Electrons in Semiconductors: How Big Are They?

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1. Introduction

Electron transport in nanoscale semiconductor devices is of increasing interest as CMOS is scaled toward 10-20 nm characteristic lengths. In this regime, the transport is expected to be dominated by quantum effects throughout the active region, even though quantum transport is not well established within a consistent conceptual framework [1]. Nevertheless, several approaches to simulation of semiconductor devices have appeared in which the transport is handled quantum mechanically [2]. In these small structures, one must begin to worry about the effective size of the carriers themselves. In recent publications, at least one author has estimated that the effective size should be given by the inelastic mean free path (called the *coherence length*) [3,4]. This size can be many 10s of nanometers, and such a definition leads to a great many inconsistencies. Indeed, in some ballistic quantum dots, the inelastic mean free path can be hundreds of nanometers, much larger than the dot itself [5]. As these dots contain many hundreds of electrons, the above definition cannot be reconciled with the experimental facts, and a smaller size must be considered. In this paper, the arguments for various sizes will be considered for electrons in semiconductor devices. In particular, in the quasi-two-dimensional electron gas of the ballistic quantum dots, it will be argued that the effective size of the electron packet is only λ_F/π, a value providing an almost minimum uncertainty packet. This size also reflects the "squeezing" of the packet in two dimensions as the carrier density is increased (and resulting in a greater extent in the third dimension).

2. Common Considerations

In general, the idea behind the semi-classical picture, which has been heavily utilized in device modeling and in ensemble Monte Carlo treatments of electron transport, is that the dephasing length l_ϕ is much smaller than the size scale L of the device. (Here, l_ϕ is the inelastic mean free path and will also be referred to as the coherence length, but this is different from the often referred to coherence length in disorderd materials [6].) Thus, one may describe the electron in terms of its position $\mathbf{r}_c$, but the extent of the wave packet is given by l_ϕ [3,4]. The rationale lies in the fact that the electron is mainly described as a plane wave state of momentum $p = \hbar k$, and it is argued this plane wave remains coherent over a distance of the order of the inelastic mean free path. By coherent, it is generally meant that the plane wave is a single entity over this length, and it is impossible to describe where the electron actually is located by this wave. Hence, the size is equated to the coherence length. If the phase breaking process within the active device is characterized by an imaginary part of the Hamiltonian, given by $i\hbar/2\tau_\phi$, then *for weak phase breaking*, the wave vector contains an imaginary term $i/2l_\phi$. This term causes the probability to decay over the phase breaking length, and this becomes an effective localization length.

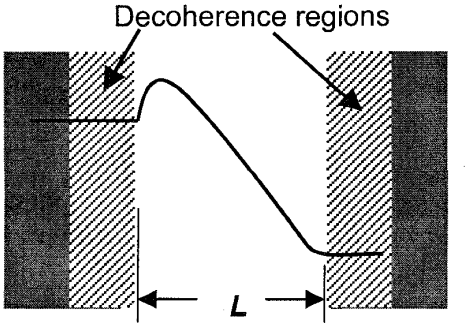

Fig. 1 A conceptual device under bias. The source is at the left and the drain at the right, as indicated by the two gray areas, which may be considered to be the "contacts." The areas to the left and right of the traditional active length L, indicated here as the decoherence regions, *must now be considered part of the active device.*

The scattering-induced broadening of the energy spectrum is given by $\delta E \approx \hbar v/2l_\phi = \hbar/2\tau_\phi$. This description can be considered to arise from the assertion that the uncertainty in position is defined by the packet size l_ϕ as $\Delta p \approx \hbar/2l_\phi$, and $\delta E \approx [E(p+\Delta p) - E(p-\Delta p)]/2 \approx p\Delta p/m \approx \hbar v/2l_\phi$. Even though this argument is consistent with the above introduction of the coherence length, this is a misleading argument. Indeed, when the description of the

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electron is a plane wave in momentum space, it is difficult to talk about spatial variation at all, a point to which we return in the next section. This argument assumes that a momentum uncertainty *automatically* relates to an energy uncertainty, which is not the case.

First, let us consider the prototypical device as an active region of length L, bounded by two *contact* regions in which the electrons must lose their coherence completely (see Fig. 1). We have argued earlier about the need to properly introduce decoherence effects for the carriers in order to bound the device properties within the active region [1]. If the decoherence is introduced by adding an imaginary potential term to the Hamiltonian only in the contact regions, the size of this potential is inversely proportional to the phase coherence lifetime τ_ϕ. For rapid decoherence, one needs a very large imaginary potential (short phase-breaking time) which gives rapid damping of the electron wavefunction within the contact (to cause the wave function of a realistic device to de-cohere over 1 nm in the contact requires $\tau_\phi \sim 0.01$ ps, which provides a barrier of order 3 V). In essence, *this leads to bound states in the active region of the device*, and the momentum is quantized into values given approximately by

$$k_n \approx \pm \frac{n\pi}{L} \quad . \tag{1}$$

This leads to an uncertainty in the momentum of $\Delta p \approx n\hbar\,\pi/L$, but there is no energy spread within the active region, as the energy levels are quite sharp. Indeed, *the simple presence of a momentum uncertainty does not imply a spread in the energy for that state.* For our bound state, the energy level is quite sharp, and the uncertainty arises from the two discrete values that the momentum may take.

One may summarize the above point with the observation that if the future small device is smaller than the coherence length, $l_\phi > L$, then the required decoherence in the contacts effectively pins the coherence length to the actual length (e.g., $l_\phi = L$). This has been known for quite some time in the study of disordered mesoscopic devices [6]. Within the active region, then, there is little dephasing, and little broadening of the energy levels that may arise. Because the wave function is now set by the bound states of the active region, their extent is not directly related to the coherence length itself, but to the device length; for the above situation, we can actually find the uncertainty in position as

$$\Delta x \approx \frac{L}{\sqrt{12}} \sqrt{1 - \frac{6}{n^2\pi^2}} \quad . \tag{2}$$

We will use this form below.

3. The Two-Dimensional Electron Gas

The problem, as discussed above, is that these treatments consider an *isolated* plane wave. In actual fact, the totality of the electron gas composes a range of plane waves, or momentum states. In order to describe the packet in real space, one must account for the contributions to the wave packet from all occupied plane wave states [7]. That is, the states that exist in momentum space are the Fourier components of the real-space wave packet. If we want to estimate the size of this wave packet, we must utilize all Fourier components, not just a select few. At low temperature in a 2D gas, all states up to the Fermi energy are occupied, and the Fermi wave vector is defined by the carrier density

$$k_F = \sqrt{2\pi n_s} \quad . \tag{3}$$

This means that, in the momentum representation, all states up to this value are occupied, or

$$\phi_m(k) = \frac{\sqrt{2\pi}}{k_F} u_0(k_F - k) \quad , \tag{4}$$

where u_0 is the Heavyside function. From this momentum space representation, we can now define a wave packet (centered at the origin) by taking the Fourier transform of (4), which leads to

$$\psi(r) = \frac{1}{r}\sqrt{\frac{2}{\pi}} J_1(k_F r) \quad . \tag{5}$$

These wave functions may now be manipulated to show that (it must be remembered that **k** and **r** are really two-dimensional vectors in this calculation)

$$\Delta p = \frac{\hbar k_F}{\sqrt{2}} \quad , \quad \Delta r = \frac{1}{k_F} \quad . \tag{6}$$

Hence, the spatial extent of the real-space wave packet can be estimated as the full-width at half-maximum value, or twice the uncertainty in position, which leads to

$$\delta r = 2\Delta r = \frac{2}{k_F} = \frac{\lambda_F}{\pi} \quad . \tag{7}$$

The result (7) is the central result for the two-dimensional electron gas, and tells us that the spatial extent of the wave packet is quite small and related to the DeBroglie wavelength of the electron and not to its coherence length.

One assuring feature of the value (7) for the size of the electron wave packet is that it is reduced as the electron density is increased. An increase of the density leads to an increase of k_F, which reduces the value in (7). On the other hand, the total volume of space occupied by the electron is relatively constant, so that the reduction in the two-dimensional plane must be accompanied by an expansion in the normal plane, which moves the electrons to a higher level in the confinement potential of this third dimension. This means a higher Fermi energy, which is consistent with the increased density. A similar "squeezing" of the wave functions in two dimensions, resulting in elongation in the

third dimesion, has been discussed by Kubo *et al.* [8] for the wave functions of carriers in a magnetic field. This also leads to the interesting result that the amount of area occupied by each electron in real space is approximately one-half of that given by the reciprocal of the electron density. We return to the effect of the other carriers on the wave packet below.

4. Bound States

In the case of bound states, the argument of Sec. 2 seems to make more sense; that is, if the particle is confined within a region of size L, then certainly one might think that the uncertainty (and therefore the electron size) is of this same order, since the particle is delocalized over this extent. In fact, this does not follow at all, as we must distinguish between the spatial extent of the wave function and the actual uncertainty in the electron's position, which we connect to it's size. We can demonstrate this with the bound states of Sec. 2 for (approximately) hard-wall confinement. The value of Δx in (2) is for a single pure state, while our dense electron gas has many occupied states. Hence, we must sum $(\Delta x)^2$ over these states, which leads to

$$(\Delta x)^2 \approx \frac{L^2}{12} - \frac{L^2}{2\pi^2}\sum_{n=1}^{N}\frac{1}{n^2} = \frac{L^2}{2\pi^2}\Psi'(N+1) \ , \qquad (8)$$

where $\Psi(z)$ is the digamma function, and N is the highest occupied state, corresponding to the Fermi energy. The derivative of the digamma function in (8) can be approximated for large N, and

$$(\Delta x)^2 \approx \frac{L^2}{2\pi^2 N} \ , \qquad (9)$$

so that the size of the electron in this structure is approximately $(2/N)^{1/2}L/\pi$. This is considerably smaller than the confinement region, if there are a large number of electrons in the active volume.

It is obvious that the higher-lying wave functions, which contribute to the total wave function, are rather sharply peaked, which leads to electrons remaining at nearly precise points. It is this factor which leads to the small value of the uncertainty in position. Again, increasing the electron density raises the value of N, and this squeezes the electrons within the confinement region.

5. The Nondegenerate 3D Semiconductor

For nondegenerate semiconductors, the distribution of allowed momentum states is defined the Maxwell-Boltzmann distribution. This brings the temperature into the problem. As the temperature is increased, higher momentum states become occupied as the distribution spreads under the influence of the temperature. A wider momentum space distribution means a tighter distribution in real space for the electron wave packet.

As previously, we consider the momentum space distribution as a description of the occupied plane wave states which contribute to the electron wave packet. The normalized momentum space distribution may then be defined to be

$$\varphi(k) = 2\left(\frac{\lambda_D}{2}\right)^{3/4} \exp\left(-\frac{\lambda_D^2 k^2}{4\pi}\right) , \qquad (10)$$

where

$$\lambda_D = \sqrt{\frac{2\pi\hbar^2}{m^* k_B T}} \qquad (11)$$

is the thermal DeBroglie wavelength [9]. We can now Fourier transform this to obtain the real space wave packet

$$\psi(r) = \frac{\pi}{\left(\sqrt{2}\lambda_D\right)^{3/2}} \exp\left[-\frac{\pi r^2}{\lambda_D^2}\right] \ . \qquad (12)$$

We then find that the effective size of the electron packet is given by

$$\delta r \sim \sqrt{\frac{3}{8}}\lambda_D \sim 0.61\lambda_D \ . \qquad (13)$$

As expected, the size of the electron's wave packet is inversely proportional to the temperature, through the thermal DeBroglie wavelength.

One interesting aspect of this last result is that there is no density dependence in the thermal wavelength, and hence in the electron wave packet size. While this may seem strange at first sight, it is quite natural, as the non-degenerate limit is one of a dilute electron gas. When the density becomes sufficiently large that this limit is no longer appropriate, then the distribution changes character to that of the Fermi-Dirac distribution. In the latter situation, the density dependence re-appears through the importance of the Fermi wavelength, rather than the thermal wavelength. However, this should not be construed to mean that the other electrons have no effect on the size of the packet.

6. Discussion

The core principles of the ensemble Monte Carlo simulation is the connection of each pseudo-particle to a "typical" electron, so that issues about the size of the electron become important in the simulation of ultrasmall devices with their corresponding high carrier densities. We can estimate the above sizes with some simple structures. For the two-dimensional electron gas in a Si MOSFET, or for that in a GaAs HEMT, the typical size is about 8 nm (this depends only upon the density and not the electron mass, and the density has been taken to be 10^{12} cm^{-2}). On the other

hand, the thermal DeBroglie wavelength at room temperature in Si is about 4.3 nm, and this will be reduced at the higher electron temperatures expected in active devices. While these are not sizes of concern for today's semiconductor devices, they certainly are comparable to the sizes envisioned within the next decade. In real devices, however, there is also a consideration about the fact that the carrier density and the carrier temperature are not homogeneous quantities. Rather, these vary with position within the device. The results obtained here suggest that the effective "size" of the electron is given either by its temperature (in a non-degenerate situation) or its density (in a degenerate situation). Consequently, the situation arises in actual devices that *the effective wave packet size for the electron actually changes with position* throughout the device! Moreover, the interaction of this wave packet with a scattering "center," such as e.g. an impurity, is also a nonlocal event—some parts of the wave packet are closer to the impurity than others. With barriers, the leading portion of the packet arrives, and begins interacting with the barrier, well before the trailing part of the packet [10-12].

The above considerations mean that the size of the electron wave packet is a result of the interactions of its environment. This environment includes not only the confining potentials, but also the effective confinement provided by the repulsive forces of the other particles, whether electrons or impurities. The shape and size of the wave packet is a balance between these environmental forces and the self-force provided by the diffusive nature of the Schrödinger equation. This latter is often evaluated from the shape of the wave packet by e.g. a generalized quantum potential [13]. Since the environment changes, through changes in the confining potentials and the local carrier densities, the shape and size of the wave packet are quantities that vary throughout a real device. Moreover, the interaction with the distributed image near barriers means that the shape of the packet may well be significantly deformed at these points. The upshot of this is that any simulations of quantum effects must be carried out with the full many-electron Hamiltonian and the real environment must appear through self-consistent potentials. Moreover, the contacts, and importantly the transition regions where decoherence is expected to occur, become real parts of the device and must be considered with the entire quantum mechanical problem.

This means that simulations such as Monte Carlo techniques will have to deal with both the finite size of the electron, its distributed and deformable shape, as well as the actual phase of the electron on its trajectory. Indeed, the previous success of Monte Carlo suggests that one might hope to find a trajectory-based Monte Carlo, non-deterministic picture for the Schrödinger equation and/or the density-matrix Liouville equation *if these problems are overcome.* Even so, the nonlocal nature of quantum mechanics provides further complications, and approaches such as those of the Wigner function offer some hope [14,15]. However, the clear point is that it will no longer be adequate to consider the electron as a point particle in these future device simulations, and new approaches to kinetic pictures for transport are needed [1].

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