Exact ground-state results for a disordered-continuum model of the halogen-bridged metal complex PtI

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Abstract. By mapping a continuum model of a halogen-bridged metal complex chain to the Takayama–Lin-Liu–Maki continuum model of polyacetylene and using a supersymmetric functional integral formalism, we study the influence of both 'site' and 'bond' disorder on the nature of the ground state of this halogen-bridged metal complex PtI. We find exact results for the amplitude of the order parameter Δ and the electronic density of states as a function of the strength of the disorder. We also obtain a phase diagram of Δ versus both bond and site disorder. The critical concentration of site impurities versus average impurity scattering strength gives a fractal dimension which is very close to that of the two-dimensional Sierpinski gasket.

1. Introduction

Recently, the interest in a class of quasi-one-dimensional chains composed of transition metal ions M and (bridging) halogens X has strongly increased. There have appeared in the literature quite a number of reports, both theoretical and experimental [1–5], emphasising various interesting properties of this class of materials. For different choices of the transition metal (M can be Pt, Pd or Ni) and the halogen (X can be Cl, Br or I), the composed halogen-bridged metal complex systems exhibit quite different properties. For instance, the complex PtCl appears to have strong electron–phonon coupling, while the complex PtI appears to have just the opposite, namely it has weak electron–phonon coupling [1]. In general, the Hamiltonian describing the halogen-bridged complex chain systems can be mapped to the Su–Schrieffer–Heeger (SSH) [6] Hamiltonian with a complex order parameter [7]. Furthermore, if an appropriate set of M and X has been chosen, say, for the case of PtI complex, by making a simple gauge transformation [2], its model Hamiltonian has exactly the same continuum limit as that of the Takayama–Lin-Liu–Maki (TLM) [8] model in polyacetylene. Baeriswyl and Bishop (BB) have discussed most properties of this class of materials and even the possible relationship with the recently discovered high-T_c superconductor; we refer readers to their papers [1] for detailed discussions of these topics.

However, it is quite natural to ask questions about how disorder (both bond and site disorder) affects this system and whether the 'gap' opened owing to 'Peierl's theorem' will be closed or enhanced with the presence of various types of disorder. Intrinsically, disorder exists in the system: the bond disorder may come from, say, the bond defects of the chains and the site disorder may arise from randomly distributed charged impurities. Unfortunately, not even approximate theories dealing with random disorder in this class

of materials have been reported so far to the present author's knowledge. To answer the above questions is definitely not a easy task; however, owing to the one-dimensionality of the system and similarities of the Hamiltonians between this system and the well known SSH and TLM models in polyacetylene, we can apply the methods which work well in the SSH and TLM models to this system as the first step.

By using a supersymmetric functional integral formalism, Xu and Trullinger (XT) [9] were able to solve a disordered model of polyacetylene in continuum limit, i.e. the disordered TLM model, exactly. We herewith apply their method to investigate a disordered continuum model of the halogen-bridged metal complex PtI chain system. We find exact results for the dependence of the gap parameter Δ and electronic density of states on the strength (concentration) of both 'bond' and 'site' random disorder (impurities). We find that the Peierl gap will be suppressed for a sufficient amount of either bond or site (attractive impurities) disorder, or both types of disorder. However, in this paper, we restrict ourselves to the ground-state configuration only, i.e. $\Delta(x) = \Delta$ is a constant without considering lattice relaxation effects and excitations such as the kink and polaron discussed in [1] as well as the Coulomb interaction. The paper is organised as follows: we introduce the supersymmetric functional integral formalism in § 2, present our results in § 3 and give conclusions in § 4.

2. Supersymmetric functional integral formalism

Treating random-disorder problems, the supersymmetry method (see, e.g., [9–15] and references therein) proves to be very useful. In general, by taking advantage of both Grassmann and conventional integrals (supersymmetry integrals), one is able to average over the disorder potential at an early stage in calculations and to arrive at an effective quantum field theory with a supersymmetric Lagrangian. This method was explicitly used in [9, 12–15] to treat some disordered systems in detail.

In this section, we specify both bond (off-diagonal) and site (diagonal) random disorder in the continuum model of the BB [1] Hamiltonian. We use the supersymmetric functional integral formalism to average over random disorder at the very beginning of computing the averaged Green function and thus convert the original Lagrangian to an effective supersymmetric Lagrangian involving superfields which is similar to the usual quantum field Φ^4 Lagrangian; therefore the transfer operator method can be applied to obtain exact results.

Our starting point is the continuum model of the BB Hamiltonian in [1] (equation (2.1)) with $\lambda_1 = 0$, $\lambda_2 \ll 1$, i.e. the weak-coupling limit (λ_i are electron–phonon coupling constants), which represents the PtI complex and is equivalent to the TLM [8] model after an appropriate gauge transformation [2]. The Hamiltonian is

$$H = \frac{\omega_Q^2}{2g^2} \int dx\, \Delta^2 + H_{el} \tag{2.1}$$

where ω_Q is the maximum phonon frequency in the discrete lattice model of BB, g is a scaled electron–phonon coupling constant and Δ is proportional to the amplitude of the displacement of X atoms, which will be regarded as a static classical field in the rest of this paper since only ground-state properties are of interest to us.

The electronic part H_{el} of the Hamiltonian after introduction of the random-disorder potentials $U_b(x)$ (bond disorder) and $U_s(x)$ (site disorder) is given by

$$H_{el} = \int dx\, \Psi^\dagger(x) \left(-i\sigma_3 \frac{\partial}{\partial x} + (1 + \sigma_2)U_s(x) + [\Delta + U_b(x)]\sigma_1 \right) \Psi(x) \tag{2.2}$$

where we set $v_F = k_F = 1$ when passing to the continuum limit, $\{\sigma_i\}$ are Pauli matrices, and $\Psi(x)$ is a two-component pseudo-spinor field composed of right- and left-moving electron fields $u(x)$ and $v(x)$. It is exactly the same as that of the disordered TLM model studied by XT.

We also note that, when the present case is compared with the XT model [9], the bond disorder in the former case corresponds to the site disorder in the latter case and the site disorder in the former case to the bond disorder in the latter case, because of the gauge transformation [2]. The bond disorder that we introduced may originate from randomly distributed lattice defects. It is assumed to be Gaussian randomly distributed with zero average and totally uncorrelated in the spatial variable x, i.e. $\langle U_b(x)U_b(x')\rangle = \gamma_b\delta(x - x')$, where the angular brackets denote the average over random realisations of the disorder and the constant γ_b represents the strength of the bond disorder. For site disorder, we cannot simply assume $U_s(x)$ to have zero average, since $U_s(x)$ usually arises from an external potential (e.g. the Coulomb potential of randomly distributed charged impurities); instead, one can assume it to be non-zero mean Gaussian distributed. Here we choose $\langle U_s(x)\rangle = U_0$, and also we set $U_s(x) = U_0 + \tilde{U}_s(x)$, where $\langle \tilde{U}_s(x)\tilde{U}_s(x')\rangle = \gamma_s\delta(x - x')$. The average value U_0 can be either negative or positive denoting attractive or repulsive impurities, respectively. Generally γ_s and U_0 are treated as independent parameters, but for the purpose of plotting representative results we consider the specific simple case of attractive δ-function impurities with average strength κ_0 and concentration c [16]. Then U_0 and γ_s can be simply related via $U_0 = -c\kappa_0$, $\gamma_s = c\kappa_0^2$. To simplify the problem further, we assume the site impurities to be 'isoelectronic', which means that the system accommodates the same number of electronic charges before and after introducing random impurities.

The component functions $u(x)$, $v(x)$ of Ψ satisfy coupled Bogoliubov–de Gennes (BDG) equations [8] obtained by varying equation (2.2). These equations can be decoupled by linear transformations ($f_\pm = u \pm iv$) to yield

$$[\![-\partial^2/\partial x^2 + [\Delta + U_b(x)]^2 - \{2[\Delta + U_b(x)]\partial U_s/\partial x\}/(E - 2U_s)$$
$$- 2(\partial U_s/\partial x)(\partial/\partial x)/(E - 2U_s)]\!]f_+$$
$$= (E^2 - 2U_sE)f_+\{-(\partial^2/\partial x^2) + [\Delta + U_b(x)]^2 + \partial U_b/\partial x\}f_-$$
$$= (E^2 - 2U_sE)f_- \tag{2.3}$$

where we note that, for a certain set of $\{x\}$, a random potential $U_s(x)$ may take its value equal to E; as it happens, one cannot simply divide the factor $E - 2U_s(x)$ from both sides of the above equation. Fortunately, for $E = 2U_s(x)$, we have a trivial case giving zero density of states (see Appendix).

The above equations define a set of effective Schrödinger equations, $Hf_\pm = \varepsilon f_\pm$ which we shall use later instead of equation (2.2). Equation (2.2) is a Dirac-type equation; thus it is difficult for us to use the transfer operator technique to perform the supersymmetric functional integrals. Of course, both sets of equations are equivalent and the resulting density of electronic states is related simply by $\langle \rho(E)\rangle = (\partial\varepsilon/\partial E)\langle\rho(\varepsilon)\rangle$. We define ε to be

$$\varepsilon = E^2 - \Delta^2 + 2c\kappa_0E. \tag{2.4}$$

With our choice of units where $v_F = k_F = 1$, the concentration $c = N_{imp}/L$ of impurities is related to the fraction $f = N_{imp}/N$ of substituted sites by $c = (2/\pi)f$.

Although the spectrum of the electronic Hamiltonian can be found in the absence of disorder [1], in the presence of $U_i(x)$ the spectrum cannot be found. Fortunately, one is

usually interested only in quantities which are averaged over the disorder. For example, the calculation of thermodynamic quantities requires only knowledge of the averaged density of states which is well known, given by the following expression:

$$\langle \rho(\varepsilon) \rangle = -(1/\pi)\langle \mathrm{Im}[G^{\mathrm{R}}(x, x; \varepsilon)] \rangle \tag{2.5}$$

where G^{R} denotes the retarded Green function which can be formally written in terms of the (unknown) eigenfunctions $\{\varphi_k\}$ and eigenvalues $\{\varepsilon_k\}$ of the full Hamiltonian as

$$G^{\mathrm{R}}(x, x'; \varepsilon) = \sum_k \frac{\varphi_k(x)\varphi_k^*(x')}{\varepsilon - \varepsilon_k + \mathrm{i}\delta} = \sum_k \varphi_k(x)\varphi_k^*(x') G^{\mathrm{R}}(k; \varepsilon). \tag{2.6}$$

By noting the properties of Grassmann and conventional integrations, after employing the supersymmetric functional integral method, we can represent $G^{\mathrm{R}}(k; \varepsilon)$ as a functional integral over supervectors

$$\Phi = \begin{pmatrix} \chi \\ S \end{pmatrix}$$

$(\Phi^\dagger = (\chi^*, S^*) = (\Phi^*)^{\mathrm{T}}$, where T is the transpose):

$$G^{\mathrm{R}}(k, \varepsilon) = -\mathrm{i} \int \mathrm{d}\Phi_k^* \, \mathrm{d}\Phi_k \, \Phi_{\alpha k} \Phi_{\alpha k}^\dagger \exp\{\mathrm{i}\Phi_k^\dagger[(\varepsilon - \varepsilon_k) - \mathrm{i}\delta]\Phi_k\} \tag{2.7}$$

where the subscript α takes one of two values which indicate the fermionic (χ) or bosonic (S) components of Φ (each of the components χ and S is itself a two-component vector containing 'right- and left-moving' fields so that the Φ superfield is a four-component object).

On introduction of the field variables Φ, $\Phi^\dagger$ according to the formulae

$$\Phi(x) = \sum_k \Phi_k \varphi_k(x) \qquad \Phi^\dagger(x) = \sum_k \Phi_k^\dagger \varphi_k(x) \tag{2.8}$$

the Green function $G^{\mathrm{R}}(x, x'; \varepsilon)$ can be written as

$$G^{\mathrm{R}}(x, x'; \varepsilon) = -\mathrm{i} \int \Phi_\alpha(x)\Phi_\alpha^\dagger(x') \exp\left(-\int L \, \mathrm{d}y\right) \mathrm{D}\Phi^* \, \mathrm{D}\Phi \tag{2.9}$$

$$L = \mathrm{i}\Phi^\dagger(\varepsilon - H - \mathrm{i}\delta)\Phi. \tag{2.10}$$

Writing out the Green function for our model, and remembering that equations (2.3) and (2.4) define H and ε, we have

$$G^{\mathrm{R}}(x, x'; \varepsilon) = -\mathrm{i} \int \Phi_\alpha(x)\Phi_\alpha^\dagger(x') \exp\left(-\int L \, \mathrm{d}y\right) \mathrm{D}\Phi^* \, \mathrm{D}\Phi \tag{2.11}$$

$$L = \mu\Phi^\dagger(\varepsilon - H - \mathrm{i}\delta)\Phi \tag{2.12}$$

where μ will be set equal to i later in an analytic continuation process for solving the effective Schrödinger equation (2.17) to obtain the density of electronic states. μ is treated as a real parameter just for convenience to solve equation (2.17) in a real domain instead of a complex domain.

Now the average over random potentials can be done easily (we give the details in the Appendix to yield

$$\mathcal{L} = \mu\Phi^\dagger[(\partial^2/\partial x^2) + \varepsilon - \mathrm{i}\delta]\Phi + (2\Delta^2\gamma_{\mathrm{b}} + 2E^2\gamma_{\mathrm{s}} + \gamma_{\mathrm{b}}^2/2)(\Phi^\dagger\Phi)^2. \tag{2.13}$$

Equation (2.13) is a typical Lagrangian of the supersymmetric Φ^4 model in field theory.

We note that the inclusion of auxiliary boson fields demands no essential changes, which was proved explicitly in [11] in 1979. Following the method in [17] for $x_1 < x_2$, our averaged Green function becomes

$$\langle G(x_1, x_2; \varepsilon) \rangle = -\mathrm{i} \int \mathrm{d}R_0 \, \mathrm{d}R_1 \, \mathrm{d}R_2 \, \Gamma(0, x_1; R_0, R_1)$$

$$\times \chi_1 \Gamma(x_1, x_2; R_1, R_2) \chi_2^* \Gamma(x_2, L; R_2, R_0) \tag{2.14}$$

where we define

$$R \equiv \{\chi, \chi^*, S, S^*\} \qquad \mathrm{d}R \equiv \mathrm{d}\chi^* \, \mathrm{d}\chi \, \mathrm{d}S^* \, \mathrm{d}S/\pi. \tag{2.15}$$

The kernel Γ appearing in equation (2.14) satisfies the Schrödinger equation

$$[-\partial/\partial x + \mathcal{H}(R)]\Gamma(x, x'; R, R') = \delta(x - x')\delta(R - R') \tag{2.16}$$

with

$$\mathcal{H} = -(1/\mu)[\partial^2/(\partial S^* \, \partial S) + \partial^2/(\partial \chi^* \, \partial \chi)] + \mu(\Delta^2 - E^2 - 2Ec\kappa_0)\Phi^\dagger \Phi$$

$$+ (2\Delta^2 \gamma_\mathrm{b} + \gamma_\mathrm{b}^2/2 + 2E^2 \gamma_\mathrm{s})(\Phi^\dagger \Phi)^2 \tag{2.17}$$

where we note that $\Phi^\dagger \Phi \equiv S^* S + \chi^* \chi$. The averaged density of electronic states is obtained from the imaginary part of the Green function according to equation (2.5).

3. Results and discussion

Our task is to find first the imaginary part of the averaged Green function (i.e. equation (2.14)) which is the density of electronic states. In the thermodynamic limit $L \to \infty$, performing the supersymmetric functional integrals in equation (2.14) is equivalent to finding the lowest energy of the effective Schrödinger equation (2.17), which gives the only contribution to the Green function.

To do this, we can expand the kernel Γ over orthogonal eigenfunctions ψ_n of the Schrödinger equation

$$\mathcal{H}\psi_n = \nu_n \psi_n \tag{3.1}$$

as

$$\Gamma(x, x'; R, R') = \theta(x' - x) \sum_n \psi_n(R)\psi_n^*(R') \exp[-\nu_n(x' - x)]. \tag{3.2}$$

Recall that any Grassmann function can be expanded as a finite polynomial of Grassmann variables χ, χ^* and $\chi^2 \equiv (\chi^*)^2 \equiv 0$; thus ψ_n can be expanded as

$$\psi_n(S, S^*, \chi, \chi^*) = \psi_n^0(S, S^*) + \psi_n^+(S, S^*)\chi + \psi_n^-(S, S^*)\chi^* + \psi_n^{(2)}(S, S^*)\chi^*\chi. \tag{3.3}$$

Substituting this into equation (3.1), we obtain

$$\{-(1/\mu)[\partial^2/(\partial S^* \, \partial S)] + V(|S|^2)\}\psi_n^0 + (1/\mu)\psi_n^2 = \nu_n \psi_n^0$$

$$\{-(1/\mu)[\partial^2/(\partial S^* \, \partial S)] + V(|S|^2)\}\psi_n^2 + (\mathrm{d}V/\mathrm{d}|S|^2)\psi_n^0 = \nu_n \psi_n^2$$

$$\{-(1/\mu)[\partial^2/(\partial S^* \, \partial S)] + V(|S|^2)\}\psi_n^\pm = \nu_n \psi_n^\pm \tag{3.4}$$

where $\quad V(|S|^2) = \mu(-E^2 + \Delta^2 - 2Ec\kappa_0)|S|^2 + (\gamma'/2)|S|^4, \quad \gamma' = 4\Delta^2 \gamma_\mathrm{b} + \gamma_\mathrm{b}^2 + 4E^2 \gamma_\mathrm{s}.$

Following similar procedures to those in [13] and introducing polar variables as $S = r \exp(i l \theta)$, we have $\psi_{nl} = \exp(i l \theta) \, \eta_{nl}(r)$. We choose the ground-state eigenfunction as $\psi_0 = \psi_0(\sqrt{\chi^* \chi + S^* S})$, which is assumed to depend only on the 'length' in the super-space. We obtain

$$-(1/\mu)[\mathrm{d}^2/\mathrm{d}r^2 + (1/r)(\mathrm{d}/\mathrm{d}r)]\eta_0^0 + V(r)\eta_0^0 = \nu_n \eta_0^0. \tag{3.5}$$

We note that the above equation has the lowest eigenvalue $\nu_0 = 0$ and the corresponding eigenfunctions [18] are the Airy functions†

$$\eta_0^0(r) = \mathrm{Ai}\{\tfrac{1}{2}r^2(2\gamma')^{1/3}(2\mu)^{1/3} + \mu(2\mu)^{1/3}[(\gamma')^2/2]^{-1/3}(\Delta^2 - E^2 - 2Ec\kappa_0)\}. \tag{3.6}$$

Inserting equation (3.2) in equation (2.14) yields

$$\langle G(x - x'; \varepsilon) \rangle = -\mathrm{i} \sum_{m,n} |J_{mn}|^2 \exp[-L\nu_n - (x - x')(\nu_m - \nu_n)] \tag{3.7}$$

where $J_{mn} = \int \psi_n^*(R) \chi \psi_m(R) \, \mathrm{d}R$.

For $x = x'$, we obtain the density of electronic states by taking the imaginary part of equation (3.7). As $L \to \infty$, only the lowest state $\nu_0 = 0$ contributes to the density of states; hence we obtain

$$\langle \rho(\varepsilon) \rangle = \frac{2}{\pi} \mathrm{Re} \left[\lim_{\mu \to i} \left(\int_0^\infty r \, \mathrm{d}r \, [\eta_0^0(r)]^2 \Big/ [\eta_0^0(0)]^2 \right) \right]. \tag{3.8}$$

We note that all the formulae are obtained by using $\chi\chi^*$ representation, e.g. equation (2.14). It was proved in [12] that the same results could be obtained with the use of SS^* representation.

Integrating equation (3.8) by parts and using the facts that $\mathrm{Ai}''(z) - z \, \mathrm{Ai}(z) = 0$, $[\mathrm{Ai}^2(z)]''' - 4z[\mathrm{Ai}^2(z)]' - 2 \, \mathrm{Ai}^2(z) = 0$ [18], as well as the relation between $\rho(\varepsilon)$ and $\rho(E)$, we obtain the electronic density of states

$$\langle \rho(E) \rangle = [4|E + c\kappa_0|/\pi^2(\gamma'/2)^{1/3}]\{[\mathrm{Ai}'(z)\,\mathrm{Ai}(z) + \mathrm{Bi}'(z)\,\mathrm{Bi}(z)]/[\mathrm{Ai}^2(z) + \mathrm{Bi}^2(z)]^2\} \tag{3.9}$$

with $z \equiv \varepsilon/(\gamma'/2)^{2/3}$, where $\gamma' = 4\Delta^2\gamma_b + 4E^2\gamma_s + \gamma_b^2$, and Ai and Bi are Airy functions of first and second type, respectively. This result is very similar to that obtained some time ago in [19] for the one-dimensional free-electron gas in the presence of disorder. This similarity comes from the facts that we use, instead of the Dirac-type equation (2.2), equation (2.3) which is a Schrödinger-type diagonalised equation; also, since the gap parameter Δ is a constant which can be absorbed as a part of the eigen-energy, we thus get a free-electron random system with modified energy eigenvalues. We note that, in the limiting cases $\gamma_b \to 0$, $\gamma_s \to 0(c\kappa_0 \to 0)$, using the asymptotic properties of Airy and Biry functions, equation (3.9) reproduces the pure system electronic density of states exactly. For $z > 0$, Airy functions decay exponentially, giving band tails within the gap which can be seen in the density of states (see figures 3 and 4); it is a general feature of one-dimensional disordered systems.

The density of states given by equation (3.9) depends on Δ (the order parameter) which remains to be determined. This is accomplished by minimising the total energy with respect to Δ with due regard to the fact that the energy cut-off [9] required for the electronic energy spectrum in the pure model now depends on Δ and the disorder strength γ_b, γ_s because of the altered density of states and the requirement that the total number of electrons to be accommodated is the same as in the unperturbed model (recall

† Note that we correct the errors in [12, 13] in the solution of equation (3.5).

Figure 1. Δ against γ_b ($\gamma_s = 0$; $\lambda = 0.2$).
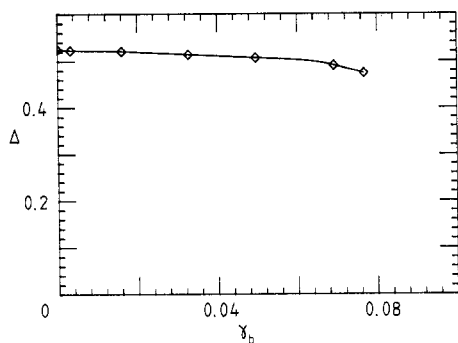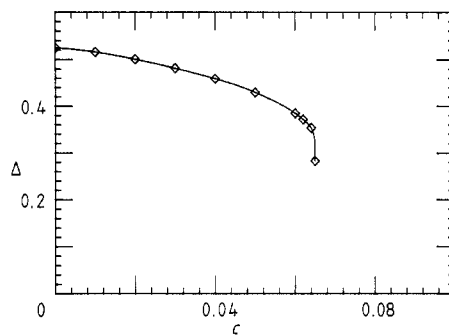
Figure 2. Δ against c (concentration) ($\gamma_b = 0$; $\lambda = 0.2$; $\kappa_0 = 1.0$).

that in the site disorder case we assumed the disorder to be the isoelectronic impurities). It is straightforward to conduct a self-consistent numerical search for the values of Δ.

In figure 1, we present the results for Δ as a function of the disorder strength γ_b, for a fixed value of λ (we choose the same set of parameters as in [1], i.e. $\Delta = 0.525$, energy cut-off $E_c = 3.2$ eV and $\lambda = 0.2$). In figure 2, we plot Δ versus impurity concentration c for the site disorder. We find that, in a similar fashion, both have an *abrupt* drop to zero†.

In figure 3, we plot the electronic density of states for the bond disorder case ($\gamma_s = 0$). An exact zero exists in the density of states (see [20–22] for a more detailed discussion). We note that the bond disorder tends to raise the valence band states of the 'pure' system in general (pushing up the energy cut-off), rounds off the square root divergence in the pure density of states and smears more states into the original 'gap'. However, the electron–phonon interaction favours keeping the 'gap' open. In addition to this competition, we require that the total number of electronic states below $E = 0$ be the same before and after introducing the disorder. Above the critical value of γ_b the competing processes can be balanced but this additional requirement can no longer be satisfied, which results in the total destruction of the order parameter, giving the abrupt drop to zero in figure 1. This discontinuity might be an artefact of the cut-off problem; one expects that in the discrete model (where there is no cut-off problem) we may not have this discontinuity.

In figure 4, we plot the electronic density of states for various impurity concentrations for the site disorder case ($\gamma_b = 0$) with $\kappa_0 = 1$ fixed. The 'diagonal' presence of the site disorder shifts the whole energy spectrum to the right or left depending on whether the mean value $\langle U_s(x) \rangle$ of the disorder potential is positive or negative. For finite c (even small) the singularity has been rounded off. We can see the asymmetric finite peaks in the broken curve in figure 4(a). In figure 4(b), we plot situations in which the concentration is near the critical value: the full curve is for the case $c < c_c$ and the broken curve for $c > c_c$. We can see dramatic changes in the density of states which correspond to the discontinuity in figure 2. Note that for $c > c_c$ a power-law divergence ($\rho \simeq E^{-2/3}$) occurs as $E = 0$ is approached from above. Physically this is because of the collapse of the original 'gap'. Recall that we have two peaks as $c < c_c$ but that the 'gap' suddenly disappears as $c > c_c$. All the states populate at $E = 0$, giving the divergence; we also note that this divergence is still integrable. From the broken curve in figure 4(c), we can see that a peak occurs at $E = 0$, followed by a very rapid exponential drop just below $E = 0$ to a very small value

† Note that we correct an error in figure 1 of [9] for bond disorder results.
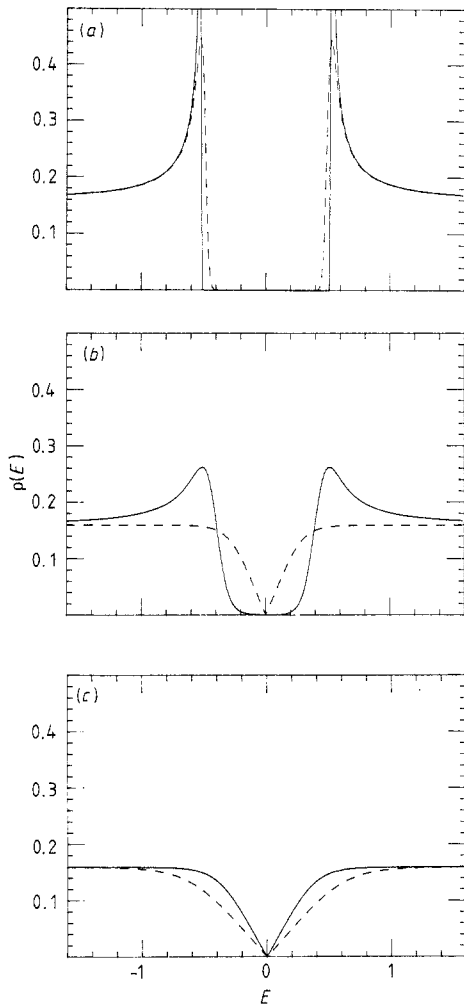
Figure 3. Density of states for the bond disorder cases $(\lambda = 0.2)$. (a) ——, $\gamma_b = 0.0$; ---, $\gamma_b = 0.0162$. (b) ——, $\gamma_b = 0.0760$ $(<\gamma_{bc}$, critical value); ---, $\gamma_b = 0.0764(>\gamma_{bc})$. (c) ——, $\gamma_b = 0.423$; ---, $\gamma_b = 0.846$.
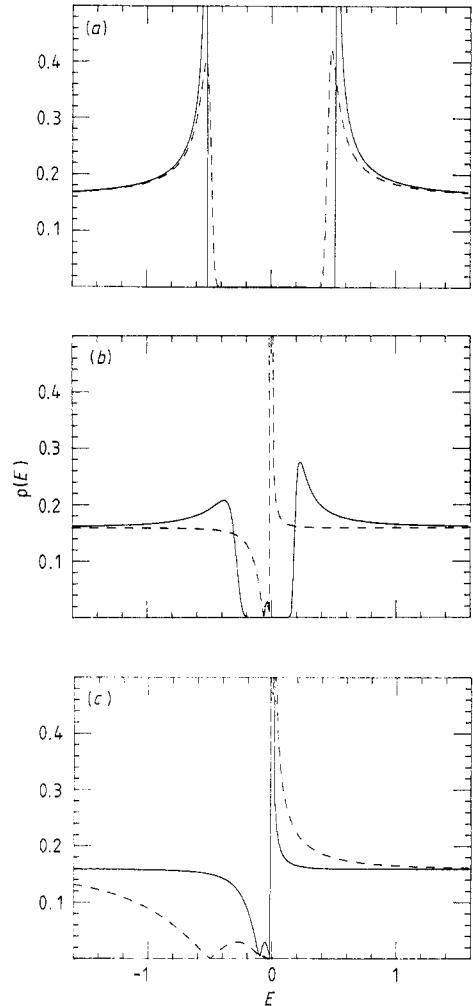
Figure 4. Density of states for site disorder cases $(\kappa_0 = 1.0;\ \lambda = 0.2)$. (a) ——, $c = 0$; ---, $c = 0.02$. (b)——, $c = 0.064(<c_c$, critical value); ---, $c = 0.065(>c_c)$. (c) ——, $c = 0.1$; ---, $c = 0.5$.

for large concentrations. This is because of the competition between the E^2 and $2c\kappa_0 E$ terms defined in equation (2.4). For very small negative E and large concentrations the latter will be dominant, yielding a positive argument of the Airy function; thus it decays like an exponential. As $|E|$ increases the E^2 term will become dominant and the whole argument of Airy function becomes negative; we then obtain the usual power law behaviour, decreasing to the exact zero at $E = \langle U_s \rangle$. This competition also results in the small peak in between the exact zero and the sharp drop just below $E = 0$. The existence of an exact zero can still be expected because of the even distribution of the random disorder; the pair splitting gives the exact zero at the mean value of the distribution of the random potential [23].

The shifting of the gap centre actually explains the discontinuity in figure 2. As $\gamma_s \to 0$ $(c\kappa_0 = \gamma_s/\kappa_0 \to 0)$, the centre of the gap is exactly at $E = 0 = E_F$. As γ_s increases, the
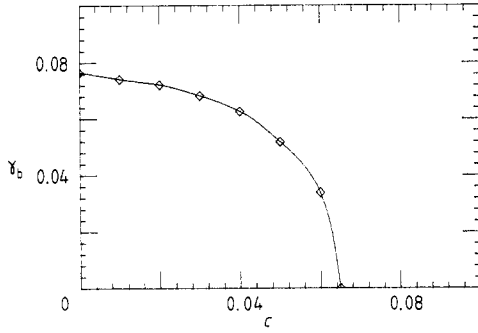
Figure 5. Phase diagram for Δ against both bond and site disorder strength ($\lambda = 0.2; \kappa_0 = 1.0$).
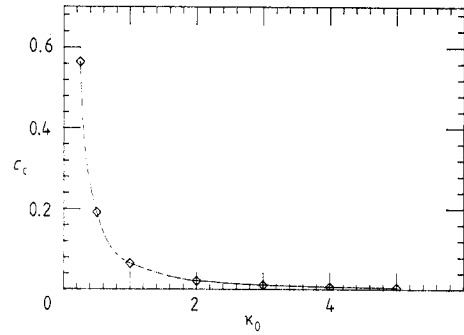
Figure 6. Critical site disorder concentration c_c against impurity strength κ_0 for $\lambda = 0.2$.

energy E is effectively shifted by an amount $c\kappa_0$. We know that increasing γ_s will decrease Δ; meanwhile, the electron–phonon interaction tends to open up the Peierl gap at the Fermi level, i.e. at $E_F = 0$. Owing to these competing effects the edge of the shifted shrunken 'gap' cannot pass the Fermi level, i.e. $E = 0$. Thus, at a certain value of γ_s, the 'gap' has to be totally destroyed which results in the discontinuity in figure 2.

In figure 5, we present the phase diagram of the bond plus site disorder case. Above the phase boundary, Δ vanishes while, within the phase boundary, the Peierl state is favoured. As either of the disorder strengths tend to zero, we reproduce the results for the single type of disorder cases.

Figure 6 shows the critical impurity concentration of the site disorder against the impurity scattering amplitude κ_0 for $\lambda = 0.2$; the best least-squares fitting shows that $c_c = \kappa_0^{-d}$, where $d = 1.58 \pm 0.05$. The appearance of the fractal dimension is because of the restriction $\gamma_s = c\kappa_0^2$, i.e. even c or κ_0 goes to zero; the product $c\kappa_0^2$ has to be finite. We can understand this by considering γ_s as an area and κ_0 as the length of a segment a set of which will encircle the area. Each individual length κ_0 can go to zero but the total area must remain finite just like the area–length relation in usual fractals. One can go even further by obtaining an equation analogous to the formula of fractal dimensions, i.e. $\ln c_c / \ln(1/\kappa_0) \to \ln N / \ln(1/r) = d$ where c_c is identified as N and κ_0 as r. Here d is very close to the fractal dimension of the two-dimensional Sierpinski gasket in which $d = 1.5849$ [24]. However, because of the discontinuity of Δ against c at c_c, we cannot find an exact analytic expression for this fractal dimension d and also the physical emphasis is not clear yet. Whether it is related to the fractal dimension and the strange attractors found in one-dimensional disordered systems [25, 26] is still an open question.

4. Concluding remarks

By using a supersymmetric functional integral formalism, we have solved the problem of the disordered-continuum BB model of a metal complex chain completely and exactly for the ground-state configuration which reproduces the previous BB model results in the limiting cases. We find the electronic density of states and gap order parameter Δ as a function of disorder strength and impurity concentration. The gap parameter Δ undergoes an abrupt drop to zero, implying the destruction of the Peierl gap. The critical impurity concentration c_c against impurity scattering strength κ_0 gives a fractal dimension that is very close to the two-dimensional Sierpinsky gasket. We also find the phase

diagram of bond disorder strength against site disorder concentration.

So far we have treated only the attractive potential case and the method also works for the repulsive potential. The model has the virtue that it can be solved exactly and hence provides a starting point for more realistic models of disorder in this class of materials. However, for a more realistic model, one has to consider effects such as lattice relaxation and higher-order corrections from the discreteness; also this treatment works just for one type of this class of materials and one has to devise some new approaches to deal with the opposite cases ($\lambda_2 \simeq 1$) which is also interesting.

Acknowledgments

Appendix. Averaging over random disorder

In this Appendix, we give the detailed steps of averaging over random-disorder potential. We need to perform the following average in equation (2.13):

$$I = \left\langle \exp\left(- \int dx \, \Phi^{\dagger}[i2\Delta U(x)]\Phi \right) \right\rangle. \tag{A1}$$

Since $U(x)$ is uncorrelated, we have in general [17]

$$\langle U(x_1)U(x_2) \ldots U(x_{2n+1}) \rangle = 0 \tag{A2}$$

and

$$\langle U(x_1)U(x_2) \ldots U(x_{2n}) \rangle = \sum_{(i_1 \ldots i_{2n})} \gamma^n \delta(x_{i_1 - x_{i_2}}) \ldots \delta(x_{i_{2n-1}} - x_{i_{2n}}) \tag{A3}$$

where we note that the summation extends over all possible partitions of the $2n$ indices $(1, 2, \ldots 2n)$ into n pairs $(i_2, i_2) \ldots (i_{2n-1}, i_{2n})$, γ is the correlation coefficient [17] and owing to the uncorrelated property of U we have

$$I = \sum_{\nu=0}^{\infty} \frac{(i2\Delta)^{\nu}}{(\nu)!} \int \ldots \int dx_1 \ldots dx_{\nu} \, \langle U(x_1) \ldots U(x_{\nu}) \rangle$$
$$\times \Phi^{\dagger}(x_1)\Phi(x_1) \ldots \Phi^{\dagger}(x_{\nu})\Phi(x_{\nu}). \tag{A4}$$

Using equation (A2), we have

$$I = \sum_{\mu=0}^{\infty} \frac{(i2\Delta)^{2\mu}}{(2\mu)!} \gamma^{\mu}(2\mu - 1)!! \left| \int dx \, [\Phi^{\dagger}(x)\Phi(x)]^2 \right|^{\mu}$$
$$= \exp\left(-(2\Delta^2\gamma) \int dx \, [\Phi^{\dagger}(x)\Phi(x)]^2 \right) \tag{A5}$$

where the identity $(2\mu)! = 2^{\mu}(2\mu - 1)!!\mu!$ has been used. Similarly

$$I_1 \equiv \left\langle \exp\left(- \int dx \, \Phi^{\dagger}(i2E\tilde{U}_s)\Phi \right) \right\rangle$$

$$= \exp\left(-(2E^2\gamma_s)\int dx\,[\Phi^\dagger(x)\Phi(x)]^2\right) \tag{A6}$$

where we use the shifted potential $\tilde{U}_s$ [17].

For integrals involving U^2, we recall that physically, although the correlation strength γ has been squared, its randomness and uncorrelated property have still been preserved. Thus we have

$$I_2 \equiv \left\langle \exp\left(-\int dx\,\Phi^\dagger iU^2\Phi\right)\right\rangle = \sum_{\nu=0}^{\infty} \frac{(i)^\nu}{(\nu)!}\int\ldots\int dx_1\ldots dx_\nu\,\langle U^2(x_1)\ldots U^2(x_\nu)\rangle$$

$$\times\,\Phi^\dagger(x_1)\Phi(x_1)\ldots\Phi^\dagger(x_\nu)\Phi(x_\nu)$$

$$= \sum_{\mu=0}^{\infty} \frac{(i)^{2\mu}}{(2\mu)!}\,\gamma^{2\mu}(2\mu-1)!!\left|\int dx\,[\Phi^\dagger(x)\Phi(x)]^2\right|^\mu$$

$$= \exp\left(-\frac{\gamma^2}{2}\int dx\,[\Phi^\dagger(x)\Phi(x)]^2\right). \tag{A7}$$

All the integrals involving $U'(x)$ give no contributions when averaged, simply because $\langle U'(x)\rangle = 0$, $\langle U'(x)U'(x')\rangle = 0$, ... The reason for this is that $\langle U'(x)\rangle = (\partial/\partial x)\langle U(x)\rangle = (\partial/\partial x)\times$ constant $= 0$, since averaging over U is only with respect to U and not x. Similarly $\langle U'(x)U'(x')\rangle = 0$. To prove this, we note that the correlation between $U(x)$ and $U(x')$ depends only on the relative distance $x - x'$ and also has to be the absolute value of the distance $|x - x'|$; in addition, the derivative of this correlation function has also to be an absolute value, i.e. its derivatives with respect to x or x' have to be the same to incorporate this translation invariance. Bearing these in mind, we have

$$\langle U'(x)U'(x')\rangle = (\partial/\partial x)(\partial/\partial x')\langle U(x)U(x')\rangle$$

$$= \lim_{\Delta x'\to 0}\{(\partial/\partial x)|[\delta(x - x' - \Delta x') - \delta(x - x')]/\Delta x'|\}$$

$$= \lim_{\Delta x',\Delta x\to 0}\{[1/(\Delta x'\,\Delta x)][|\delta(x + \Delta x - x' - \Delta x') - \delta(x + \Delta x - x')|$$

$$-\,|\delta(x - x' - \Delta x') - \delta(x - x')|]\}$$

$$= \lim_{\Delta x',\Delta x\to 0}\{[1/(\Delta x'\,\Delta x)][|\delta(x - x')| - |\delta(x - x')|]\} = 0 \tag{A8}$$

where properties of δ functions have been used as well as the assumption that Δx and $\Delta x'$ have the same rates when approaching zero. All the derivatives of higher-order moment are products of the derivatives of second or first moment and, hence, vanish.

The term involving $\langle U'/(E - 2U)\rangle$ can be treated in the following way. We use $\langle U'/(E - 2U)\rangle = (\partial/\partial x)\langle-\frac{1}{2}\ln(|E - 2U|)\rangle = (\partial/\partial x)\times$ constant $= 0$, because the average again is not a function of x. We note that we exclude the point at $U = E/2$ in performing the average, i.e. our average is defined as $\int_{-\infty}^{E/2-\delta}dU\,F(U) + \int_{E/2+\delta}^{+\infty}dU\,F(U)$ where $F(U) = p(U)(-\frac{1}{2}\ln|E - 2U|)$ and $p(U)$ is the probability distribution function of U. It is clearly not a function of x but δ which is in any case a constant. All the higher-order moments can be obtained in a similar way as in equation (A8) and again vanish. Thus all the terms involving U' give no contribution to the average.

Next, we determine the density of states at $E = 2U_s$. For the value $E = 2U_s$, we need to go back to the original equation (2.3) which becomes simpler in this case. Since all the non-quadratic terms vanish, we have only quadratic terms left and thus

one can easily perform the functional integral to obtain the density of states. We need to carry out the following functional integral:

$$G = -\mathrm{i} \int D\Phi^* \, D\Phi \, \Phi\Phi^\dagger \exp\left[-\mathrm{i} \sum_i \Phi^\dagger(x_i)\left(\frac{\partial^2}{\partial x^2} - \Delta^2 - \mathrm{i}\delta\right)\Phi(x_i)\right] \qquad (A9)$$

where $\{x_i\}$ are the set of points at which $U_s = E/2$ and $(\partial^2/\partial x^2)\Phi(x_i)$ means that derivatives are at these points. Since the exponent is a quadratic functional, we can perform the integration explicitly to obtain

$$\mathrm{Im}(G) = \mathrm{Im}\left[-\mathrm{i}\,\mathrm{Tr}\left(\frac{\mathrm{i}}{-p^2 - \Delta^2 - \mathrm{i}\delta}\right)\right] = \mathrm{Im}\left(\int \mathrm{d}p \, \frac{1}{p^2 + \Delta^2 + \mathrm{i}\delta}\right) = 0. \qquad (A10)$$

We see that at $E = 2U_s(x)$ the density of states is zero.

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