The use of Bohm trajectories and the effective potential in probing quantum mechanical behavior in 2-D and spintronic sub-micron devices+

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ABSTRACT

We utilize an effective potential to reproduce Bohm (quantum) trajectory behavior using purely classical trajectories. The effective potential is a novel method for including certain quantum phenomena into classical simulations by projecting the non-zero dimensions of the quantum electron onto the classical background potential via a smoothing function. We show that the choice of smoothing length, which is related to the "size" of the electron, is crucial to the success of the method. Bohm trajectories are used to study the properties of novel spintronic devices. Our simple study illustrates that magnetic fields can be used to effectively reproduce electrical gates in a quantum point contact device as well as showing promise used as a logic type device.

Keywords: Effective Potential, Spintronics, Bohm Trajectories

1 INTRODUCTION

n-channel MOSFETs with effective gate lengths below 25 nm [1,2] have been fabricated, showing these feature sizes are feasible. In the sub-micron regime, quantum effects should dominate electron transport and one needs to worry about the effective size introduced by the wavelike nature of the carriers [3]. To aid in the development of such devices, efficient simulation methods need to be developed to gain insight into problems arising from quantum mechanical effects. One such method that can be used is the effective potential. Other methods to include such quantum effects tend to be complicated and computationally intensive. Moreover, they tend to be unattractive from an industrial point of view, since the most advanced industrial simulation tools currently used are still particle based. The effective potential is a good method for including quantum effects into semi-classical simulations. It incorporates the effective size of the electron into the problem and therefore can be used to introduce the non-point like behavior of quantized electrons into standard Monte Carlo techniques.

Spintronics is the use of magnetic fields and the utilization of an electron's quantum spin to realize logic devices. Certain materials lend themselves better to spintronics than others, due to large g factors. One such material is InSb, which has a g factor of −51. To illustrate these points, simulations of a tunable quantum point contact are presented which demonstrate the logic ability of spin-split systems [4]. The Stern-Gerlach experiment is also reproduced which demonstrates its ability to reproduce the effects of a electrically applied quantum point contact, further illustrating the ability of spintronics to replicate voltage device technologies. These effects will be shown with the aid of Bohm trajectories. Bohm trajectories are rarely used in the field of computation, but it will be shown that their usefulness provides valuable understanding to all quantum device problems.

2 METHOD

2.1 Bohm Trajectories

Following the de Broglie-Bohm model [5,6,7], electron trajectories are determined by a velocity field given by [8]:

$$\mathbf{v}(\mathbf{x},t)=\frac{\nabla S(\mathbf{x},t)}{m^*}=\frac{\hbar}{m^*}\frac{\mathrm{Im}\left(\psi^*\nabla\psi\right)}{|\psi|^2}, \tag{1}$$

or alternatively by the acceleration field:

$$\mathbf{a}(\mathbf{x},t)=-\frac{\nabla V(\mathbf{x},t)+\nabla Q(\mathbf{x},t)}{m^*}. \tag{2}$$

In the above, V is simply the classical potential that occurs in the original Hamiltonian. The additional term

$$\mathbf{Q}=\frac{\hbar^2}{2m^*}\frac{\nabla^2|\psi|}{|\psi|}, \tag{3}$$

is the Bohm potential.

2.2 Effective Potential

In an inhomogeneous system, the potential enters the Hamiltonian as

$$V=\int d\mathbf{r}V(\mathbf{r})n(\mathbf{r}) \quad . \tag{4}$$

If we assume that the charge has a non-local Gaussian form, this can be rewritten as [7]

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$$V = \int d\mathbf{r} V(\mathbf{r}) \sum_i n_i(\mathbf{r})$$
$$= \sum_i \int d\mathbf{r} \delta(\mathbf{r} - \mathbf{r}_i) \int d\mathbf{r}' V(\mathbf{r}') \exp\left(- \frac{|\mathbf{r} - \mathbf{r}'|^2}{\alpha^2} \right), \quad (5)$$

where the summation over i is a summation over the carriers themselves. The term in the primed integration is now the *effective potential*. As can be seen, this is a smoothing of the real classical potential, where the finite size of the electron wave packet defines the smoothing length, α, which is given by [3]

$$\alpha = \frac{\lambda_F}{\pi}. \quad (6)$$

There is also a mathematical connection between our effective potential and the Bohm potential that can be demonstrated by using a Taylor series expansion. Expanding eqn. (5) in a Taylor series in one dimension yields

$$V_{eff}(x) = \frac{1}{\sqrt{2\pi}\alpha} \int_{-\infty}^{\infty} V(x+\xi) e^{-\xi^2/2\alpha^2} d\xi$$
$$\cong \frac{1}{\sqrt{2\pi}\alpha} \int_{-\infty}^{\infty} \left[V(x) + \frac{\xi^2}{2} \frac{\partial^2 V}{\partial x^2} + \ldots \right] e^{-\xi^2/2\alpha^2} d\xi. \quad (7)$$

due to the symmetry of the Gaussian. Furthermore, the dependance of the density upon the potential is as a factor $exp(-\beta V)$. Using this along with some manipulation, we arrive at [11]

$$V_{eff}(x) = V(x) - \frac{2\alpha^2}{\beta\sqrt{n}} \frac{\partial^2 \sqrt{n}}{\partial x^2} + \ldots. \quad (8)$$

Within a factor of 2, the second term is now recognized as Bohm potential [6].

2.3 Self-Consistent Solutions

Our simulations were performed on a discrete lattice using a numerically stabilized variant of the transfer matrix approach to solve a finite difference version of the Schrödinger equation [9], which is then coupled to an iterative Poisson solver. For self-consistency, we assume an infinite wire. However, Poisson's equation is solved only in the active region, under the assumption that, at the entrance and exit slices of this region, the density satisfies

$$\frac{dn}{dx} = 0. \quad (9)$$

While only strictly true when the transmitted and reflected waves are subjected to damping, this assumption is sufficiently accurate to allow a convergent solution to Poisson's equation. It has been used previously in calculations of similar quantum wires [10,11]. To stabilize the calculation during the iteration to solve Poisson's equation, we fix the one-dimensional density at the entrance and exit slices [12,13]. The Fermi energy is allowed to adjust itself in order to keep the number of propagating modes constant via:

$$N = \frac{2}{\pi} \sum_{E_l < E_F} \left[\frac{2m^*(E_F - E_l)}{\hbar^2} \right]^{\frac{1}{2}}, \quad (10)$$

where N is the number density and E_l are the energy levels associated with the one-dimensional subbands.

The full self-consistent potential is a combination of the Hartree, exchange and correlation potentials. The Hartree potential is of course given by the solution to Poisson's equation:

$$\nabla^2 \phi(\mathbf{r}) = -\frac{e}{\varepsilon} \rho(\mathbf{r}) \quad (11)$$

where ρ, the density, is given by

$$\rho(\mathbf{r}) = n_{eq} - n(\mathbf{r}). \quad (12)$$

Here, n_{eq} is the average electron density of the entire structure and is included to represent, in an approximate way, the positive charge background created by the ionized donors that had given up the electrons that form the 2DEG.

3 RESULTS

3.1 Validating the Effective Potential

We intend to show that, in the case of a quantum wire constriction, there is a correspondence between the classical trajectories obtained using our effective potential and the quantum trajectories obtained using the Bohm method. We begin by solving Schrödinger's equation assuming hard-wall boundaries and including the self-consistent solution for the potential [13]. Using Eqn. (1), the Bohm trajectories are calculated for this case, and are plotted against the quantum potential in Fig. 1(a). Note that none of the Bohm trajectories cross. This is expected since the velocity field is uniquely defined for each value of x [6,7]. Note also that the Bohm trajectories are bent around the constriction, a consequence of the diffraction that the electron waves are subjected to when exiting the constriction. Note that the original Fermi energy assumed in the hard-wall case was 18.84 meV, which gives rise to 5 propagating modes for the given dimensions in this wire, while the constriction allows only two propagating modes. When we include the self-consistency, the net self-consistent potential is negative [14]. This is a result of correlation in the system. The tendency is for the density in

the structure to increase, giving rise to more propagating modes. However, as discussed previously, since we constrain the number of modes and the density to be constant, we must adjust the local Fermi energy after each iteration of the Schrödinger equation. Once the iteration has converged, the Fermi energy in the device is 5.46 meV. Given the self-consistent potential, we can use eqn. (7) to calculate the effective potential. The result of this convolution is shown as the background to Fig. 1(b). 4 propagating modes result in the wire in this case, which is less then the 5 modes previously seen. Note also that the effective potential yields a narrower constriction and a wider potential barrier wall. From Fig. 1(b) we also can see that the general flow of the Bohm trajectories is similar to the previous result. However, the trajectories are more meandering, which to a certain extend suggests the quantum behavior has been amplified.

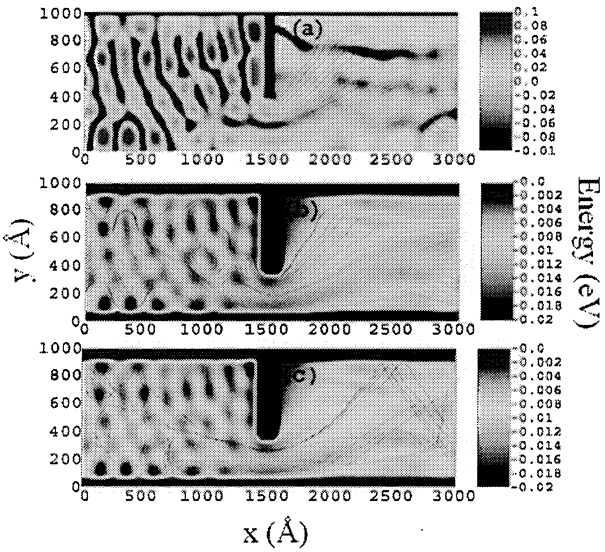

Figure 1: (a) Bohm trajectories are plotted on top of quantum + self-consistent potential; (b) Bohm trajectories are plotted on top of the effective potential; (c) Classical trajectories are plotted on top of the effective potential.

The goal of this is ultimately to "reproduce" the Bohm trajectories using purely classical mechanics. To illustrate this in this system, we now calculate classical trajectories directly from the effective potential, using the classical acceleration:

$$\mathbf{a}(\mathbf{x},t) = -\frac{\nabla V_{eff}(\mathbf{x},t)}{m^*}, \qquad (13)$$

where we have replaced the self-consistent and quantum potential with just the effective potential. In Fig. 1(c), classical trajectories have been plotted for a smoothing length, α, of 2 nm. The smoothing length calculated from eqn. (6) is roughly equal to 2 nm for the given Fermi energy, which corresponds to the case shown in Fig. 1(c). In contrast to the Bohm trajectories, which reflected the diffraction effect produced by the constriction, when the smoothing length is not correct, the resulting classical trajectories show little bending towards the upper boundary of the wire [13]. Smoothing with too small a value of α produces more bending, but not enough to really reproduce the diffraction effect. Over smoothing over compensates for the effective size of the electron and results in a system that is almost closed. However, if the correct smoothing length is used, as shown in Fig. 1(c), we are able to generate trajectories that have the desired properties to mimic the quantum system [13].

3.2 Spintronics

We now examine spin effects. It is well known that a quantum point contact (QPC) is tunable. That is, different biases allow more or less electrons to propagate through the QPC. However, it is also possible to use magnetic fields to tune a QPC [4]. The basic concept behind this is that when a magnetic field is applied to a semi-conductor material, spin-splitting occurs.Instead of one degenerate energy level, we now have two energy levels, one with higher and one with lower energy. Following methods used in previous studies [15], we looked at two very interesting cases, the first being a standard QPC, and the second being a magnetically applied QPC.

Results of a magnetically tunable QPC can be seen in Fig 2. Again we use Bohm trajectories to further understand the problem at hand. In Fig 2., it is clear that if we bias the QPC such that we are on the 0/1 mode transmission transition, applying a magnetic field will cause one spin-state to have propagating density while the other shows no propagation, which we can think of of logic 0 and logic 1. This is also shown by the Bohm trajectories where no trajectories flow through the device at the lower energy.

It is also interesting to look at what extent magnetic fields and electron spins can be used for real device applications. One famous experiment regarding electron spins is the Stern-Gerlach experiment, in which a non-uniform magnetic field, which has the form of a linearly varying vector potential, is used to separate electrons with different spins. We implemented this magnetic field and the results are seen on the left hand side of Fig 3. As a visual aid, we use Bohm trajectories to show that the spin up and spin down states force the electrons to either move up or down through the device. What is interesting about these results is that they can be qualitatively reproduced using quantum point contacts, which are shown on the right of Fig 3. Therefore, what essentially has occured is that the magnetic field generates a magnetic force on the electrons which is similar to the confinement forces generated by the QPC. While applications of spin devices are still in their infancy, novel results such as these can be seen as a stepping stone for a larger and broader approach to spintronic devices.

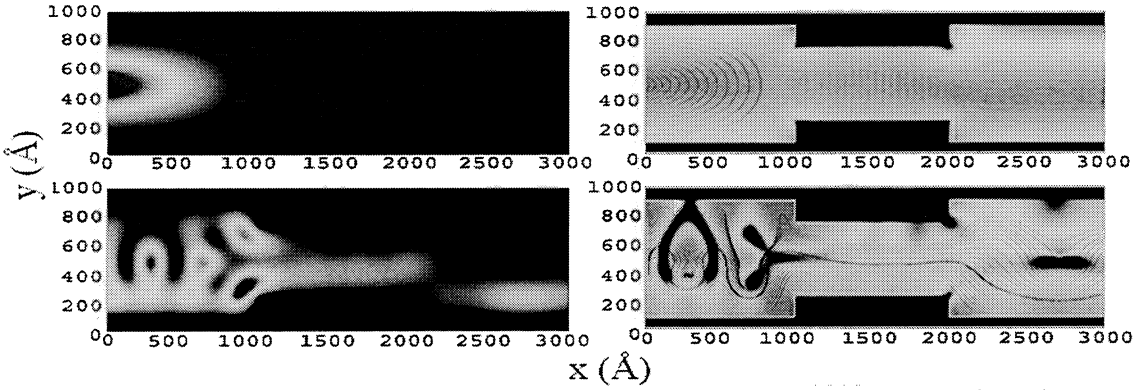

Figure 2: LEFT: Density in the device. The top figure is the spin down state, the bottom picture is the spin up state. RIGHT: The corresponding Bohm trajectories plotted against the quantum potential

4 CONCLUSION

We have shown that by using an appropriate effective potential, obtained by convolving the electrostatic potential with a Gaussian, we can replicate certain quantum behavior by using classical physics. Significantly, in contrast to the Bohm potential method, one is not required to actually solve Schrödinger's equation in all situations using this method. While densities entering into the Poisson equation were obtained quantum mechanically in this case (necessitated by the strong quantization in this particular quasi one dimensional system), more generally, one can obtain good results simply by convolving the potentials obtained from a particle-based Poisson solver. This effective potential approach has already been successfully incorporated into a particle-based ensemble Monte Carlo simulation of a silicon MOSFET [16]. Furthermore, it has been shown that the use of magnetic fields can be used to not only produce viable logic type devices, but also to replicate current/voltage type devices. These types of devices (spintronics) are a new device technology that is currently getting much attention. In order to fully understand these devices, quantum simulation is required. However, the use of Bohm trajectories in the analysis of these devices has again proved to be very useful and provide insight.

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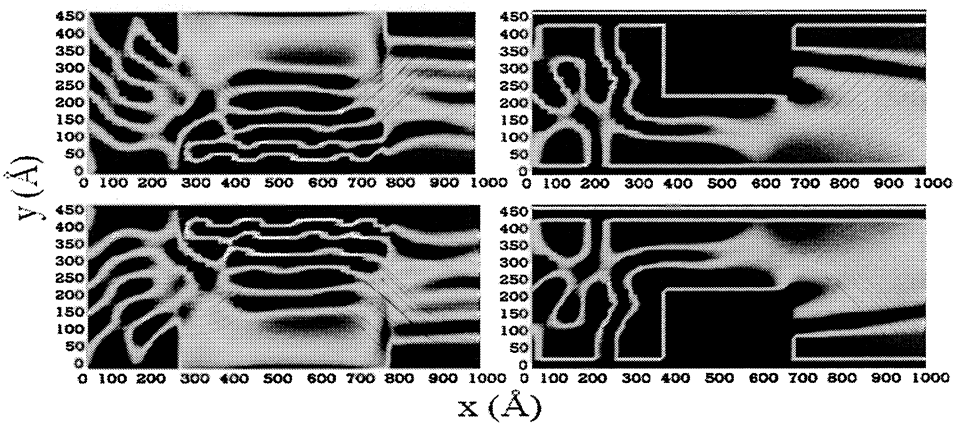

Figure 3: LEFT: Bohm trajectories plotted against the quantum potential for the spin up and spin down states for a Stern Gerlach magnetic field. RIGHT: Bohm trajectories plotted against the quantum potential for a top and bottom quantum point contact