \to \infty$. The former limit corresponds physically to a domain of localized states ($\Delta_{\mathrm{mp}}(E) \propto \eta \to 0+$); and, with η vanishingly small, the large μ limit corresponds to a domain of strongly extended states of energy E, associated with predominantly coherent transport. In addition, as discussed in Ref. 2, retention of a finite η in the second order RPS for the self-energy mimics in a simple but physically transparent manner the effects of dephasing interactions (where $2\eta/\hbar$ is a sum of the rates of all dephasing processes); in this case the large η and hence large μ limit describes the (Förster or master equation) domain of extremely rapid dephasing interactions, with incoherent transport. Having examined the limiting behaviour of $\Delta_{\mathrm{mp}}(E;\mu)$ in the small and large μ domains, an interpolation is made between these limits via a simple Padé approximant which correctly preserves the small μ analyticity of $\Delta_{\mathrm{mp}}(E;\mu)$. The $\eta \rightarrow 0+$ localization transition and, for $\eta > 0$, the influence of dephasing interactions, can then be examined starting from this basic self-consistency relation.

Although formulated at the level of the conventional second-order RPS, in which screening effects embodied in the renormalized transfer matrix elements Φ_{ij} are omitted, it is straightforward to incorporate these effects into the above theory. For, within a most probable value approach, it is clear from (5) that in the $\mu \rightarrow 0+$ regime of localized states, $\Delta_i(E)$ is given by

$$\Delta_i(E) \simeq \sum_j{}' \frac{|\Phi_{ij}|^2}{(E - \varepsilon_j - E_j)^2}\,\mu : \mu \rightarrow 0+ \tag{6a}$$

This is almost identical to that considered in Ref. 2, but with the bare V_{ij} replaced by the effective E- and ρ-dependent transfer matrix element Φ_{ij}. The situation is even simpler in the large μ limit. Conflating $S_j^{(i)}$ with S_j in (3), and writing $S_j(E) = E_j(E) - i\Delta_{\mathrm{mp}}(E)$ for all $j \neq i$, it is apparent that in the $\mu \rightarrow \infty$ limit the resultant expression for $S_i(E)$ is dominated by its second order term. In particular, the imaginary part of the self-energy for the tagged atom i reduces to

$$\Delta_i(E) \simeq \sum_j{}' \frac{|V_{ij}|^2}{\mu} : \mu \rightarrow \infty \tag{6b}$$

which is precisely that considered in Ref. 2 in the large μ limit.

The basic formal modification to the most probable value theory of Logan and Wolynes[2] thus reduces to an incorporation of the effective transfer matrix element Φ_{ij} in the $\mu \rightarrow 0+$ localized domain. This is a minor modification, and the basic results of Ref. 2 carry through, leading to the following simple self-consistency equation for the most probable value, $\Delta_{\mathrm{mp}}(E)$, of the site self-energy:

$$\Delta_{\mathrm{mp}}(E) = \frac{T(\rho; E)[\eta + \Delta_{\mathrm{mp}}(E)]}{1 + T(\rho; E)J_2^{-1}(\rho)[\eta + \Delta_{\mathrm{mp}}(E)]^2} \tag{7}$$

Here, $J_2(\rho)$ is given by

$$J_2(\rho) = \rho \int d\mathbf{R}\; g_2(R)|V(R)|^2 \tag{8}$$

and corresponds to the second moment of the bare transfer matrix element averaged over the topological disorder, where $g_2(R)$ is the structural pair distribution function for particles interacting via the chosen classical potential. The quantity $T(\rho; E)$ is given by:

$$T(\rho; E) = \frac{2\pi}{3}\,[J_1(\rho; E)D(E)]^2 \tag{9a}$$

$D(E)$ is the ensemble averaged density of states of the system, and $J_1(\rho; E)$ is the first moment of the magnitude of the renormalized transfer matrix element

$$J_1(\rho; E) = \rho \int d\mathbf{R}\, g_2(R)|\Phi(R; \rho, E)|, \tag{9b}$$

where the ρ- and E-dependence of Φ is made explicit. Assuming a knowledge of J_1, J_2 and the density of states $D(E)$, Eq. (7) is readily used to examine the pure ($\eta \to 0+$) Anderson localization problem: when $\Delta_{\mathrm{mp}}(E)$ is found to be proportional to η and thus vanishingly small, states of energy E are localized; and when states of energy E become extended Eq. (7) may be used to obtain an explicit expression for the non-vanishing $\Delta_{mp}(E)$ and hence the E-dependent transfer rate from a site, $\tau^{-1}(E) = 2\Delta_{\mathrm{mp}}(E)/\hbar$. Similarly, when the effects of dephasing interactions are included, $\eta > 0$, (7) may be used to examine the dephasing rate dependence of the transfer rate and thus, for example, to investigate the problem of Mooij correlation regarded as a weak delocalization phenomenon.

Viewed as a function of $T(\rho; E)$ and $J_2(\rho)$, Eq. (7) is identical to that of Ref. 2. The various T-domains of physical interest in the behaviour of Δ_{mp} are discussed fully therein, and we do not repeat them here. The essential difference in the present work is that screening effects arising from the higher order RPS terms in the localized domain are included in the evaluation of $T(\rho; E)$ via both the effective transfer matrix element and, implicitly, the density of states. Our primary interest here is to examine explicitly these effects at the most probable value level of description, particularly in regard to the energetic asymmetry which arises in the mobility edge trajectories as a consequence of screening. This requires consideration of suitable liquid state approximations to describe the dependence of $\Phi(R; \rho; E)$ and $D(E)$ on energy, number density and characteristic structural parameters of the system, and will be considered in detail in the following section. We note first that, with $\eta \to 0+$ and $T(\rho; E) < 1$, the solution to (7) is

$$\Delta_{\mathrm{mp}}(E) = \frac{T(\rho; E)}{1 - T(\rho; E)}\,\eta : T < 1 \tag{10}$$

corresponding to localized states of energy E, and with $n(E) = 1 + \Delta_{\mathrm{mp}}(E)/\eta = [1 - T(\rho; E)]^{-1}$ giving a rough measure of the number of sites which participate in the localized state. The criterion for a transition from localized to extended states is thus $T(\rho; E) = 1$, i.e.

$$J_1(\rho; E)D(E) = \left[\frac{3}{2\pi}\right]^{1/2} \sim 0.7, \tag{11}$$

and for $T(\rho; E) > 1$, states of energy E are extended, with $\Delta_{\mathrm{mp}}(E)$ finite.

Although derived from the detailed theory given in Ref. 2, some insight into the transition criterion may perhaps be gleaned from the following suggestive argument. Consider a localized state of energy E centred with maximum amplitude on site i, and another with energy E' centred on site j a distance R away from i. If these states are indeed to be localized and unmixed, we argue that their energy separation,

$\Delta E = |E' - E|$, must exceed the effective matrix element $|\Phi(R)|$ which connects sites i and j; if $\Delta E \lesssim |\Phi(R)|$, mixing of the two will occur. We consider then a would-be localized state of energy E, and ask for the probability $p(E)$ that we find another such that the separation in energy between the two is less than or comparable to the matrix element which effectively connects them. This gives the probability that the would-be state of interest has a "bond" or connection to another, and when this "bond percolation"-like probability is of order unity we expect delocalization to occur. To estimate $p(E)$, note that the number of states whose energies lie in the range $E \pm |\Phi(R)|$ is

$$N \int_{E-|\Phi(R)|}^{E+|\Phi(R)|} D(E)dE$$

where N is the total number of states (or, equivalently, sites). The probability that we find a site a distance R away from i is approximately $4\pi R^2 g_2(R)dR/V$ where V is the volume of the system. Thus the probability that we find a state of energy E' centred on a site a distance R away from that of energy E such that $\Delta E \lesssim |\Phi(R)|$ is roughly

$$p(R;\, E,\, E \pm |\Phi(R)|)dR \simeq (4\pi\rho g_2(R)R^2 dR) \times \left[\int_{E-|\Phi(R)|}^{E+|\Phi(R)|} D(E)dE\right] \tag{12a}$$

where $\rho = N/V$ is the number density. As R increases the relative probability of finding another state centred in the $(R,\, R + dR)$ shell increases, but the number of such states which can potentially mix with that centred on i diminishes. Assuming for dominant values of R that the range of integration in (12a) is appreciably smaller than the bandwidth (so that the energy splitting is small), we approximate:

$$p(R;\, E,\, E \pm |\Phi(R)|) \simeq 8\pi\rho g_2(R)|\Phi(R)|R^2 D(E)$$

Integrating over R gives

$$\begin{aligned} p(E) &\simeq 2D(E) \times 4\pi\rho \int_0^\infty dR\; R^2 g_2(R)|\Phi(R)| \\ &= 2J_1(\rho;\, E)D(E) \end{aligned} \tag{12b}$$

and when this is of order unity we anticipate delocalization, i.e. when $J_1(\rho;\, E)D(E) \sim \frac{1}{2}$ which is to be compared with the criterion (11).

3 SCREENING EFFECTS AND LOCALIZATION CHARACTERISTICS

We now consider the renormalized transfer matrix element in some detail. From Ref. 3, Φ_{ij} is decomposed as

$$\Phi_{ij} = V_{ij} + \Gamma_{ij}^0 \tag{13}$$

with Γ^0_{ij} specified as the following sum of liquid state interaction diagrams:

Γ^0_{ij} = the sum of all distinct connected graphs consisting of two root points labelled i and j, at least one field point (associated with a factor of $\rho\bar{X}(E)$), and such that a given graph consists of an open polygonal periphery ($i \rightarrow j$) of T_{kl}-bonds connecting adjacent points on the polygon, with zero or one interior h_2-bonds connecting all possible pairs of non-adjacent points except the pair (i, j). (14)

Sites i and j are considered fixed in space and are root points (RP) in graph theory terminology; all other points are integrated over and are field points (FP). The quantity $\bar{X}(E) = \mathrm{Re}\,\bar{G}(z)$ where, with $z = E + i0+$, $\bar{G}(z) = \bar{X}(E) - i\pi D(E)$ is the ensemble averaged Green function for the spatially disordered tight-binding model. A $T_{kl} \equiv T(\mathbf{R}_k, \mathbf{R}_l)$ bond is defined by $T_{kl} \equiv g_2(\mathbf{R}_k, \mathbf{R}_l)V(\mathbf{R}_k, \mathbf{R}_l)$, and $h_2(R) = g_2(R) - 1$ is the short-ranged structural pair distribution function. In Figure 1 we show all graphs in Γ^0_{ij} with up to three T_{kl}-bonds.

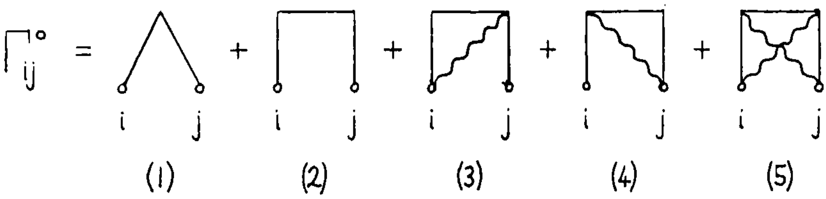

Figure 1 All graphs contributing to Γ^0_{ij} with a chain of up to three T_{kl}-bonds. $\underset{k}{\circ}$———$\underset{l}{\circ}$ denotes a T_{kl} bond, and $\underset{k}{\circ}\sim\sim\sim\sim\sim\underset{l}{\circ}$ a short-ranged $h_2(kl)$ bond. A factor of $\rho\bar{X}(E)$ (1) is associated with each FP (RP).

At this point it is helpful to note a correspondence between the above specification of Φ_{ij} and a similar quantity appearing in theories for the averaged Green functions of a topologically disordered tight-binding model. We have recently analyzed the latter problem[13] and, in particular, have given a formal specification of a "complete" single-site theory for the averaged Green functions. It was shown that differences between various approximate but tractable single site theories arise from different approximations to a particular function $S(1, 2)$ (in what follows, $i = 1, 2, \ldots$ as the argument of a function is used as a shorthand for $\mathbf{R}_i$, and $d(i) \equiv d\mathbf{R}_i$). It is easily demonstrated that a graphical specification of the exact $S(1, 2)$ is identical to that of $\Gamma^0(1, 2)$ in the present problem, except that the FP of the former have factors of $\rho\bar{G}(z)$ associated with them, as opposed to factors of $\rho\bar{X}(E)$ in the latter case. We may therefore effect tractable approximations to $\Gamma^0(1, 2)$ by direct analogy with single-site approximations used in a determination of the averaged Green functions. One such is due to Ishida and Yonezawa[14] which, in the present context, corresponds to

$$\Gamma^0(1, 2) \simeq W(1, 2) - T(1, 2) \tag{15a}$$

with $W(1, 2)$ defined by:

$$W(1, 2) = T(1, 2) + \rho\bar{X}(E) \int d(3)W(1, 3)T(3, 2) \tag{15b}$$

Graphically, this corresponds to a neglect of all diagrams contributing to $\Phi(1,2)$ which possess interior $h_2(k,l)$-bonds, such as graphs (3)–(5) in Figure 1. The above approximation was examined explicitly in Ref. 3 in the limit $g_2(R) = 1$ for all R, which is exact for a perfectly random system, and for which Eqs (15) reduce to the well-known Matsubara–Toyozawa approximation[15].

It is however known that the best single-site theory for the averaged Green functions is the effective medium approximation (EMA) of Roth[7]. Graphically, this corresponds in the present problem to neglecting only those diagrams in $\Phi(1,2)$ with crossing interior h_2-bonds, such as graph (5) in Figure 1. The EMA is equivalent to the single super chain approximation (SSCA) examined by us recently[8] which, with $\Gamma^0(1,2)$ and $\bar{X}(E)$ replacing $S(1,2)$ and $\bar{G}(z)$ respectively, may be written in the present case as

$$\Gamma^0(1,2) \simeq \Gamma(1,2) = H(1,2) - C(1,2) \tag{16}$$

where $H(1,2)$ and $C(1,2)$ are found from solution of

$$H(1,2) = C(1,2) + \rho\bar{X}(E)\int d(3)H(1,3)C(3,2) \tag{17a}$$

with:

$$g_2(1,2)C(1,2) = g_2(1,2)V(1,2) + h_2(1,2)H(1,2) \tag{17b}$$

Equation (17a) is analogous to the Ornstein–Zernike equation for the pair distribution function of a classical liquid; and (17b) provides a closure relation which, with $g_2(1,2)$ and $V(1,2)$ specified, enables us to find $H(1,2)$ and $C(1,2)$ and hence, from (13) and (16), the effective transfer matrix element.

To illustrate this we consider a bare transfer matrix element of Yukawa form,

$$V(R) = -(V_0/R)\exp(-\alpha R), \tag{18}$$

the spatial range of which is characterized by the length scale $\alpha^{-1} = a_H$. A modified exponential transfer matrix element is known to be appropriate to describe several problems of interest, such as electronic transport in tightly bound bands of certain liquid metals, and in the impurity band of a doped semiconductor. The choice of a Yukawa interaction reproduces the physical features of interest whilst allowing simple analytical results to be obtained. We consider a system with off-diagonal disorder alone i.e. $P(\varepsilon) = \delta(\varepsilon)$. And we take $g_2(R)$ to be a simple step function corresponding to the low-density limit of hard spheres with hard sphere diameter, σ i.e.

$$g_2(R) = \theta(R - \sigma) \tag{19}$$

Although the model pair distribution function (19) is simple, it introduces a second length scale, σ, which characterizes the range of structural correlations in the system. The variation of localization characteristics with both the structural length scale and the hopping length scale, α^{-1}, may thus be examined.

To evaluate $\Phi(R)$ we require $\Gamma(\mathrm{R})$, the Fourier transform of which is given from (16) and (17) by:

$$\hat{\Gamma}(k) = \frac{\rho \bar{X}(E)[\hat{C}(k)]^2}{1 - \rho \bar{X}(E)\hat{C}(k)} \tag{20}$$

For a given ρ we thus require $\bar{X}(E)$ and $\hat{C}(k)$. To be consistent with the EMA/SSCA approximation to $\Phi(R)$ we must of course evaluate $\bar{X}(E) = \mathrm{Re}\, \bar{G}(z)$ within the same framework. This problem has been examined by us in Ref. 8; $\bar{X}(E)$ is thus known. To find $\hat{C}(k)$ note that with (19) for $g_2(R)$, the closure condition (17b) reduces to:

$$H(R) = 0 : R < \sigma \tag{21a}$$

$$C(R) = V(R) : R > \sigma \tag{21b}$$

As with the related problem for the averaged Green functions[8], solution of the EMA/SSCA Eqs. (17a) and (21) is obtained directly by noting a formal correspondence of these equations to the mean spherical approximation of classical liquid state theory[16], solutions of which are known for the case of a Yukawa interaction[17,18].

It is now convenient to introduce the following reduced variables based on σ as the unit of length and $V_0^* = V_0/\sigma$ as the basic unit of energy:

$$\begin{gathered} \rho^* = \rho\sigma^3,\ \alpha^* = \alpha\sigma,\ R^* = R/\sigma \\ \tilde{X}(E) = V_0^* \bar{X}(E),\ \tilde{C}(R) = C(R)/V_0^*,\ \tilde{H}(R) = H(R)/V_0^* \end{gathered} \tag{22}$$

With $V(R)$ given by (18), the solution of Eqs (17a) and (21) is:

$$\tilde{C}(R) = -\tilde{S}(E)\frac{[1 - e^{-\alpha^* R^*}]}{\alpha^* R^*} + [\tilde{S}(E)]^2 \frac{[\cosh(\alpha^* R^*) - 1]}{2\alpha^{*2} R^*} : R^* < 1 \tag{23a}$$

where

$$\tilde{S}(E) = -4\pi\rho^* \tilde{X}(E) \int_0^\infty dR^* R^* e^{-\alpha^* R^*} \tilde{H}(R^*) \tag{23b}$$

satisfies:

$$\begin{aligned} 4\pi\rho^*\tilde{X}(E)&\left\{-e^{-\alpha^*} + \tilde{S}(E)\frac{[1 - e^{-\alpha^*}]}{\alpha^*} - [\tilde{S}(E)]^2 \frac{[\cosh\alpha^* - 1]}{2\alpha^{*2}}\right\}^2 \\ &= 2\alpha^*\tilde{S}(E) + [\tilde{S}(E)]^2 \end{aligned} \tag{23c}$$

For given ρ^* and α^*, and with $\bar{X}(E)$ known, (23c) gives $\tilde{S}(E)$. From (23a) and (21b) we thus know $C(R)$ for all R; $\Phi(R)$ follows from Eqs. (20) and (13). One potential problem with the determination of $\tilde{S}(E)$ is the multiplicity of roots associated with Eq. (23c). We know however from (23b) that $\tilde{S}(E)$ is real and must be zero when $\tilde{X}(E)$ is zero. Further, at the band edges in the density of states $D(E)$, $\bar{G}(z) = \bar{X}(E)$. The present problem is then equivalent to the averaged Green function problem mentioned above, and we may identify $\tilde{S}(E)$ as the improper self-energy at the band edges, the values of which are known[8]. These considerations are sufficient to determine uniquely the correct root of Eq. (23c).

In Figure 2 we plot $\Phi(R)$ and the bare $V(R)$, in units of V_0^*, as functions of R^* for $\rho^* = 0.007$, $\alpha^* = 0.572$ and (a) $\varepsilon \equiv E/V_0^* = 0.2$, (b) $\varepsilon = -0.4$. Figure (2a) is typical of higher energies and shows that $\Phi(R)$ is *screened* i.e. it is of shorter spatial range than $V(R)$. Conversely, Figure (2b) shows the low energy case where $\Phi(R)$ is *anti-screened* i.e. is longer ranged than the bare $V(R)$. From Eqs (20) and (13) it follows that when $\bar{X}(E) = 0$, $\Phi(R) = V(R)$, and this energy represents a crossover from screening to anti-screening behaviour. We add that, in contrast to the estimate of Ref. 3, the crossover does not in general occur at $\varepsilon = 0$, but rather at some positive energy.

To see how the screening embodied in $\Phi(R)$ affects the localization characteristics of the system we require $J_1(\rho; E)$ given by Eq. (9b). A determination of J_1 is simplified considerably if we assume $\Phi(R)$ is negative definite. This is certainly true when $\Phi(R)$ is

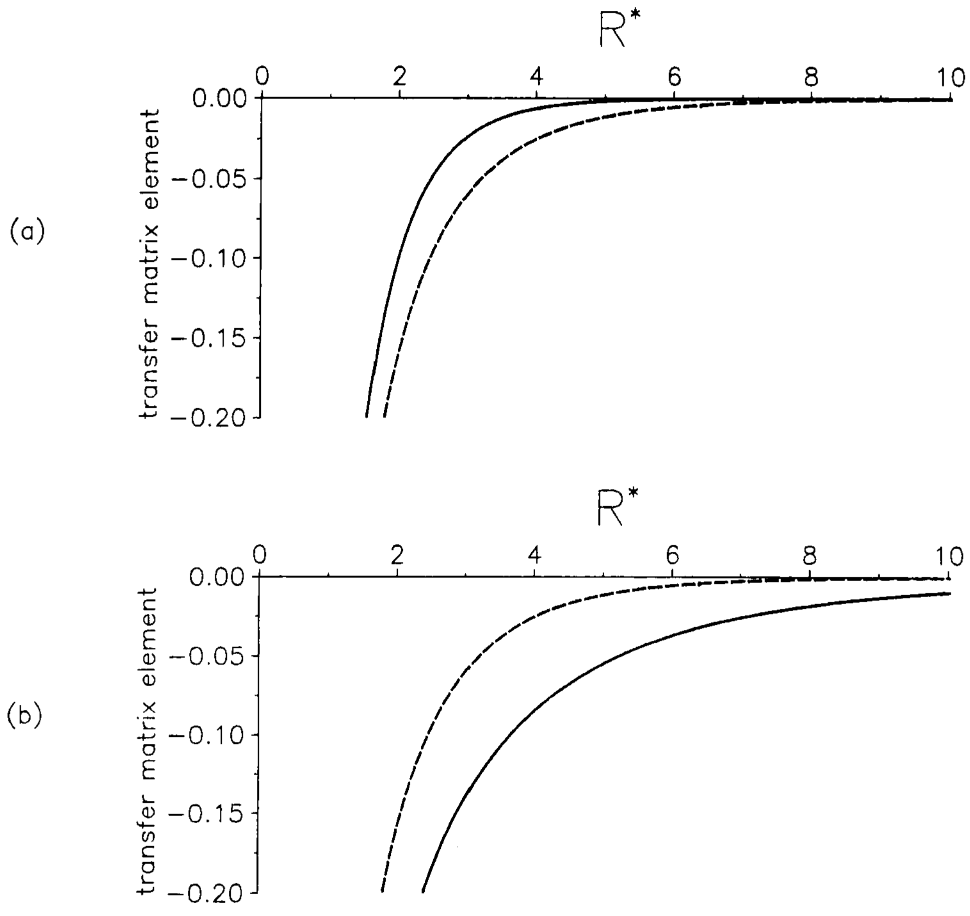

Figure 2 $\Phi(R)/V_0^*$ (full curve) at the EMA/SSCA level of description and the bare $V(R)/V_0^*$ (broken curve) as functions of R^* for $\rho^* = 0.007$, $\alpha^* = 0.572$ and (a) $\varepsilon = 0.2$, (b) $\varepsilon = -0.4$.

anti-screened, and although screening may cause $\Phi(R)$ to become positive for some small R range, the extent to which it does so is negligible. Making this assumption we have

$$\begin{aligned} J_1(\rho; E) &= -\rho \int d\mathbf{R}\, g_2(R)\Phi(R) \\ &= -\rho \int d\mathbf{R}\, H(R) \\ &= -\rho \hat{H}(0) \\ &= \frac{-\rho \hat{C}(0)}{1 - \rho \bar{X}(E)\hat{C}(0)} \end{aligned} \tag{24}$$

where Eqs (13), (16) and (17) have been used. We thus require only $\hat{C}(0)$ which from (21b) and (23a) is given by

$$\frac{\hat{C}(0)}{V_0^*} = C_1 + C_2\tilde{S}(E) + C_3[\tilde{S}(E)]^2 \tag{25}$$

where:

$$\begin{aligned} C_1 &= -4\pi(1 + \alpha^*) \exp(-\alpha^*)/\alpha^{*2} \\ C_2 &= C_1/\alpha^* + 2\pi(2 - \alpha^{*2})/\alpha^{*3} \\ C_3 &= C_2/2\alpha^* - C_1/4\alpha^{*2} - \pi(1 - \alpha^*) \exp(\alpha^*)/\alpha^{*4} \end{aligned}$$

Equations (24) and (25) give $J_1(\rho; E)$. To determine mobility edge trajectories via the localization criterion (11) we need in addition the averaged density of states, $D(E)$. Once again consistency demands that we evaluate $D(E)$ within the EMA/SSCA, as described fully in Ref. 8. All quantities appearing in the localization function $T(E; \rho)$, Eq. (9a), are thus evaluated at the EMA level of description.

A comment is perhaps in order on the use of the EMA/SSCA for $D(E)$ at reduced densities of order $\rho^* \sim 0.01$, which in the context described below is the density regime of interest in studying localization. Simulations have been performed[19] to test the accuracy of the density of states obtained from the EMA/SSCA, and from a theory applicable at very low densities, $\rho^* \lesssim 0.002$; with $\alpha^* \sim 0.5$, neither theory does particularly well at the intermediate density of $\rho^* \sim 0.01$. Use of the EMA/SSCA for $D(E)$ has however the advantage of being consistent with its use in calculating $\Phi(R; \rho, E)$; further, a calculation of both $D(E)$ and Φ via the EMA/SSCA introduces asymmetry into the mobility edge trajectories, the presence of which is confirmed computationally as we discuss below.

In Figure 3 we plot $\tilde{J}_1(\rho^*; \varepsilon) \equiv J_1/V_0^*$ and $\tilde{D}(\varepsilon) = V_0^* D(E)$, as functions of reduced energy, ε, for $\rho^* = 0.007$ and $\alpha^* = 0.572$; the shaded areas indicate localized states. The figure illustrates the competing effects of J_1 and $D(E)$ in determining mobility edges: the characteristic asymmetry of $D(E)$ (which may also be viewed in terms of screening[3]) by itself tends to favour extended states in the upper half of the band, whereas the anti-screening of $\Phi(R)$ tends to favour, via the resultant $J_1(\rho; E)$, extended

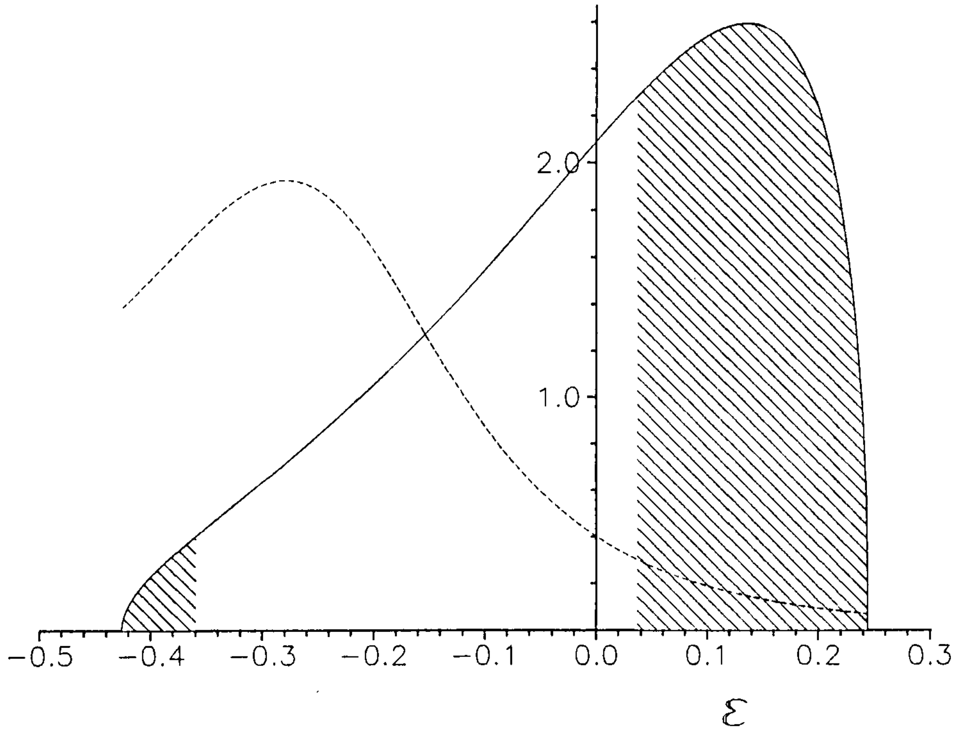

Figure 3 $\tilde{D}(\varepsilon)$ (full curve) and $\tilde{J}_1(\rho^*;\varepsilon)$ (broken curve) as functions of ε for $\rho^* = 0.007$ and $\alpha^* = 0.572$. The shaded areas indicate localized states.

states in the lower half band. We see that, although there is the usual pattern of localized states towards the edges of the band separated by a domain of extended states, the latter occur in a low-energy low-density-of-states region due to the dominating effects of anti-screening in $\Phi(R)$. The characteristic long low-energy tail in $D(E)$ is thus by itself no guarantee of localized states.

The asymmetry in the positions of the mobility edges has been confirmed by computer simulation. Ching and Huber[4] have studied a three-dimensional system specified by a tight-binding Hamiltonian, with active sites randomly distributed at low occupancy on an underlying f.c.c. lattice, and with a simple exponential transfer matrix element. Gibbons *et al.*[5] have studied an off-diagonally disordered tight-binding model with topological disorder characteristic of a quenched hard sphere fluid, also using a pure exponential transfer matrix element, $V(R) = -V'_0 \exp(-\alpha' R)$. The full effects of hard sphere structure are of course included in the latter simulation and, for $\alpha'\sigma = 0.9$, mobility edge trajectories were estimated from a study of the inverse participation ratio (IPR); these are shown in Figure 4. The estimated location of the mobility edges in the upper half of the band is statistically quite sound, but because of the large scatter in the IPR distribution for energies $\varepsilon \lesssim -0.1$, the mobility edges estimated in this region (shown as a dotted line) are somewhat tenuous; and, as argued in Ref. 5, it is likely that the regime of localized states is overestimated

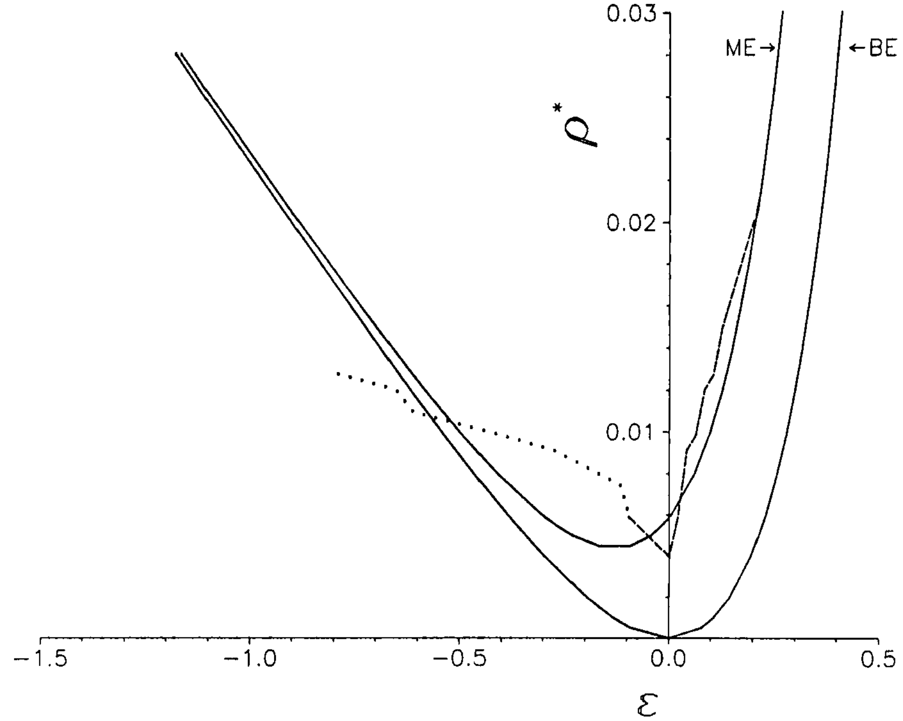

Figure 4 Mobility edge (ME) and band edge (BE) trajectories from theory (full curves) for $\alpha^* \equiv \alpha\sigma = 0.572$. Shown for comparison is the mobility edge estimated in Ref. 5 (broken curve) for $\alpha'\sigma = 0.9$ (see text for relation between α and α').

somewhat. Although the simulation has a pure exponential matrix element as opposed to a Yukawa form in the present theory, we can compare the two simply by choosing the Yukawa parameters to ensure that the first and second moments of the two transfer matrix elements are identical. This yields $\alpha = 0.636\alpha'$ (or $\alpha^* = 0.572$) and $V_0^* = 0.948V_0'$, and the resultant mobility edge trajectories obtained from the preceding theory are compared with the simulation in Figure 4. The qualitative agreement between theory and simulation in regard to mobility edge asymmetry is good; and the quantitative agreement, particularly in the upper half band, is encouraging given the simplicity of the underlying localization theory. The main discrepancy occurs in the lower half of the band and, as mentioned above, this may be a problem with the estimation of mobility edges from the simulation: the present theory would indeed suggest that simulation overestimates somewhat the range of localized states in the lower half of the band.

The effects of screening are evidently important in determining the localization characteristics of the system. Such effects would of course still be present if the structural order implicit in the hard sphere length scale were neglected. How important is it, even at the relatively low densities under consideration, to consider the short-ranged structure of the system which enters the problem via the dimensionless ratio $\alpha\sigma$ $(=\sigma/a_H)$? This is illustrated in Figure 5 where the mobility edge

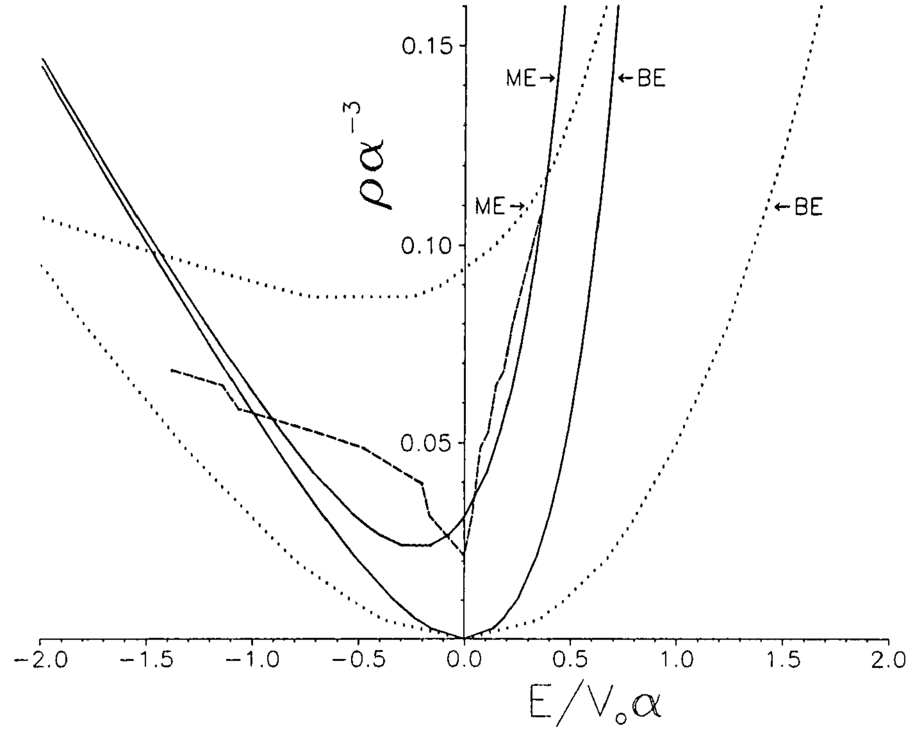

Figure 5 As Figure 4 but with the MTA result added (dotted curve) corresponding to $\alpha^* \equiv \alpha\sigma = 0$. Note the different set of units used for the density and energy scales.

trajectories of Figure 4 are reproduced but with $\rho\alpha^{-3}$ $(=\rho a_H^3)$ and $E/V_0\alpha$ as the reduced density and energy scales. Also shown for comparison is the theoretical result with σ/a_H set to zero, corresponding to complete neglect of the short range structural order; in this case the EMA/SSCA, in common with all other single site theories, reduces to the familiar Matsubara–Toyozawa approximation[15]. From the figure it is evident that an adequate treatment of structural correlations is indeed necessary to obtain agreement with simulation.

Acknowledgement

MDW is grateful for the award of a SERC postgraduate studentship.

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