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UTILIZATION OF QUANTUM DISTRIBUTION FUNCTIONS FOR ULTRA-SUBMICRON
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Résumé - La représentation de Wigner est considérée comme une méthode utilisable pour décrire les phénomènes de transport quantique dans la physique des dispositifs submicroniques. La fonction de distribution de Wigner est rappelée ici et sa non unicité est discutée, ainsi que sa généralisation aux autres fonctions de distribution quantique. L'équation du mouvement pour la fonction de distribution de Wigner est décrite et un nouveau résultat, les moments de cette équation du mouvement, est obtenu. On montre que les équations du moment contiennent des corrections quantiques par rapport aux équations classiques et que ces termes quantiques ne sont pas négligeables lorsque les longueurs de transit des porteurs sont de l'ordre de la longueur d'onde de de Broglie.

Abstract - The Wigner representation is considered as a method for describing quantum transport phenomena in connection with submicron device physics. The Wigner distribution function is reviewed, its non-uniqueness discussed; its generalization to other quantum distribution functions is examined. The equation of motion for the Wigner distribution function is described and a new result, the moments of this equation of motion, is derived. It is shown that the moment equations contain quantum corrections to the classical moment equations; these quantum terms are seen to be non-negligible when the carrier transit lengths are of the order of the particle deBroglie wavelength.

Introduction - As semiconductor technology continues to pursue the scaling-down of IC device dimensions into the submicron (less than ten thousand Angstroms) regime, many novel and interesting questions will emerge concerning the physics of charged particles in semiconductors. One of the more important topics to be considered is that of the appropriate transport¹ picture to be used for a given spatial and temporal regime. Moreover, from the point of view of device physics, it is most desirable to have a microscopic description of semiconductor transport which is computationally manageable or at least amenable to phenomenological treatment so that its properties can be meaningfully incorporated into device simulations. In this paper attention is focused on a useful transport methodology for the ultra-submicron regime. At present, electronic devices with transit lengths in the ultra-submicron region are coming to fruition due to the advent of MBE² processing so that the need for an appropriate description of transport in this regime is indeed imperative.

Semiconductor transport in the ultra-submicron regime approaches the category of quantum transport. This is suggested by the fact that within the effective mass approximation the thermal deBroglie wavelength for electrons in semiconductors (See Fig. 1) is of the order of ultra-submicron dimensions. Whereas classical transport

physics is based on the concept of a probability distribution function which is defined over the phase space of the system, in the quantum formulation of transport physics, the concept of a phase space distribution function is not possible inasmuch as the non-commutation of the position and momentum operators (the Heisenberg uncertainty principle) precludes the precise specification of a point in phase space. However, within the matrix formulation of quantum mechanics, it is possible to construct a "probability" density matrix which is often interpreted as the analog of the classical distribution function.

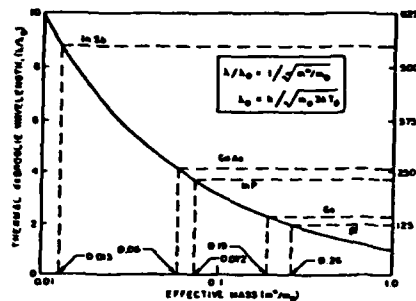


Fig. 1: Thermal deBroglie wavelength versus effective mass.

There is yet another approach to the formulation of quantum transport based on the concept of the Wigner distribution function (WDF)³. This formalism is particularly attractive for use in ultra-submicron device transport in that it contains all of the quantum mechanical information about the state of the system yet has elements of the classical picture implicitly built in. Thus, the intent of this study is to explore the potential usefulness of the WDF as well as other possible quantum distribution functions for describing quantum (ultra-submicron) device transport in semiconductors. To this end we first review the salient features of the WDF and then discuss a new result, the derivation of the first three quantum moment equations using the WDF. It is shown that the moment equations contain quantum corrections to the classical moment equations; these quantum terms are non-negligible when the transit lengths are of the order of the carrier deBroglie wavelength.

Wigner Distribution Function - The Wigner distribution function³ is generally defined in terms of all the generalized coordinates and momenta of the system as

$$P_w(x_1, \dots, x_n, p_1, \dots, p_n) = \frac{1}{(2\pi\hbar)^n} \int_{-\infty}^{\infty} dy_1 \dots dy_n \psi^* \left(x_1 + \frac{y_1}{2}, \dots, x_n + \frac{y_n}{2} \right) \psi \left(x_1 - \frac{y_1}{2}, \dots, x_n - \frac{y_n}{2} \right) e^{i(p_1 y_1 + \dots + p_n y_n)/\hbar} \quad (1)$$

However, for simplicity here in this paper we discuss the properties of a single coordinate and momentum WDF:

$$P_w(x, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \psi^* \left(x + \frac{y}{2} \right) \psi \left(x - \frac{y}{2} \right) e^{ipy/\hbar} \quad (2)$$

where $\psi(x)$ represents the state of the system in the coordinate representation. Although we will be treating the WDF for the special case of pure states, the adaptation of this formalism to include mixed states is accomplished through the generalization

$$P_w(x, p) = \sum_n P_n \left[\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \psi_n^* \left(x + \frac{y}{2} \right) \psi_n \left(x - \frac{y}{2} \right) e^{ipy/\hbar} \right] \quad (3)$$

where P_n is the probability to be in state "n". (For example, for a system in contact with a heat bath at constant temperature, $P_n = e^{-E_n/kT}$.)

The distribution function of Eq. (2) has interesting properties in that integration over all momenta leads to the probability density in real space; while integration over all coordinates leads to the probability density in momentum space³:

$$\int_{-\infty}^{\infty} P_w(x, p) dp = \psi^*(x) \psi(x) \quad \int_{-\infty}^{\infty} P_w(x, p) dx = \phi^*(p) \phi(p) \quad (4a)$$

where

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx \quad (4b)$$

It follows from Eqs. (4a,b) that, for an observable $w(x,p)$ which is either a function of the momentum operator alone, the position operator alone, or any additive combination therein, the expectation value of the observable is given by³

$$\langle w \rangle = \iint w P_w(x, p) dx dp$$

which is analogous to the classical expression for the average value. Herein lies the interesting aspect of the WDF; it is possible to transfer many of the results of classical transport theory into quantum transport theory by simply replacing the classical distribution by the Wigner distribution function. However, unlike the density matrix, the WDF itself cannot be viewed as the quantum analog of the classical distribution function since it is generally non-positive definite and non-unique.

Further resemblance of the Wigner distribution function to the classical distribution function is apparent by examining the equation of time evolution for $P_w(x,p)$. Upon assuming that $\psi(x)$ in Eq. (2) satisfies the Schrodinger equation for a system with Hamiltonian $H = p^2/2m + V(x)$, it has been shown that P_w satisfies the equation³

$$\frac{\partial P_w}{\partial t} + \frac{p}{m} \frac{\partial P_w}{\partial x} + \theta \cdot P_w = 0 \quad (5)$$

where

$$\theta \cdot P_w = - \frac{2}{\hbar} \sum_{n=0}^{\infty} (-1)^n \frac{(\hbar/2)^{2n+1}}{(2n+1)!} \frac{\partial^{2n+1} V(x)}{\partial x^{2n+1}} \frac{\partial^{2n+1} P_w(x,p)}{\partial p^{2n+1}} \quad (6)$$

Alternately, $\theta \cdot P_w$ can be expressed as $\theta \cdot P_w = - \frac{2}{\hbar} \left[\sin \frac{\pi}{2} \left\{ \frac{\partial}{\partial x} \frac{\partial}{\partial p} \right\} \right] V(x) P_w(x,p)$ where it is understood that the position gradient operates only on the potential energy, $V(x)$. In the limit $\hbar \rightarrow 0$, $\theta \cdot P_w = - \frac{\partial V}{\partial x} \frac{\partial P_w}{\partial p}$ so that Eq. (6) reduces to the classical collisionless Boltzmann equation.

The Wigner distribution function is not the quantum analog of the classical distribution function⁴ as evidenced by the fact that it is generally non-positive definite and non-unique. The non-uniqueness is clearly evident by noting that many quantum distribution functions can be constructed which obey the sum rules of Eqs. (4a,b). One other distribution function which we have examined in detail is^{4,5}

$$P_{w_1} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \psi^*(x) \psi(x-y) e^{ipy/\hbar} = \frac{1}{\sqrt{2\pi\hbar}} \psi^*(x) e^{ipx} \phi(p) \quad (7)$$

where $\phi(p)$ is given by Eq. (4b). In actuality the non-uniqueness and non-positive definiteness of the Wigner distribution function can be traced to the non-commutation of the position and momentum operators.

Moment Equations - In this section, we derive the first three moments of a "Wigner-Boltzmann"-like transport equation,

$$\frac{\partial P_w}{\partial t} + \frac{p}{m} \frac{\partial P_w}{\partial x} + \theta \cdot P_w = \left(\frac{\partial P_w}{\partial t} \right)_{\text{coll.}} \quad (8)$$

This equation was constructed to include an ad-hoc collision term which may not necessarily express the same phenomenology as that of the classical Boltzmann transport equation, since P_w is not a true probability distribution function. These problems are conceptually reduced when dealing with moments in a relaxation approximation. The moment equations are obtained by multiplying Eq. (8) by an appropriate function of momentum, $\tilde{\phi}(p)$, and then integrating over all momenta to obtain:

$$\frac{\partial \langle \tilde{\phi} \rangle}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} \langle \tilde{\phi} p \rangle - \sum_{n=0}^{\infty} \left(\frac{\hbar}{2i} \right) \frac{1}{(2n+1)!} \frac{\partial^{2n+1}}{\partial x^{2n+1}} V(x) \int \tilde{\phi}(p) \frac{\partial^{2n+1}}{\partial p^{2n+1}} P_w dp = \langle \tilde{\phi} \left(\frac{\partial P_w}{\partial t} \right)_{\text{coll.}} \rangle \quad (9)$$

where $\langle \rangle$ refers to an integration over momentum. In making the assumptions that $\tilde{\phi}(p)$ be an analytic function of momentum and that $P_w(x,p)$ vanish at the momentum limits, it follows that

$$\int \tilde{\phi}(p) \left(\frac{\partial^{2n+1}}{\partial p^{2n+1}} P_w \right) dp = (-1)^{2n+1} \int \left(\frac{\partial^{2n+1}}{\partial p^{2n+1}} \tilde{\phi}(p) \right) P_w dp \quad (10)$$

and that Eq. (9) becomes

$$\begin{aligned} \frac{\partial \langle \tilde{\phi} \rangle}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} \langle \tilde{\phi} p \rangle \\ + \sum_{n=0}^{\infty} \left(\frac{\hbar}{2i} \right)^{2n} \frac{1}{(2n+1)!} \left(\frac{\partial^{2n+1}}{\partial x^{2n+1}} V(x) \right) \langle \frac{\partial^{2n+1} \tilde{\phi}}{\partial p^{2n+1}} \rangle = \langle \tilde{\phi} \left(\frac{\partial P_W}{\partial t} \right)_{\text{coll.}} \rangle \end{aligned} \quad (11)$$

For specific values of $\tilde{\phi}(p) = p^0, p$, and $\frac{p^2}{2m}$, Eq. (11) becomes

$$\frac{\partial \rho}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} \langle p \rangle = 0, \quad (12a)$$

$$\frac{\partial \langle p \rangle}{\partial t} + \frac{1}{m} \frac{\partial}{\partial x} \langle p^2 \rangle + \rho \frac{\partial V}{\partial x} = \langle p \left(\frac{\partial P_W}{\partial t} \right)_{\text{coll.}} \rangle, \quad (12b)$$

$$\frac{1}{2m} \frac{\partial}{\partial t} \langle p^2 \rangle + \frac{1}{2m^2} \frac{\partial}{\partial x} \langle p^3 \rangle + \frac{\langle p \rangle}{m} \frac{\partial V}{\partial x} = \langle \frac{p^2}{2m} \left(\frac{\partial P_W}{\partial t} \right)_{\text{coll.}} \rangle \quad (12c)$$

where upon reduction

$$\langle p^n \rangle = \left(\frac{\hbar}{2i} \right)^n \sum_{j=0}^n (-1)^j \frac{n!}{(n-j)! j!} \frac{\partial^j \psi^*(x)}{\partial x^j} \frac{\partial^{n-j} \psi(x)}{\partial x^{n-j}} \quad (13)$$

thereby showing the dependence of $\langle p^n \rangle$. For $n=0,1,2,3$ we show $\langle p^n \rangle$ explicitly:

$$\langle p^0 \rangle = \psi^* \psi, \quad \langle p^1 \rangle = \frac{\hbar}{2i} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \quad (14a)$$

$$\langle p^2 \rangle = \left(\frac{\hbar}{2i} \right)^2 \left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - 2 \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi^*}{\partial x^2} \psi \right) \quad (14b)$$

$$\langle p^3 \rangle = \left(\frac{\hbar}{2i} \right)^3 \left(\psi^* \frac{\partial^3 \psi}{\partial x^3} - 3 \frac{\partial \psi^*}{\partial x} \frac{\partial^2 \psi}{\partial x^2} + 3 \frac{\partial^2 \psi^*}{\partial x^2} \frac{\partial \psi}{\partial x} - \frac{\partial^3 \psi^*}{\partial x^3} \psi \right) \quad (14c)$$

Note that use of Eqs. (14a) in Eq. (12a) results in the correct quantum mechanical continuity equation.

In order to see the transition between the quantum and classical regimes, we invoke a wavefunction of the form $\psi(x,t) = A(x,t) e^{iS(x,t)/\hbar}$, and so,

$$A^2(x,t) \equiv \psi^* \psi = \rho(x,t) \quad , \quad \frac{1}{m} \frac{\partial S(x,t)}{\partial x} = v(x,t) \quad (15)$$

where $\rho(x,t)$ is the probability density and $v(x,t)$ is the ensemble velocity. Inserting the wavefunction of Eq. (15) into Eq. (14) results in

$$\langle p^0 \rangle = \rho(x,t) \quad \langle p^1 \rangle = mv\rho \quad (16a)$$

$$\langle p^2 \rangle = (mv)^2 \rho - \frac{\hbar^2}{4} \rho \frac{\partial^2}{\partial x^2} \ln \rho \quad (16b)$$

$$\langle p^3 \rangle = (mv)^3 \rho - \frac{\hbar^2}{4} \rho \left\{ 3mv \frac{\partial^2}{\partial x^2} \ln \rho + \frac{\partial^2}{\partial x^2} (mv) \right\} \quad (16c)$$

It is evident from Eq. (16) that the terms possessing an explicit dependence on " \hbar " are the quantum corrections to the classical momentum-density moments. Furthermore, insertion of these momentum-moments into Eqs. (12) results in a set of moment equations which contain explicit quantum corrections as well. Of course, as $\hbar \rightarrow 0$, these moment equations reduce to the classical, zero temperature, moment equations.

The logarithmic derivative term appearing in Eqs. (16) is not uncommon; such a term appears in the real part of the Schrodinger equation when the wavefunction associated with Eq. (15) is used⁶. In the limit where this term is negligible, the Schrodinger equation goes over to the Hamilton-Jacobi equation.

We have made order of magnitude estimates of the strengths of the quantum correction term appearing in Eq. (16). Using a Gaussian spatial variation for $\rho(x)$, and a thermal ensemble value for $\frac{1}{2}mv^2$, typical of central valley GaAs electrons, we find that the quantum correction is substantial for widths of the order of 80 Å.

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