A Critical Examination of the Basis of Macroscopic Quantum Transport Approaches

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The density gradient, effective potential and smooth quantum hydrodynamic approaches have been proposed in recent years as promising candidates for the efficient simulation of quantum effects in semiconductor devices [1-3]. The microscopic justifications for these three approaches are based on, in that order, very specific approximations to the equilibrium Wigner function, the average carrier energy and the equilibrium density matrix. The validity of these approximations is however very questionable in realistic devices containing material heterojunctions. For example, the density gradient method is derived from the equilibrium Wigner function for a slowly varying device potential, but it is often applied to model MOS inversion layer transport near an abrupt barrier where the approximation is invalid. Furthermore, attempts to extend it to the treatment of tunneling phenomena [4,5] have been made for which it is expected to have even lesser applicability.

In this work, we directly examine the microscopic basis for the density gradient and the smooth quantum hydrodynamic approaches in one dimension using the Green's function formalism. These approaches are both predicated upon particular equilibrium relationships between the stress tensor and the local carrier gas density [1,3] to close the hydrodynamic hierarchy at the current transport equation (Eqns.1). We therefore derive the equilibrium density matrix for different barrier potentials, and then explicitly construct the stress tensor to compare it with the forms postulated in the two approaches. We show, that as expected the two forms are inaccurate near the barrier for realistic abrupt barrier heights (Fig 1) and are thus of questionable validity as such for transport simulations in the barrier direction.

The underlying problem with the stress tensor forms employed in the above two approaches [1,3] is that they are derived assuming perturbations on the solution of the free carrier Bloch equation. The resulting solutions are therefore accurate only under nearly free carrier like situations. The density gradient method assumes a slowly varying potential (through a suitably defined perturbation parameter [1]) while the smooth quantum hydrodynamic model assumes a potential that is small compared to the thermal voltage [3], both of which are violated in typical tunneling problems where the barrier plays a central role. To elucidate this further, we analytically derive the density matrix for a single-barrier structure using the scattering state solutions of the Schrödinger equation and show that the density/stress-tensor relationship can be written in a different form from those given above and that they have to be different inside and outside the barrier (Eqns. 2). We will also discuss using this form as the unperturbed solution for a perturbation analysis of the Bloch equation to derive new forms for the equilibrium Wigner function.

References :

1.) M.G, Ancona et. al, Phys. Rev. B, Vol. 39, No. 13, May 1989.
2.) D.K. Ferry et. al, Superlattices and Microstructures, Vol. 27, No.2/3, 2000.
3.) C. Gardner et. al, Phys. Rev. E, Vol. 53, No. 1, Jan. 1996.
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a.) $P = -nkT + \frac{\hbar^2}{12m^*}\left[\nabla^2 n - \frac{|\nabla n|^2}{n}\right]$

b.) $P = -nkT + \frac{\hbar^2 n}{4m^* kT}\nabla^2 V_{eff}$, where $V_{eff}(x) = \int_0^1 y^2 dy \int \frac{dz}{\sqrt{\pi}} e^{-z^2} V[x + [\frac{\beta(1-y)\hbar^2}{2m^*}]^{1/2} z]$

Eqns 1. The 1-D stress tensor forms used for closing the hydrodynamic hierarchy in a) Density gradient theory [1] and b) Smooth QHD model [3]. All the variables used above have their usual meanings.

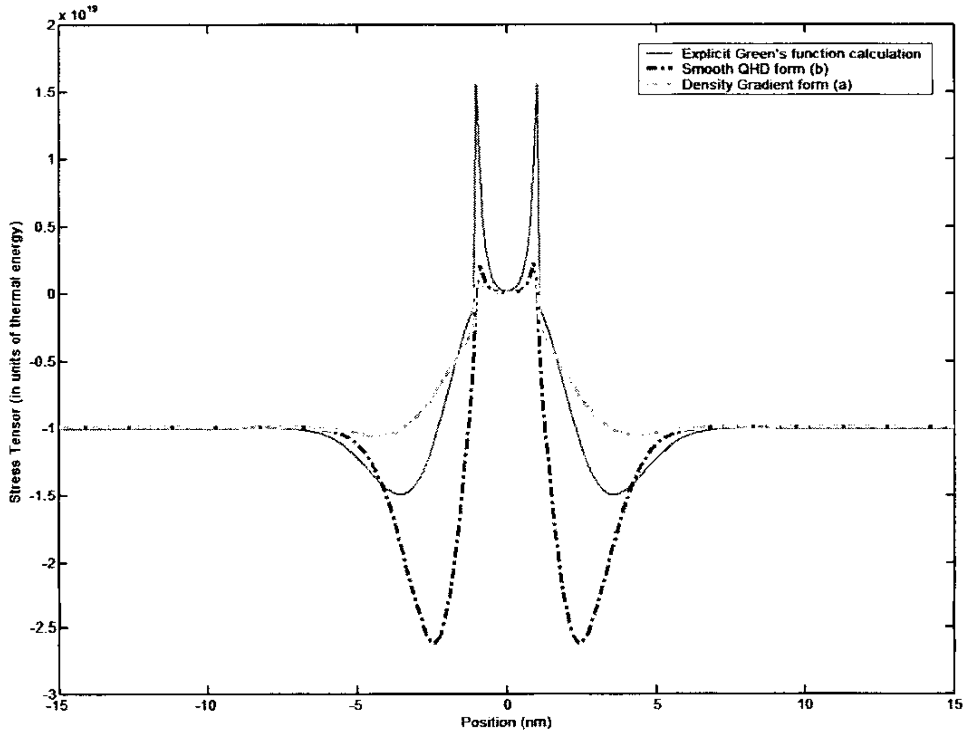

Fig 1. A comparison of the stress tensor in equilibrium from a) Green's function calculation (red, solid line) b) the form used in closing the hydrodynamic hierarchy in density gradient theory (green, dashed line) and c) the form derived for the smooth quantum hydrodynamic model (blue, dot-dashed line). The potential is a single 1 eV, 2 nm located symmetrically around the origin and the densities are constant at 10^{19}/cc on either side

$$\rho(x,x') = \int_{-\infty}^{\infty} \psi_k^*(x')\psi_k(x) e^{-\beta E(k)} dk \qquad \text{With} \qquad \lambda_{th} = \sqrt{\frac{\hbar^2 \beta}{2m^*}}\ ,\ \tilde{r} = \frac{x+x'}{2\lambda_{th}} \ \text{and}\ \tilde{s} = \frac{x-x'}{\lambda_{th}},$$

$$\rho(\tilde{r},\tilde{s}) = \frac{1}{2\sqrt{\pi}\lambda_{th}}\left[e^{-\tilde{s}^2} - e^{-(\tilde{r}\pm\tilde{a})^2}\left(1 + \frac{H_1(\tilde{r}\pm\tilde{a})}{\sqrt{\beta E_b}} + \frac{H_2(\tilde{r}\pm\tilde{a})}{\beta E_b}\right)\right], \qquad |\tilde{r}|,|\tilde{s}| \geq |\tilde{a}|$$

$$= \frac{e^{-2k_b\tilde{a}}}{2\sqrt{\pi}\lambda_{th}}\left[\cosh(2k_b\tilde{r}) + e^{-2k_b\tilde{a}}\cosh(k_b\tilde{s})\right] \quad \text{with} \quad k_b\lambda_{th} = \sqrt{\frac{2mE_b}{\hbar^2}} \qquad |\tilde{r}|,|\tilde{s}| < |\tilde{a}|$$

Eqns. 2 Density matrix derived from an explicit sum of scattering states for the barrier problem in Fig.1. The barrier (height, E_b) is between [-a,a] and it can be seen that the two forms (outside and inside the barrier) are very different and not free-carrier like near the barrier.