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Determine the Lower-State Energy of (GaMn)As/GaAs Quantum Well using Localization Landscape Method

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ABSTRACT

The current research presented the value of the lowest state energy for (GaMn)As/GaAs Quantum Well by using the Schrodinger equation and the localization landscape method, and a comparison between the quantum confinement potential and the wavefunction localization of both the landscape method and the Schrödinger method, a great match was found between the two methods, where the Landscape method 0.1% greater than Schrodinger method. From the Hamiltonian function analysis, it was found that the quantum eigenvalues in the discrete wells interact only when the corresponding eigenvalues are close to each other. Localization appears clearly in the sub-regions of quantum well, so, we prove damping in quantum wells, especially near the boundaries of the well. The effective quantum potential W was determined.

Introduction

For the last years, the calculation of the electronic structure of nanoscale semiconductors such as quantum wells and quantum dots has received wide and exciting interest, as knowing these properties helps improve the performance and design of those devices that vary according to their function, such as light-emitting diodes and some semiconductor lasers [1].

In order to modelling individual particle states of quantum dots, wells, and even superlattice structures, it requires solving the time-independent Schrödinger equation for these systems that contain millions of atoms, it is difficult to apply theory of standard function density and use experimental models for this huge number of atoms. Even if it can be applied, this requires solving the problem of the large eigenvalue of energy which remains an important numerical requirement [2]. When calculating the characteristics of the transmitter in its LED device, the numerical potential doubles very largely, making the process of self-numerical calculations more difficult.

In the 2012 year, [3] presented the concept of the landscape function mathematically by solving the function u in the form of $\hat{H}u = 1$, since $\hat{H}$ is an elliptical effect operator, and he demonstrated that this function has the ability to predict the shape and position of the localization of the low-energy eigenfunctions of the $\hat{H}$operator. Whether the localization was due to voltage disturbance or due to field geometry, or both [4]. Recently, [6,5] developed a landscape function theory that was originally used to compute Anderson's localization, in order to circumvent the problem of large eigenvalue computations to obtain wave functions in-ground and excitable states instead of solving the time-independent Schrödinger equation [7,8].

Since then this method has been used in theoretical and experimental physics to predict plate vibration and the dual Laplace spectrum with Dirichlet boundaries [9], to study the quantitative efficiency of GaN light-emitting devices and the spectral properties of the Schrödinger equation with the Anderson potential within the specified range [10].

The research idea is summarized in the solution of the equation $\hat{H}u = 1$, where $\hat{H}$is the Hamiltonian effect in the time-independent Schrödinger equation $\hat{H}\psi_i = E_i\psi_i$, Ψ is the wave function for the state (i), and E is the eigenvalue of energy. In order to calculate the eigenvalue of the energy of the ground state, as well as the wavefunction in Schrodinger's equation, the problem of the large eigenvalue can be

addressed through the Hamiltonian matrix, which corresponds to the $\hat{H}$effect, which will be accurately constructed depending on the basic electronic structure. This structure is for contrasting semiconductor structures according to the k.p method or effective mass approximations of the beam, where the dimension of the matrix depends on the number of atoms in the system. Where the landscape theory divides the system into weakly connected sub-regions to form areas of the spatial distribution of self-vibrating shapes, which are derived from the value of the eigenvalue of energy. Where it can reduce the linear behavior of the system to knowing its patterns of vibration, which means the functions and the eigenvalues of the spatial differential factor associated with the wavenumber itself [11].

According to this theory, the precise spatial location of the quantum states in the potential well V(r) can be predicted using u(r) solution of the simplified Dirichlet problem, which is called the localization scene.

Theoretical Model

Localization phenomenon is defined as the concentration of the system's eigenfunctions in a small part of the surrounding original field and is close to or equal to zero in the rest of the regions, which leads to preventing its spread completely. The wave localization occurs in all vibrating systems in nature, starting with traditional mechanics and ending with quantum mechanics, where it arises. In irregular geometrical systems (weak localization) as well as in disordered systems (Anderson localization).

There are several types of localization, each of which exhibits a specific behavior. First: When it is caused by the irregular geometry of the vibration field, here it is classified as weak localization characterized by a slow decay of the amplitude pattern away from its generating region. Secondly, it can arise due to a dampening disturbance in the system which is called the localization of Anderson who discovered it in 1958 [12]. The amplitude decay pattern moves away from the region of its generation where there is strong localization. Finally, there is localization that differs from high-frequency localization in specific domains possessing stable orbits such as ball bounce mode [13].

To investigate the localization of the wave function in these structures, the carrier wave functions are computed by solving the Schrödinger equation and the landscape method. This method requires knowledge of the potential energy of the well. The present calculation of the carrier potential energy includes band displacement effects between GaAs and GaMnAs (see Figure 1).

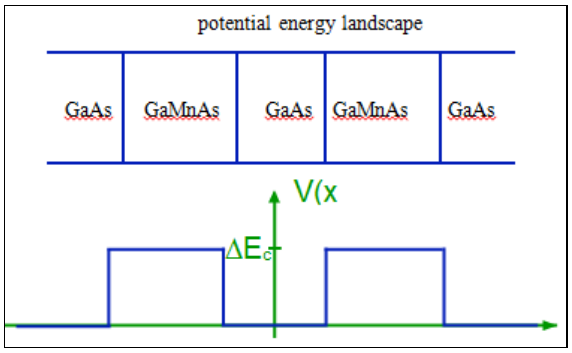

Fig. 1: illustrates a landscape method for the potential energy of a GaAs quantum well, the effective mass was taken in the calculations.

The state function u can be formulated on the basis of the wave function ψ where H is the Hamiltonian operator:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla + V \dots\dots\dots\dots (1)$$

The landscape function can be defined by solving the equation:

$$\hat{H}u = -\frac{\hbar^2}{2m}\nabla \mathrm{u} + Vu = 1 \dots\dots\dots\dots (2)$$

Ref. (12), shows that the sub-regions in which the localization of the eigenfunctions delimited by the valleys occurs in the Figure (2). This property is obtained from the fundamental inequality satisfied by the eigenfunction (ψ) of the Hamiltonian influence with the eigenvalues of energy whose amplitude is equal to one.

$$|\psi(r)| \leq Eu(r) \dots\dots\dots\dots\dots (3)$$

In the other formulation, the small values of $(u(r))$ along the valley lines restrict the amplitude of the function (ψ) to be small on the same lines, and therefore the lowest energy eigenfunctions reside within the regions surrounded by these lines, and thus the Landscape (u) gives a division of the field into a set of sub-regions that Each one determines the localization the carrier.

Where u(r) s the landscape function in the quantum well width, E is the energy eigenvalue.

The eigenvalue and its corresponding energies can be determined from the function u itself from equation (2). All details are available at [9].

The landscape function can be expressed by the function u (r) on the basis of the eigenvalues of the wave function ψ of the H operator:

$$\langle 1|u\rangle = \sum_i \alpha_i \langle 1|\psi_i\rangle \dots\dots\dots\dots\dots\dots\dots\dots\dots (4)$$

Where:

$$\alpha_i = \langle u|\psi_i\rangle = \iiint u(r)\psi_i(r)d^3r \dots\dots\dots\dots\dots (5)$$

Due to the self-adjacent condition of the Hamiltonian H, α_i (is expansion coefficient) can be determined by the equation:

$$\alpha_i = \langle u|\psi_i\rangle = \frac{1}{E_i}\langle u|H\psi_i\rangle = \frac{1}{E_i}\langle 1|\psi_i\rangle \dots\dots\dots (6)$$

Observing equation (6), it is showed that the contributions of high energy states appear to be fake of the wavefunction u and depends on factor $1/E_i$, so if there is an energy interval between the ground states i and the irritant (i+1), then many of these states contribute to the expansion of the localization scene, and this is not desirable because this leads to a large difference in the ground state value of the wave function when compared to that result by application Schrödinger's equation.

In the case of a quantum square well, the wave function is located in the sub-regions close to the potential barriers as in the figure (1) and away from the main areas inside the well because that results from the strengthening of the less active quantitative functions in those sub-regions.

In many cases, when we consider the radioactive recombination within the voltage well of the vectors in each sub-wave localization region, the value of u can be estimated by:

$$\langle 1|u\rangle \cong \frac{\langle 1|\psi_1^m\rangle}{E_1^m}|\psi_1^m.\rangle = \alpha_i|\psi_1^m.\rangle \dots\dots.. (7)$$

Where: $|\psi_1^m.\rangle$ Is the general basic case in the sub-region Ωm Accordingly to the hypothesis [4], the spread of u in the sub-region can be considered as:

$$\langle 1|\psi_1^m\rangle \approx \frac{|u\rangle}{\|u\|} \dots\dots\dots\dots\dots (8)$$

By using equation (8), the ground state energy in the sub-region can be approximated:

$$E_1^m = \langle\psi_1^m|\hat{H}|\psi_1^m\rangle \approx \frac{\langle u|\hat{H}|u\rangle}{\|u\|^2} = \frac{\langle u|1\rangle}{\|u\|^2} = \frac{\iiint_{\Omega_m} u(r)d^3r}{\iiint_{\Omega_m} u^2(r)d^2r} \dots\dots.. (9)$$

From equation (9) we can estimate the eigenvalue of the ground state: $u(r) = \langle r|u\rangle$

The landscape function u(r) is not only for determining the ground state of energy and the wave function but also for determining the effective quantum confining potential W, where w=1/u. Where the exponential decay of the localization status is determined, starting from the sub-region towards the barriers, to start a new concept called the tunnel.

Solution of localization landscape equation

The Schrödinger equation gives the ground state of energy En the wave equation ψ in the form:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}\psi(x) + V\psi(x) = E\psi(x) \dots\dots\dots\dots\dots (10)$$

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} \dots\dots\dots (11)$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L \dots.. (12)$$

E_1 represent the ground state energy, $\psi_n(x)$ is the wavefunction of n state.

By equation (11) and Concept of localization scene theory according to Hilbert space we can get:

$$u = \sum \alpha_n\psi_n \dots\dots\dots\dots\dots (13)$$

By seen the equations (6) and (13), we can conclude three main observations. Firstly, the quantum states of low energy contribute more to u function than the high energy states, secondly, in a certain sub-localization region, the lower energy functions enter (i) In the analysis of equation (6) which is basically the local quantum states of this sub-region, thirdly, in each sub-region, the ground state has a shape similar to a small protruding protrusion, while the higher-energy state takes orthogonally, positive and negative values, so that the numerical results become From the equation (13) it almost fades away.

Note that this cancellation also occurs for non-specified system states with high power. As a result, substituting (13) by ($\hat{H}u = E_i u$) we get:

$$\hat{H}u = \sum_n E_n\alpha_n\psi_n = 1 \dots\dots.\dots. (14)$$

And substituting (12):

$$\sum_n \alpha_n E_1 n^2\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi z}{L}\right) = 1 \dots\dots\dots. (15)$$

We can rewrite equation (15) as [14]:

$$\frac{4}{\pi}\sum_{n_{ood}}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi z}{L}\right) = 1 \dots\dots. (16)$$

From above equations, α_n equal to zero for even value of n, but it taken odd value, where:

$$\alpha_n = \frac{2\sqrt{2L}}{E_1 n^3\pi} \dots\dots\dots\dots\dots\dots. (17)$$

So, from eq. (13) and eq. (17) we can get:

$$u(z) = \sum_{n_{odd}}^{\infty}\frac{2\sqrt{2L}}{E_1 n^3\pi}\psi_n(z)$$

$$u(z) = \frac{2\sqrt{2L}}{E_1\pi}\sum_{m=1}^{\infty}\frac{\psi_{2m-1}(z)}{(2m-1)^3} \Rightarrow$$

$$= \eta\left[\psi_1(z) + \frac{1}{27}\psi_3(z) + \frac{1}{125}\psi_5(z) + \cdots\right] \dots\dots\dots\dots (18)$$

Where: $\eta = \frac{2\sqrt{2L}}{E_1\pi}$. From equation (18) it is noticed that the series u converges for every $1/n^3$. This means that the Landscape method gives a satisfactory approximation of the ground state within the range [0, L].

To calculate the value of ground state energy E_1^m for a square one-dimensional potential well:

$$E_1^m = \frac{\int u.H.u^*dz}{\|u\|^2} = \frac{2\eta\sqrt{2L}}{\pi\eta^2}\frac{\sum_{m=1}^{\infty}\frac{1}{(2m-1)^4}}{\sum_{m=1}^{\infty}\frac{1}{(2m-1)^6}} = \frac{20\sqrt{2L}}{\eta\pi^3} \dots\dots\dots. (19)$$

$$E_1^m \cong 1.0210\ E_1$$

We notice that the ground state energy within the range (0, r) is largely consistent with the result obtained from solving the time-independent Schrödinger equation, and it is greater than it by 9%.

Results and discussion

The numerical solution by Landscape method will be compared to the time-independent Schrödinger analytical solution, using tables and graphs as comparison tools, and we will verify whether the Landscape solution, which has been mathematically constructed for the wavefunction, is physically acceptable with regard to the energy of the ground state of well width, with respect Equation (10) and boundary conditions. The results obtained for the lowest eigenvalues inside the potential well represent the first family of what would be expected from the effect of quantum well width on the lower energy eigenvalue .

In numerical terms, we have seen more exponential separation and decay than what mathematical equations express. The approximate solutions

generated through the Landscape method show the energy quantization characteristic at each wavefunction with a slight error due to the calibration of the Hamiltonian factor, and there is another condition that the approximate solution must fulfill, which is the continuity property for the range (0, r), where it appears that solutions are physically acceptable, see Table.(1)

Figure (2) shows the localization landscape method, where Figure (a) shows the limits of localization for the function u, while Figure (b) represents the landscape function u as solutions to the equation (2), (c) represents a two-dimensional view of the gradient of the bound states inside the potential quantum well, (d) represent the effective localization potential W for the sub-regions shown in (a).

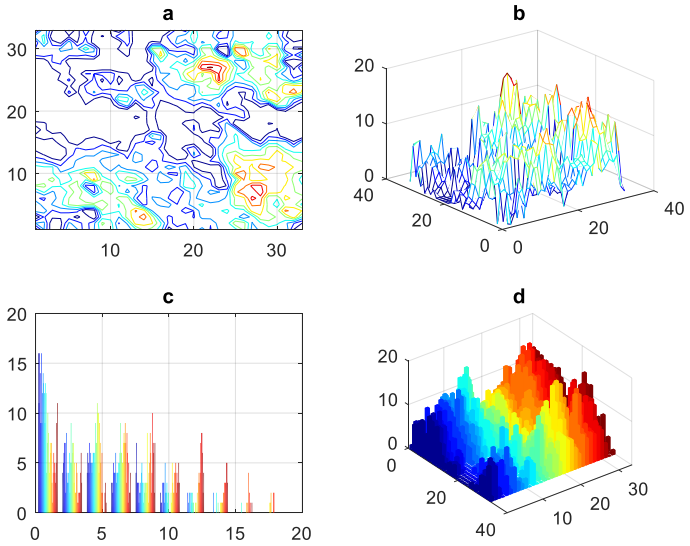

Fig. 2: The localization landscape method: (a) the valley network with blue lines represents the localization limits for the function (u), (b) the landscape function (u) represents the solutions of equation (2), (c) represents a two-dimensional view of the bound states gradient inside the quantum potental well., (d) represents the effective localization potential (W) for the sub-regions shown in (a) where $W = u^{-1}$.

Localization appears clearly in the sub-regions in the quantum well, Therefore, we prove the presence of decay in quantitative wells, especially near the boundaries of the well. By Comparing of the effective potential of a square well with infinitely high potential bollards. The infinite square well potential is given by the Black line. The effective confining potential calculated by the landscape is given by the red dotted line. Ground states of Energy obtained for Localization Landscape via two different Method. is given by the green and blue lines, see Figure (3), noting that up to this moment the resonance tunneling was not taken into account, as it was found that there is a strong interaction between the eigenfunctions in the separate wells when the eigenvalues are close.

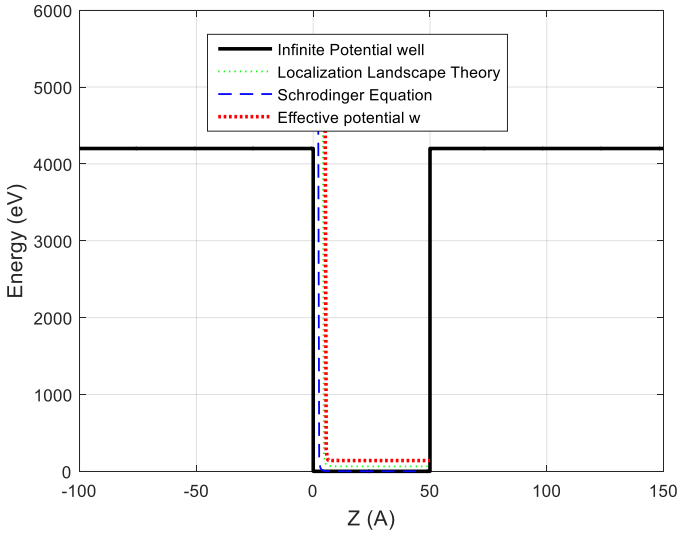

Fig. 3: Shows a comparison between the possibility of quantum confinement and wavefunction localization for the Landscape and Schrodinger method, it is clearly that there is a high congruence in the two methods, as the error rate is approximately 0.1% between the two methods, width of the well is 50 A with infinite barriers.

As presented from numerical and analytical solutions, it clear that there is congruence with the exact solution of the time-independent Schrödinger equation (see Figure 4), but in order for the Landscape solution to be physically acceptable, it must achieve a state of quantization energy and thus the emergence of bound states and wave localization Inside the potential well, through the probability density of the wavefunction which is related to the quantization of energy, as in Figure (5).

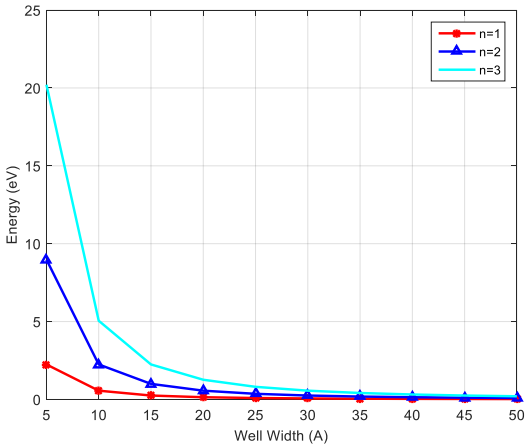

Fig. 4: Shows the lowest three states of energy eigenvalue in a GaAs potential well, width of 50 A surrounded by infinite barriers. It is clearly that all three states appear coherent with decreasing energy value during increasing the well width.

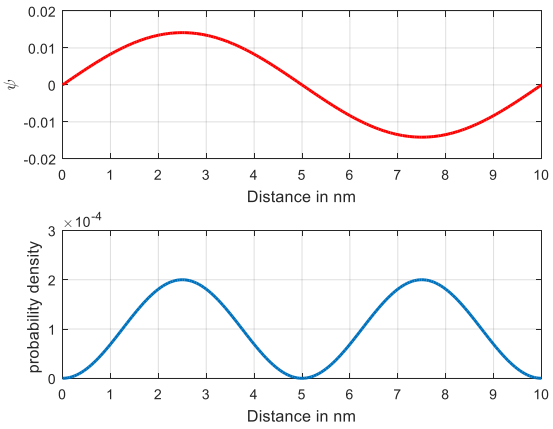

Fig. 5: Shows the approximate solution and the probability density of the wave function at the ground state energy n = 1, for a single potential well (GaAs) width of 10 nm.

While, Figure (6) Shows the wavefunction for the first three quantum states of energy as a function of the well width, as it is observed that the wave function is decay continuously when increasing the quantum well width, which predicts the need to adhere to the limits of the quantum well to produce the bound states that located inside the quantum well.

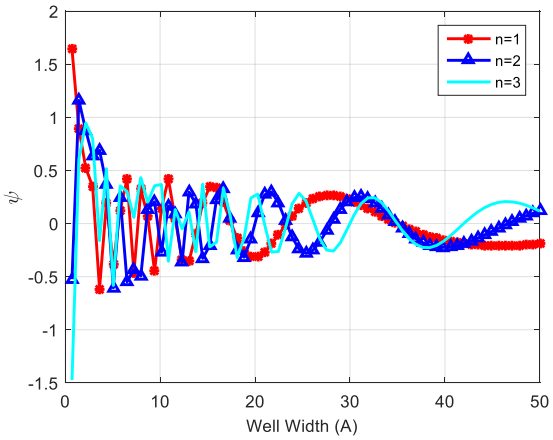

Fig. 6: The eigenfunctions of the ground state (n=1) and the excited states (n=2,3), corresponding to the self-energy states computed using the time-independent Schrödinger equation.

In this and other Similar studies, the ground state energy is the desired goal in all semiconductor applications, as it is concerned with the stability of the device's operation.

Table 1: A comparison between the landscape method of localization and the Schrödinger method to calculate the lowest eigenvalue of energy for a GaAs potential square well, width 50A surrounded by infinite walls. The effective mass was taken into Schrödinger's equation, 0.067m0.

Energy by SE (eV)	Energy by LLT (eV)	Well width (Å)	Index n
22.503282	22.953348	5	1
5.625821	5.738337	10	
2.500365	2.550372	15	
1.406455	1.434584	20	
0.900131	0.918134	25	
0.625091	0.637593	30	
0.459251	0.468436	35	
0.351614	0.358646	40	
0.277818	0.283375	45	
0.225033	0.229533	50	

Conclusions

In this work we applied the landscape method to build a mathematical model for quantum semiconductor devices. The Schrodinger equation was replaced by the landscape equation whose solution is called the (u) localization landscape. The inverted (u) gives us the effective landscape localization potential (W). We were able to provide a good picture of wave function localization in a GaAs potential well of finite width and surrounded by GaMnAs infinite using the scene method and Schrödinger's equation.

Landscape method provides a convenient method for determining the decay of a quantum state far from its point of origin. This decay corresponds to the tunnel effect and is more common in quantum mechanics.

The results showed a great agreement between the ground state energy E_1^m in the region (0, L) by Landscape method and the exact solution of Schrödinger's equation, it is about 1% greater than (E_1) and it is acceptable from a physical point of

view, especially with regard to the ground state energy of the infinitely high potential well and the limited width.

Calculation time is reduced with Localization Landscape Method compared to the traditional Schrödinger equation, making this model ideal for simulating and designing quantum devices.

Nevertheless, we believe that this work is a profound fundamental step towards explaining the localization of all the values of the eigenvalues in the (1/u) sub-regions strongly defined by [8,9]. The emission and absorption in the quantum system can also be framed precisely in terms of calculating the intrinsic energy depending on this concept.

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تحديد طاقة الحالة الأرضية لبئر الجهد الكمي (GaMn)As/GaAs باستخدام طريقة لاند سكيب المحددة

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الملخص

في البحث الحالي تم تحديد طاقة الحالة الارضية لبئر الجهد (GaMn)As/GaAs بواسطة معادلة شرودنجر غير المعتمدة على الزمن وطريقة لاندسكيب المحددة، ومقارنة بين إمكانية الحصر الكمي وتوطين دالة الموجة لكل من طريقة لاندسكيب وطريقة شرودنجر، تم العثور على تطابق كبير بين الطريقتين، حيث ان طريقة لاندسكيب المحددة اكبر من طريقة شرودنجر بحدود 0.1%. من تحليل الهاميلتون، وجد أن القيم الذاتية الكمية في الآبار المنفصلة تتفاعل فقط عندما تكون القيم الذاتية المقابلة قريبة من بعضها البعض .اذ يظهر التحديد بوضوح في المناطق الفرعية للبئر الكمي، لذلك، نثبت وجود الاضمحلال في الآبار الكمية، خاصة بالقرب من حدود البئر. تم تحديد الجهد الكمي الفعالW.