Order amidst Disorder in 2D+3D Quantum Dragon Composite Nanodevices with varying Breadth

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Abstract. A disordered quantum dragon nanodevice from a composite of 2D and 3D graphs is constructed. The nanodevice has a different number of atoms in every slice, in other words has a varying breadth. When connected to appropriate uniform semi-infinite leads, the device is shown to be a quantum dragon, namely the transmission probability is unity for all energies of incoming electrons. The device shows order amidst disorder, in that the local density of states as obtained from the Green’s function is ordered for the disordered device. For additional uncorrelated on site disorder in the tight-binding model, universal scaling of the average transmission is shown to be an effective analysis method.

1. Introduction
There is a great interest in nanoelectronics and molecular electronics, including entire books related to the subjects [1-6], that reflect the large volume of theoretical, computational, and experimental work on the science and engineering of electrical currents in nanodevices. Nevertheless, there are still surprises in electron transport in nanosystems, such as the prediction of the existence of quantum dragon nanodevices [7-9]. A quantum dragon is a nanodevice which may be strongly disordered but when connected properly to leads has total electron transmission for a wide range of energies, namely $T(E)=1$ for a wide range of $E$. Thus a quantum dragon in a two-probe measurement would have the electrical resistance equal to the inverse of the quantum of conductance, while in four-probe measurements the electrical resistance is zero. Quantum dragon nanodevices may lack any type of translational invariance, and hence the normal theoretical tools of Bloch wavefunctions and band structure are not applicable. Analysis of the electrical transmission in quantum dragon nanodevices is accomplished by finding a unitary transformation that gives in a rotated basis in Hilbert space a uniform wire connected to the leads, and a number of degrees of freedom that are disconnected from the leads. A quantum
dragon nanodevice is one that in a ball-and-stick model of the nanodevice has an underlying disordered graph and/or a disordered Hamiltonian. Only atypical disorder exhibits the quantum dragon behavior, while typical disorder has $T(E) \ll 1$.

In this paper examples of quantum dragons with both disordered graphs and disordered Hamiltonians are presented. The underlying graph is a combination of partially ordered 2D and 3D subgraphs, with different breadths of the device perpendicular to the direction of electron flow. Nevertheless, the device exhibits ‘order amidst disorder’ in that the local density of states (LDOS) is uniform even though the device graph and Hamiltonian is extremely disordered.

2. Quantum Dragon Nanodevices

A quantum dragon nanodevice can be obtained by considering only nearest-neighbor (nn) interactions. Then the device can be arranged in $\ell$ ‘slices’ labeled by the index $j$. Atoms in slice $j$ only interact with atoms in the same slice or in slices $j \pm 1$. The Hamiltonian thus is a block tri-diagonal matrix of the form (written for $\ell=4$)

$$
H = \begin{pmatrix}
A_1 & B_{1,2} & 0 & 0 \\
B_{1,2}^\dagger & A_2 & B_{2,3} & 0 \\
0 & B_{2,3}^\dagger & A_3 & B_{3,4} \\
0 & 0 & B_{3,4}^\dagger & A_4
\end{pmatrix}
$$

where the $B_{j,j+1}$ matrices contain the inter-slice portions of the Hamiltonian and the $A_j$ the intra-slice portions of the Hamiltonian. A quantum dragon nanodevice is one with atypical disorder where all $A_j$ and $B_{j,j+1}$ blocks have a common eigenvector $\vec{v}_{\text{Dragon}}$ [7]. For devices with varying breadth the $B_{j,j+1}$ are not square, and then the dragon condition is generalized to common left-singular and right-singular vectors. All $A_j$ must have a common eigenvalue associated with $\vec{v}_{\text{Dragon}}$. All $B_{j,j+1}$ must have a common singular value associated with the common singular vectors. In this paper we take a uniform $\vec{v}_{\text{Dragon}}$, namely we take all elements to be equal to $m_j^{-1/2}$ when slice $j$ encompasses $m_j$ atoms.

3. Device Tight-Binding Hamiltonian

The standard single-band tight binding model [10], also sometimes called the Anderson model, is studied. The device is based on a graph with $N$ vertices (locations of the atoms) and edges (bonds between nn atoms). The total device graph will be obtained by joining 2D (two dimensional) and 3D graphs. The graph vertices are partitioned into $\ell$ slices, with the slice labeled by the index $j$. Every site has the associated on site energy $\epsilon_{i,j}$. The creation (annihilation) operators at each site are $\hat{c}_{i,j}$ ($\hat{c}_{i,j}^\dagger$). Every bond has a hopping term of strength $t_{i,j,i',j'}$, with the second sum being over all edges of the graph. The subgraphs will be disordered 2D or 3D graphs formed by some bonds being cut from a regular lattice.

The Hamiltonian on the graph has the form

$$
\mathcal{H} = \sum_{j=1}^{\ell} \sum_{i=1}^{m_j} \epsilon_{i,j} \hat{c}_{i,j}^\dagger \hat{c}_{i,j} - \sum_{(i,j,i',j')} t_{i,j,i',j'} \left( \hat{c}_{i,j}^\dagger \hat{c}_{i',j'} + \hat{c}_{i',j'}^\dagger \hat{c}_{i,j} \right),
$$

The graph has $N = \sum_{j=1}^{\ell} m_j$ vertices ($N$ atoms in the device). Every site has the associated on site energy $\epsilon_{i,j}$. The creation (annihilation) operators at each site are $\hat{c}_{i,j}$ ($\hat{c}_{i,j}^\dagger$). Every bond has a hopping term of strength $t_{i,j,i',j'}$, with the second sum being over all edges of the graph. The subgraphs will be disordered 2D or 3D graphs formed by some bonds being cut from a regular lattice.

The tight binding model we study in Eq. (2) is a traditional model to study electron transport through nanodevices [10]. Although the model is a low-level approximation for actual materials,
it nevertheless has been well studied and applied to understanding properties of materials. The hopping terms \( t_{i,j,i',j'} \) are taken to be real since here only zero external magnetic fields are studied.

Most researchers study typical disorder, and models with locally-correlated but arbitrarily-strong disorder were expected to have \( T(E) \ll 1 \) in 2D, 3D, or 2D+3D. Our study is restricted to quantum dragon nanodevices, namely devices with strong atypical disorder but which have \( T(E)=1 \) for all electron energies that propagate in the leads. We furthermore study the effects of uncorrelated on site disorder being added to the quantum dragon device, which gives a device which is nearly a quantum dragon. This additional on site disorder is chosen randomly at every site using a uniform distribution of width \( \delta \). In particular, at every site a quantum dragon has a particular on site energy \( \epsilon_{\text{dragon}} \), and this is replaced for a device which is nearly a quantum dragon to a value chosen uniformly at random in \( \left[ \epsilon_{\text{dragon}} - \frac{1}{2} \delta, \epsilon_{\text{dragon}} + \frac{1}{2} \delta \right] \).

The uniform semi-infinite leads also have a tight-binding Hamiltonian. The on site energy of every lead atom is \( \epsilon_{\text{Lead}} \), and \( t_{\text{Lead}} \) is the hopping strength between nn pairs of atoms in the uniform wires. The right lead has the tight binding Hamiltonian

\[
H_{\text{R,Lead}} = \epsilon_{\text{Lead}} \sum_{j=\ell+1}^{\infty} c_j^\dagger c_j - t_{\text{Lead}} \sum_{j=\ell+1}^{\infty} \left( c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right)
\]

with \( \ell \) the slice index of the right-most slice of the nanodevice. The zero of energy is chosen to be \( \epsilon_{\text{Lead}} = 0 \). The unit of energy is set by choosing the hopping strength \( t_{\text{Lead}} = 1 \). The Hamiltonian for the left lead is similar, and also has \( \epsilon_{\text{Lead}} = 0 \) and \( t_{\text{Lead}} = 1 \). Let \( a \) be the nn distance between lead atoms. A Bloch wavefunction analysis for the uniform leads gives the dispersion relation

\[
E = -2t_{\text{Lead}} \cos \left( q_{\text{Lead}} a \right)
\]

with electron wavevector in the leads \( q_{\text{Lead}} \). We take our unit of length by setting \( a=1 \).

4. NEGF (NonEquilibrium Green’s Function)

The nanodevice, with Hamiltonian of Eq. (2), is connected to a semi-infinite incoming lead and a semi-infinite outgoing lead, with the lead Hamiltonian as in Eq. (3). The leads are connected to a macroscopic source of electrons at \(-\infty\) and a macroscopic sink for the electrons at \(+\infty\).

The NEGF method is used to calculate the electron transmission \( T(E) \), the probability of transmission of an electron to propagate to the end of the right lead (to \(+\infty\)) if it was injected with energy \( E \) from the end of the left lead (from \(-\infty\)). Connect the end atom of the left lead to each of the \( m_1 \) atoms in the first slice of the nanodevice, and form the vector \( \vec{v}_{\text{Dragon},1} \) of length \( m_1 \) with each element being the hopping element with strength \( m_1^{-1/2} \). Similarly connect the right lead to the device using the vector \( \vec{v}_{\text{Dragon},\ell} \) of length \( m_\ell \) with each element being the hopping element with strength \( m_\ell^{-1/2} \), being the strength of the hopping between each of the \( m_\ell \) atoms in the right-most slice of the nanodevice to the end atom of the right-hand lead. One could use different ‘dragon vectors’, but here we will use uniform connections between the end lead atoms and the device atoms. The transmission probability can be obtained from the solution of the time-independent Schrödinger equation for the infinite system of leads plus device.

Alternatively the NEGF method utilizes the \( N \times N \) matrix of the device Hamiltonian \( H \) of Eq. (2) [1, 2, 5, 10]. Define \( \xi = e^{-i q_{\text{Lead}} a} \), with \( q_{\text{Lead}} \) the electron wavevector in the leads. For the 1D semi-infinite leads, define the self-energy for the incoming (left) lead to be \( \Sigma_L = -\xi^* \vec{L} \vec{L}^\dagger \), with the \( N \)-dimensional vector \( \vec{L} \) having the first \( m_1 \) elements from the vector \( \vec{v}_{\text{Dragon},1} \) of hopping terms connecting the end atom of the incoming wire with the \( m_1 \) atoms in the first slice of the nanodevice, and all other elements zero. The self-energy of the outgoing (right) lead
is similarly given by $\Sigma_R = -\xi^* \vec{R} \vec{R}^\dagger$ with the $N$-dimensional vector $\vec{R}$ having all elements zero except the last $m_\ell$ elements from the vector $\vec{v}_{\text{Dragon},\ell}$ of hopping terms connecting the end atom of the outgoing wire with the $m_\ell$ atoms in the last slice of the nanodevice. The left and right broadening functions are defined to be $\Gamma_k = i \left( \Sigma_k - \Sigma_k^\dagger \right)$ for attached leads $k = L, R$. The Green’s function for an incoming electron with energy $E$ is defined by

$$G(E) = (EI - \mathcal{H} - \Sigma_L - \Sigma_R)^{-1} \quad (5)$$

with the device Hamiltonian $\mathcal{H}$ the $N \times N$ matrix from Eqs. (1,2). Here $I$ is the $N \times N$ identity matrix. The NEGF approach gives the electron transmission as the trace over four $N \times N$ matrices $[1, 5, 10]$,

$$\mathcal{T}(E) = \text{Tr} \left( \Gamma_L G \Gamma_R G^\dagger \right) \quad (6)$$

Once the transmission $\mathcal{T}(E)$ is calculated via the NEGF method of Eq. (6), the electrical conductance is given using the normal Landauer formula $[1, 5, 10]$. In two-probe measurements in the limit of low temperature and low bias the electrical conductance is $G = G_0 \mathcal{T}(E_F)$ with $E_F$ the Fermi energy. The quantum of conductance is $G_0 = 2e^2/h$ with $e$ the charge of an electron and $h$ Planck’s constant.

From the Green’s function, the imaginary part of the diagonal elements gives the local density of states at the atomic sites

$$\text{LDOS}_{i,j}(E) = -\frac{1}{\pi} \text{Im} \left( G_{i,j,i,j}(E) \right) \quad (7)$$

The LDOS is experimentally observable, via scanning probe techniques. The LDOS as calculated using Eq. (7) is the traditional NEGF definition $[10]$.

We say a nanodevice exhibits order amidst disorder if the device Hamiltonian of Eq. (2) is disordered (the parameters $\epsilon_{i,j}$ and $t_{i,j,j',j''}$ are not all the same) and/or are not in a regular pattern) while the LDOS$_{i,j}(E)$ is ordered. More accurately, for the quantum dragons studied here the LDOS$_{i,j}(E)$ shows order amidst disorder for all energies in $-2 < E < 2$, except at a set of energies of measure zero which are some of the eigenvalues of the device Hamiltonian. At these energies there may be a delta function contribution to LDOS$_{i,j}(E)$ due to the wavefunction on the degrees of freedom in the rotated Hilbert space basis that are disconnected from the leads.

5. Nanodevices with varying breadth

There are many choices that can be made to construct a quantum dragon nanodevice of varying breadth (a varying number of atoms in the slices). The quantum dragon nanodevices discussed here will be composed of graphs formed from a 2D ribbon connected to a two-layer 3D system, which breaks up into two 2D ribbons which is then connected to a four-layer 3D portion. If each 2D ribbon has $n_{\text{ribbon}}$ atoms, the 3D layered systems have widths $\kappa m_{\text{ribbon}}$ where $\kappa = 2, 4$ is the number of layers.

An example of the disordered 2D ribbon, which is based on a 2D hexagonal graph, is shown in Fig. 1, shown for $n_{\text{ribbon}} = 20$. Figure 1 has $\ell_{\text{ribbon}} = 36$ slices. If all Hamiltonian parameters corresponded to those of carbon, Fig. 1 would be a zigzag graphene nanoribbon. However, we have introduced disorder both in the graph and in the Hamiltonian parameters. All inter-slice bonds, those making angles of $\pm 30^\circ$ from the horizontal, had the hopping strength $t_{i,j;i+1,j} = 1$ (the same as the hopping in the leads). At random 20% of the intra-slice (vertical) bonds were removed (cut), and the rest were given values chosen uniformly at random $t_{i,j;i+1,j} \in [0.5, 1.5]$. The width of the (cyan) cylinders in Fig. 1 is proportional to the hopping strength $t_{i,j;j',j''}$. The quantum dragon nanodevice requires the two on site energies connected to an intra-slice bond to have the values $\epsilon_{i,j} = \epsilon_{i+1,j} = t_{i,j;i+1,j}$ $[9]$. The radii of the red spheres in Fig. 1 are proportional.
Figure 1. (TOP): The 2D hexagonal graph portion of a disordered quantum dragon, connected to the left lead. (MIDDLE): The LDOS at $E = \sqrt{29}/5 \approx 1.08$ for the shown portion of the quantum dragon device in the top figure. This shows order amidst disorder, since the LDOS is the same for all atoms. (BOTTOM): The LDOS at $E \approx 1.08$ for the device shown in the top figure. The device is nearly a quantum dragon with added uncorrelated on site disorder of strength $\delta = 0.05$, while the electron transmission probability is $T(\sqrt{29}/5) = 0.994$.

to the on site energy $\epsilon_{i,j}$. The yellow spheres denote atoms with on site energy zero, which includes the lead atoms.

The 3D portion of the nanodevices are based on regular 3D graphs, with each slice a 2D graph with some randomly chosen missing bonds. The 2D slices are in a $\kappa \times n_{\text{ribbon}}$ arrangement, with $\kappa$ the number of layers. The $\kappa=2$ subgraph was chosen to have the 2D cross section of a triangular graph, while the $\kappa=4$ subgraph has the 2D cross section of a square lattice. All inter-slice bonds, those parallel to the direction of the electron propagation, were chosen to be $t_{i,j,i,j+1} = 1$ (the
same value as the hopping in the leads). An example of a $\kappa = 4$ layer portion of the quantum dragon nanodevice is shown in Fig. 2, with only ten slices shown. In Fig. 2, 20% of the intra-slice bonds were set to zero (the edges of the 2D square graph were removed), and the remaining nn bonds were chosen uniformly at random in $t_{i,j,i',j} \in [0.5, 1.5]$. To obtain a quantum dragon the local correlation condition [9] is that the on site energies satisfy

$$\epsilon_{i,j} = \sum_{\text{intra}} t_{i,j; i',j}$$

where the sum is over all intra-slice bonds that couple to the atom indexed by $(i, j)$. The maximum number of terms in the sum in Eq. (8) is four. In Fig. 2 the radii of the cyan cylinders that represent the bonds are proportional to the hopping strength $t_{i,j; i',j}$, and the radii of the red spheres are proportional to $\epsilon_{i,j}$ (or are represented by a yellow sphere if $\epsilon_{i,j} = 0$). The number of atoms in each slice of the 3D portion of the quantum dragon is $\kappa m_{\text{ribbon}}$.

**Figure 2.** An example of a 3D 4-layer portion of the composite quantum dragon, based on a simple cubic graph with some missing bonds. This $\kappa$=4 subgraph has $m_j = 80$. Each layer is based on a 2D $4 \times 20$ square graph with some missing bonds. The direction of electron flow is upward-and-to-the-right.

The remaining portion of the constructed nanodevice is two 2D ribbons, each of width $m_{\text{ribbon}}$ and each ribbon having the same length (same number of slices). They are each based on a 2D rectangular graph, with 20% of randomly chosen intra-slice bonds missing. The intra-slice nn hopping strengths for the bonds present were randomly chosen with $t_{i,j; i+1,j} \in [0.5, 1.5]$, and the quantum dragon condition of Eq. (8) gives the on site energies. Each ribbon is connected to one layer of the $\kappa$=2 3D subgraph and two layers of the $\kappa$=4 3D subgraph. The number of atoms in each slice is thus $2m_{\text{ribbon}}$.

**Figure 3.** A depiction of the connection between two 2D ribbons and a $\kappa = 4$ layer 3D portion of the quantum dragon. The direction of electron flow is upward-and-to-the-right.

The coupling between the 2D ribbons and 3D portion of the quantum dragon is more complicated because the inter-slice matrices $B_{j,j+1}$ of Eq. (1) are not square. Consider connecting the 2D ribbon in the first region to the 2-layer 3D graph in region 2. Since the number of atoms in each slice of the ribbon is $m_{\text{ribbon}}$, and the number of atoms in each slice of the $\kappa = 2$ layer 3D portion is $2m_{\text{ribbon}}$ the inter-slice hopping Hamiltonian $B_{\text{connect}}$ has
dimensions $m_{\text{ribbon}} \times 2m_{\text{ribbon}}$. It is easy to understand the required form of a proper connection by using a singular-value-decomposition (SVD) of $B_{\text{connect}}$. Require the SVD have a singular value $\sigma_{-1} = -1$ associated with the dragon vectors in the two regions. Both regions here have uniform dragon vectors, but they are of different lengths. The two conditions are

$$\begin{align*}
B_{\text{connect}}^\dagger \vec{v}^{(2D)}_{\text{Dragon}} &= \sigma_{-1} \vec{v}^{(2D)}_{\text{Dragon}} \\
B_{\text{connect}} \vec{v}^{(3D)}_{\text{Dragon}} &= \sigma_{-1} \vec{v}^{(3D)}_{\text{Dragon}}.
\end{align*}$$

(9)

In order to make a simple and physical connection we use the method in [7], which uses the generalizations of the Kronecker matrix product and notation of [11]. In particular, we choose

$$B_{\text{connect}} = -\frac{1}{\sqrt{2}} \left\{ J_{m_{\text{ribbon}} \times 2} I_{m_{\text{ribbon}} \times m_{\text{ribbon}}} \right\}$$

(10)

with the identity matrix $I$ and matrix $J$ with all values unity, both of the shown dimensions. Here in region 4 (the $\kappa = 4$ 3D region) the atoms in the top layer are numbered $1, 2, \cdots, m_{\text{ribbon}}$, and the bottom layer is numbered $3m_{\text{ribbon}} + 1, 3m_{\text{ribbon}} + 2, \cdots, 4m_{\text{ribbon}}$. In words, the end atoms from region 3 (the top 2D ribbon) is connected with hopping strengths $1/\sqrt{2}$ to the two associated end atoms in the top two layers in region 4 (the $\kappa = 4$ 3D region). Similarly, the bottom ribbon in region 3 is connected to the bottom two layers in region 4. For the case $m_{\text{ribbon}} = 4$, explicitly one has the matrix

$$B_{\text{connect}} = -\frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1
\end{pmatrix}.$$ 

(11)

See Fig. 3 for a graphical depiction. We use the same type of connection between the 2D hexagonal ribbon in region 1 and the adjoining $\kappa = 2$ 3D region (region 2).

Figure 4. Two views of a large 2D+3D quantum dragon. The device is composed of four regions, numbered 1 through 4 reading from left to right. The nanodevice has $m_{\text{ribbon}}=18$, a total of $\ell=86$ slices, and $N=3456$ atoms. See the text for further details.

With the description of the four different regions of the device, and the connections between nn atoms in different regions, it is possible to build many different quantum dragons from 2D and 3D sub-graphs with varying numbers of atoms in each slice. One example is shown in Fig. 4, with $\ell = 86$ slices. The device is composed of four different regions with the number of atoms in a slice in region $k$ given by $m_k$ and the number of slices in that region $\ell_k$. The total number of atoms in Fig. 4 is $N = 3456 = \sum_{k=1}^{4} m_k \ell_k$. In region $k$ the intra-slice Hamiltonian $A_k$ and the inter-slice Hamiltonians $B_{j,j+1}$, defined in Eq. (1), are of size $m_k \times m_k$. For simplicity we take
the common eigenvector in region $k$ to be $\vec{v}^{(k)}_{\text{Dragon}} = 1/\sqrt{m_k}$ and the $B_{j,j+1}$ within any region to be the negative of the $m_k \times m_k$ identity matrix.

The four regions in Fig. 4, from left to right, are

(i) Zigzag 2D hexagonal graph; $m_1 = m_{\text{ribbon}} = 18$ and $\ell_1 = \ell_{\text{ribbon}} = 20$;

(ii) 3D triangular 2-layer ($\kappa = 2$) graph; $m_2 = 36 = 2m_{\text{ribbon}}$ and $\ell_2 = 18$; each layer has 18 atoms in every slice;

(iii) Two ribbons formed by 2D rectangular graphs; $m_3 = 36 = 2m_{\text{ribbon}}$ and $\ell_3 = 28$; each ribbon has 18 atoms in every slice;

(iv) 3D simple cubic 4-layer ($\kappa = 4$) graph; $m_4 = 72 = 4m_{\text{ribbon}}$ and $\ell_4 = 20$; each layer has 18 atoms in every slice.

All intra-slice hopping terms were chosen so 20% of the bonds were missing, with other intra-slice hopping terms chosen uniformly at random with $t_{i,j}$; $i, j \in [0.5, 1.5]$. The on site energies were then assigned as in Eq. (8), with the radii of the red spheres proportional to $\epsilon_{i,j}$. Note the 3D regions have typically larger on site energies because they typically have a larger coordination number than the 2D regions. The first region, on the left in Fig. 4, has the lead end atom connected to each of the $m_1$ atoms in slice $j = 1$ with hopping of strength $1/\sqrt{m_1}$. The fourth region, on the right in Fig. 4, has the lead end atom connected to each of the $m_4$ atoms in slice $j = \ell$ with hopping of strength $1/\sqrt{m_4}$.

Even though there is significant disorder in both the Hamiltonian parameters and in the underlying graphs, the nanodevice in Fig. 4 is a quantum dragon, and has $T(E) = 1$ for all energies in the range $-2 < E < 2$.

6. Order amidst disorder

A disordered nanodevice exhibits order amidst disorder when its LDOS is regular. For our choice of uniform dragon vectors, at every energy the LDOS is

$$\text{LDOS}_{i,j}(E) = \left[\pi m_j \sqrt{4 - E^2}\right]^{-1}$$

and is ordered since it is independent of the index $i$. The order amidst disorder is demonstrated in the middle figure of Fig. 1, with the radii of the blue spheres proportional to LDOS$_{i,j}$. Any energy in $-2 < E < 2$ could be chosen for the plot, and a uniform LDOS would be observed. Figure 1(Middle) also shows that the LDOS for the lead atoms is $m_{\text{ribbon}}$ times larger than those of the atoms in the device, as predicted by Eq. (12).

It is easy to derive Eq. (12), by considering the uniform wire in the rotated basis, and every atom in a uniform wire has a LDOS equal to $[\pi \sqrt{4 - E^2}]^{-1}$ which can be found from the Green’s function of a uniform wire. Rotating back to the real space of the device Hamiltonian, the similarity transformation includes the dragon vector $\vec{v}_{\text{dragon},j}$ when written in the original basis. Because in our case $\vec{v}_{\text{dragon},j}$ has elements equal to $m_j^{-1/2}$ the rotation back to the device basis divides the LDOS of a uniform wire into $m_j$ equal values, giving the LDOS$_{i,j}(E)$ of Eq. (12).

A quantum dragon has locally correlated disorder in the device, and exhibits order amidst disorder. If a small amount of extra uncorrelated disorder of strength $\delta$ is added to the dragon value, then the LDOS is no longer uniform, as shown in Fig. 1(Bottom). The example in Fig. 1(Bottom) used $\delta = 0.05$, and is nearly a quantum dragon. The uncorrelated disorder was added only to the region 1 nanoribbon, and had $T(\sqrt{29}/5) = 0.994$. Although the transmission probability is very close to unity, the LDOS is disordered as seen in Fig. 1(Bottom).

Even for the much larger device in Fig. 4, the device exhibits order amidst disorder. The disorder is present in that every slice is different from every other slice, and the sub-graphs in the four regions are different and have a different value for $m_k$. Furthermore the subgraphs
are disordered, since about 20% of the intra-slice bonds of a regular graph have been cut. Nevertheless, the nanodevice in Fig. 4 shows order amidst disorder in the LDOS_{i,j}(E) for any $-2 < E < 2$, as seen in Fig. 5 for the energy $E = 1$. Here the radii of the blue spheres are proportional to LDOS_{i,j}. Every atom in each region has the same value for the LDOS, and furthermore the sum over all atoms within a slice $j$ all have the same value for $\sum_{i=1}^{m_j} LDOS_{i,j}$. The lead end atoms (the largest spheres) have a LDOS which is $m_k$ times larger than the individual LDOS_{i,j} of the atoms in region $k$ for any slice. These findings agree with the predictions for the LDOS of Eq. (12). This is shown in Fig. 6 for the large nanodevice in Fig. 4.

The effect of additional uncorrelated on site energy disorder on the LDOS is illustrated in Fig. 6 for the large 2D+3D quantum dragon nanodevice of Fig. 4, with 200 atoms of each lead also shown. The atoms are numbered from slices left-to-right and within a slice top-to-bottom. The energy is chosen to be $E = \sqrt{4 - \pi^2} \approx 1.9745$ so the leads have a LDOS value of unity, but any energy in $-2 < E < 2$ has similar behavior. In Fig. 6 the red points have $\delta = 0$ and hence the device has $T(E) = 1$. The red points thus have the prediction from Eq. (12) that for this energy $LDOS_{i,j} = m_j^{-1}$, which is born out by the plot. The other points in Fig. 6 have a different uncorrelated random variant of on site disorder of strength $\delta$ added to each quantum dragon on site energy. No uncorrelated disorder is added to any lead atom. The cyan points in Fig. 6 are for $\delta = 0.01$ where for this energy and random variant $T = 0.9910$. The gray points in Fig. 6 are for $\delta = 0.1$ where for this energy and random variant $T = 0.1514$. The transmission probability can be very large, but the added uncorrelated on site disorder makes the LDOS_{i,j} quite disordered as seen in Fig. 6.
7. Universal scaling near a quantum dragon

One important question is how the transmission probability approaches unity as one approaches a quantum dragon. For a device with a uniform $\vec{v}_{\text{Dragon}}$, in [9] the prediction is made that averaging over different uncorrelated on site disorder of very small strength $\delta$ gives the average transmission $T_{\text{ave}}(E, \delta)$

$$T_{\text{ave}}(E, \delta) = 1 - \left( \frac{1}{4 - E^2} \frac{\ell}{m_{\text{scale}}} \right) \delta^2$$  \hspace{1cm} (13)

for a nanodevice with $\ell$ slices. This relationship is predicted to be valid in the limit $\delta \rightarrow 0$. The prediction is universal in that it is independent of the disorder in the quantum dragon nanodevice, the underlying graph of the nanodevice, or the eigenvalues of the device Hamiltonian $H$. The average transmission only depends on the electron energy through the factor $4 - E^2$.

Eq. (13) predicts that for small $\delta$ $1 - T_{\text{ave}} \propto \ell$, and this shows how the average transmission changes with the number of slices in the nanodevice (which is proportional to the length of the nanodevice). Eq. (13) predicts that for small delta $1 - T_{\text{ave}} \propto \delta^2$. If the number of atoms in every slice of the nanodevice were equal to $m$, for such uniform breadth nanodevices $m_{\text{scale}} = m$ and Eq. (13) predicts that for small delta $1 - T_{\text{ave}} \propto m^{-1}$. For a nanodevice with varying breadth the number of atoms in the $j^{th}$ slice, $m_j$, may be different for each slice. We find empirically that for quantum dragons based on uniform $\vec{v}_{\text{Dragon}}$ vectors $m_{\text{scale}}$ is given by

$$\frac{1}{m_{\text{scale}}} = \frac{1}{\ell} \sum_{j=1}^{\ell} \frac{1}{m_j}. \hspace{1cm} (14)$$

In Eq. (13) it is important to keep in mind the range of validity for the scaling. For example, although for large $m_{\text{scale}}$ one has $T(E) \rightarrow 1$, this result is valid only when the average transmission is predominantly from the way a single Fano resonance changes for different instances of the random uncorrelated on site disorder. As $m_{\text{scale}}$ or $\ell$ increase for a given type of Hamiltonian, the density of the Fano resonance singularities [9], the DOS($E$), also increases. Hence, the validity of Eq. (13) is then only for smaller values of $\delta$ which implies smaller values of $1 - T_{\text{ave}}(E, \delta)$.

We can rewrite Eq. (13) in a slightly different scaling form. The universal scaling form is predicted to be

$$[1 - T_{\text{ave}}(E, \delta)] \frac{(4 - E^2) m_{\text{scale}}}{\ell \delta^2} = 1. \hspace{1cm} (15)$$

See Fig. 7 for a test of Eq. (15). The data are for three types of nanodevices:

- **Black symbols**: Linear chains with $m = 1$ and two values of $\ell$.
  - With $(m, \ell)$ given by (1, 37):disks, (1, 18):squares.
  - For $\ell = 18$ at the smallest $T_{\text{ave}}(E, \delta)$ values ten different averages are shown, each using a different $10^4$ configurations of uncorrelated site disorder.

- **Green symbols**: Single-walled nanotubes (SWNT) with three values of $(m, \ell)$.
  - With $(m, \ell)$ given by (12, 37):circles, (6, 37):squares, and (12, 18):triangles.

- **Red symbols**: 2D+3D nanodevice, a nanodevice similar to Fig. 4 but for a smaller $N$, with varying values of $m$ in slices and hence using $m_{\text{scale}}$ from Eq. (14).
  - Here $m_{\text{ribbon}}=6$, and $N = \sum_{j=1}^{\ell} m_j = 372$ denoted by the red open disks and circles.
  - The four regions of the 2D+3D quantum dragon nanodevice with varying breadth has $\ell_1=\ell_2=\ell_4=6$ and $\ell_3=10$ with the total number of slices $\ell=28$.
  - The $N=372$ quantum dragon nanodevice, without disorder in the four subgraphs or the Hamiltonian, is shown in Fig. 8.
Figure 7. Scaling plots to test Eq. (15) for the two energies (A) $E = 1$ and (B) $E = -\sqrt{2}$. The color of the points are for 1D linear chains (black), armchair single-walled 2D hexagonal nanotubes (green), and 2D+3D devices with varying $m$ (red). See text for full description.

In all cases in Fig. 7 the filled plotting symbols are for regular subgraphs (no missing bonds) and all $t_{i,j,i',j'} = 1$, while the open plotting symbols are for corresponding graphs with 20% of the intra-slice bonds cut and the other intra-slice hopping terms $t_{i,j,i',j} \in [0.5, 1.5]$. In all cases the dragon condition Eq. (8) is used to obtain the $\epsilon_{i,j}$ on site energy values. The averages are over $10^4$ Gaussian-distributed uncorrelated values added to each dragon condition on site energy. The Gaussian distribution has mean zero and width unity, and is then multiplied by $\delta$. The averages must be over a large number of disorder configurations, due to the narrow Fano resonance dips to $T(E) = 0$ [9]. The same dragon Hamiltonians and graphs are plotted for all three types of nanodevices in Fig. 7, for the two energies (A) $E = 1$ and (B) $E = -\sqrt{2}$. With no adjustable parameters in Fig. 7 we see for small $1 - T_{\text{ave}}(E, \delta)$, so for small $\delta$, excellent agreement with Eq. (15) for all nanodevices. We do not have a prediction for when the quantum dragon universal scaling breaks down as $\delta$ becomes larger. This breakdown is probably a complicated function of $\ell$, $m_j$, $\text{DOS}(E)$, $E$, and perhaps the precise location of the disorder in the quantum dragon nanodevice. In Fig. 7(A) the energy $E = 1$ shown is near a minimum for the DOS($E$) for the armchair single-walled nanotubes (green points). For a given quantum dragon nanodevice the universal scaling breaks down as $\delta$ increases at different values of $\delta$, and hence at different values of $T_{\text{ave}}(E, \delta)$, at different energies as seen most readily by comparing the SWNT (green) symbols in (A) and (B). We observed very similar behavior for all energies we tested in $-2 < E < 2$, with the only difference from Fig. 7 how large $\delta$ had to be before the universal scaling of Eq. (15) broke down.
Figure 8. A small 2D+3D device with $m_{\text{ribbon}}=6$ and $N = 372$, used for the filled red symbols in Fig. 7.

8. Conclusions and Discussion

We have demonstrated by construction that quantum dragon nanodevices with varying breadth based on 2D+3D graphs exist. In particular, we have studied the single-band tight binding model on these 2D+3D graphs. In our units, for all energies $-2 < E < 2$ of the incoming electron, we find unit transmission $T(E)=1$. Furthermore these quantum dragons show ‘order amidst disorder’ in that a disordered device shows an ordered local density of states LDOS), as in Figures 1, 5, and 6. The 2D+3D quantum dragon nanodevices have strong disorder, but the disorder is correlated in such a fashion that the device has unit electron transmission. This requires only local correlation of parameters in the tight binding Hamiltonian. We have further demonstrated that for small random amounts $\delta$ of added uncorrelated on site energies the predicted universal scaling of Eq. (15) is valid, while for devices with varying width the effective scaling breadth is given by Eq. (14).

These quantum dragons with varying breadth allow researchers in nanoelectronics, optoelectronics, and molecular electronics to devise many different types of devices and circuits that have high electron transmission over a wide range of energies.

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