Preferential Interaction Paths for Localized Wave Functions in Disordered Media

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***Abstract*—GaN-based alloys are characterized by important spatial composition inhomogeneities resulting from the random distribution of Indium atoms. These variations can induce carrier localization and strongly influence the performance of the devices. We present here a work based on the recent theory of the localization landscape, whose main result is the derivation of an effective potential W. The basins of this effective potential define the localization subregions of carriers. The exponential decay of the wave functions outside these regions is controlled by the Agmons distance, which is calculated on 2D landscape map. Interactions between bound states are shown to happen along very well defined preferential paths within the system.**

I. The localization landscape theory

We first briefly review the main results of the localization landscape theory, described for the first time in [1]. In this theory, the spatial position of the quantum states in a random potential field V (such as the potential energy resulting from the compositional fluctuations of an InGaN disordered layer) can be precisely predicted without the need of solving the Schrödinger equation

$$\hat{H}\psi = E\psi, \quad \text{with} \quad \hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V} \tag{1}$$

Instead, we solve a much simpler linear Dirichlet problem whose solution u is called the *localization landscape*:

$$\hat{H}u = 1\ . \tag{2}$$

The main feature of this landscape is that its valley lines delimit the localization regions of the wave functions, following the inequality [1]:

$$|\psi(\vec{r})| \leq Eu(\vec{r}) \tag{3}$$

where ψ is an eigenfunction of $\hat{H}$ and E is its associated eigenenergy. Indeed, Eq. (2) ensures that ψ is small along the valley lines of the landscape (where u is small), which constrains ψ to be confined within the subregions defined by the valley network of u. Furthermore, the landscape also provides information on the shape of the fundamental state in each localization subregion Ω_i, as well as its associated eigen-energy [2]:

$$\psi_0^i \approx \frac{u}{||u||} \tag{4}$$

$$E_0^i = \frac{\langle u|1\rangle}{||u||^2} = \frac{\iiint_{\Omega_i} u(\vec{r})\ d\vec{r}}{\iiint_{\Omega_i} u(\vec{r})^2\ d\vec{r}} \tag{5}$$

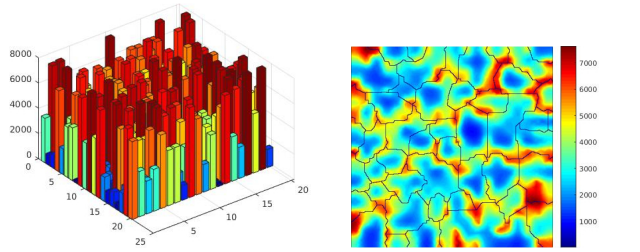

Fig. 1. (a) 3D representation of the original disordered potential V. (b) The valley lines of the landscape $1/u$ (black lines) delimit the various localization regions.

In the following, we compute localized states on a 2D unitary square domain divided into 20×20 smaller squares on which V is piecewise constant and randomly determined between 0 and 8000 (Fig. 1a).

Recently, Arnold et al. [3] showed that the inverse of u, here called W and homogeneous to an energy (Fig. 1b), acts as an effective confining potential seen by the localized eigenstates, and that its basins (delimited by the valley lines of u) correspond to the localization subregions. Indeed, the following equality, satisfied by any quantum state $|\psi\rangle$

$$\langle\psi|\hat{H}|\psi\rangle = \frac{\hbar^2}{2m}\,\langle u\vec{\nabla}(\frac{\psi}{u})|u\vec{\nabla}(\frac{\psi}{u})\rangle + \langle\psi|\hat{W}|\psi\rangle \tag{6}$$

shows that its energy can never be smaller than the one it would have in a potential $W(\vec{r})$. This result also shows that the quantity $(W-E)_+$ can be used to construct an Agmon distance which controls the long-range exponential decay of the localized wave function in the barrier regions where $E < W$.

II. Agmon's decay of wave functions

The Agmon distance between two points $\vec{r_0}$ and $\vec{r}$ is defined as the length of the shortest geodesic path connecting the two points when using the Agmon metric $\sqrt{(W-E)_+}$ (with $f(x)_+ = \max(f(x), 0)$). Considering a state $|\psi\rangle$ of energy E centered in $\vec{r_0}$, the Agmon distance between the points $\vec{r_0}$ and $\vec{r}$ is:

$$\rho_E(\vec{r_0}, \vec{r}) = \min_{\gamma}\Big(\int_{\gamma} \sqrt{(W(\vec{r}) - E)_+}\ ds\Big) \tag{7}$$

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where the minimum is computed on all paths connecting the two points. It can be shown [4] that the problem of finding the Agmon distance from a given point $\vec{r_i}$ to any other point $\vec{r}$ is equivalent to solving the eikonal equation:

$$|\nabla \rho_{E_i}(\vec{r_i}, \vec{r})|^2 = \frac{2m}{\hbar}(W(\vec{r}) - E_i)_+ \ . \tag{8}$$

This eikonal equation is solved using a Fast Marching Algorithm with an upwind gradient scheme (Fig. 2a). In addition, the Agmon distance governs the decay of a wave function ψ_i through the following inequality [5]:

$$|\psi_i| \leq c_i e^{-\rho_{E_i}(\vec{r_i},\vec{r})} \quad \text{with} \quad c_i = \frac{1}{\sqrt{\int e^{-2*\rho_{E_i}(\vec{r_i},\vec{r})} d\vec{r}}} \tag{9}$$

where E_i is the energy of the state, and $\vec{r_i}$ is the position of the minimum of $W = \frac{1}{u}$ in this region. The coefficient c_i is obtained by normalizing the wave function over the entire space.

III. Preferential interaction paths

Interaction matrix elements between bound states are now calculated from Agmon distance maps. Hopping-assisted transport from one state to another happens through absorption or emission of phonons, with the following eletron-phonon Hamiltonian:

$$H_{ep} = \sum_q a_j^+ a_i b_q^\eta \ \left(-i\eta \ c_q \ \langle \psi_j | e^{(-i\eta \vec{q}.\vec{r})} | \psi_i \rangle\right) \ , \tag{10}$$

where a_j^+ and a_j are the creation and annihilation operators of an electron on site j (resp. i), b_q^η is the creation ($\eta = +1$ for emission process) or annihilation ($\eta = -1$ for absorption process) operator of a phonon of mode $\vec{q}$, and c_q is a coupling factor. The bracket elements are then, at first order:

$$\langle \psi_j | e^{-i\eta \vec{q}.\vec{r}} | \psi_i \rangle = \int \psi_j^* e^{-i\eta \vec{q}.\vec{r}} \psi_i \ d\vec{r} \tag{11}$$

$$\approx -ic_i c_j \eta \int e^{-(\rho_i(\vec{r}) + \rho_j(\vec{r}))} \ \vec{q}.\vec{r} \ d\vec{r} \tag{12}$$

The integrand in the above equation remains significantly large only along a preferential path that minimizes simultaneously both Agmon distances ρ_i and ρ_j. This defines a most favorable path of interaction between two bound states that can be directly read on the map of W, since this path essentially goes through the saddle points of this landscape. Fig. 2b displays an example of several preferential paths between localized states. Together, these paths define a subnetwork of connected sites, equivalent to the Miller and Abrahams [6] resistor network model for localized carriers transport.

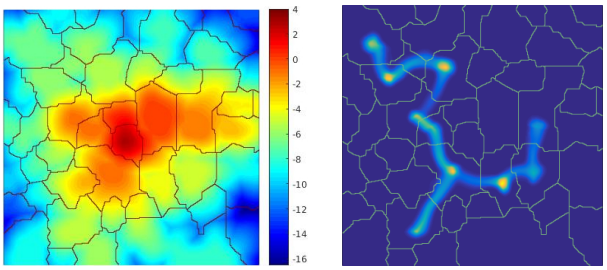

Fig. 2. (a) Agmon distance computed from the center of a localization subregion located inside the domain (log scale). (b) Examples of preferential interaction paths determined by the sum of Agmon distances (see Eq. 12). These paths essentially go through the saddles of the effective potential W displayed in Fig. 1b.

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