Appendix

Appendix A

Comments on the model of Tsuchiya, Ogawa and Miyoshi

The numerical model of Tsuchiya et al. (1991) for the Wigner transport equation in a spatially varying parabolic energy band suffers from severe problems. These problems manifest themselves in the physically unreasonable prediction that as the effective mass in the barrier increases, the peak current density does too. In this appendix, their equation is rewritten in a form that lends itself to proper numerical treatment, and to comparison with our work.

Here we ignore the fact that the equation of Tsuchiya et al. (1991) is inconsistent with the Weyl transform. It will be shown that except for one term, their equation is identical to ours. The numerical model developed here, for their transport equation, turns out to be very similar to that based on the transport equation presented in chapters 3 and 4. Our numerical treatment shows that the predictions of both models are very similar, as should be expected: different correspondence rules yield similar results. This comparison emphasizes the importance of proper numerical discretization.

Using the von Neumann equation for the "minimal Hermitian" Hamiltonian

$$\frac{\partial \rho}{\partial t} = \frac{\imath\hbar}{2}\left[\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z} - \frac{\partial}{\partial z'}\frac{1}{m^*(z')}\frac{\partial}{\partial z'} - \frac{2}{\hbar^2}\left[v(z) - v(z')\right]\right]\rho(z,z'), \tag{A.1}$$

Tsuchiya et al. (1991) correctly derive the equation of motion for the Wigner function

$$f(q,k) = 2\int dr\, e^{2\imath kr}\rho(q+r,q-r)$$

where $q=(z+z')/2$ and $r=z-z'$:

$$\begin{aligned}
\frac{\partial f}{\partial t} &= \frac{\hbar}{8\pi}\int dk'\, M_1(q,k-k')\frac{\partial f(q,k')}{\partial q} - \frac{\hbar}{4\pi}\int dk'\, k' M_2(q,k-k')f(q,k') \\
&+ \frac{\hbar}{16\pi}\int dk'\, M_3(q,k-k')\left[\frac{\partial^2 f(q,k')}{\partial q^2} - 4k'^2 f(q,k')\right] \\
&- \frac{\hbar}{4\pi}\int dk'\, k' M_4(q,k-k')f(q,k') \\
&- \frac{2}{\pi\hbar}\int dk'\, f(q,k')V_T(q,k-k'). \qquad \text{(A.2)}
\end{aligned}$$

The kernels M_1, M_2, M_3, M_4 and V_T, as given in Eqs. 7–13 of Tsuchiya et al. (1991), are in an undesirable form in that they depend on derivatives of the inverse effective-mass. After some manipulations, however, they can be written in terms of $\mathcal{M}^e$, $\mathcal{M}^o$ and $\mathcal{V}$ (the kernels in Eq. 3.21):

$$\begin{aligned}
M_1(q,k) &= -8(k-k')\mathcal{M}^e(q,k), \\
M_2(q,k) &= -8(k-k')\mathcal{M}^o(q,k), \\
M_3(q,k) &= -4\mathcal{M}^o(q,k), \\
M_4(q,k) &= 4\mathcal{M}^e(q,k), \\
V_T(q,k) &= -4\mathcal{V}(q,k). \qquad \text{(A.3)}
\end{aligned}$$

Substituting Eq. A.3 in Eq. A.2, we get

$$\begin{aligned}
\frac{\partial f}{\partial t} &= -\frac{\hbar}{\pi}\int dk'\, k'\frac{\partial}{\partial q}\left[f(q,k')\mathcal{M}^e(q,k-k')\right] \\
&- \frac{\hbar}{4\pi}\int dk'\, \frac{\partial^2}{\partial q^2}\left[f(q,k')\mathcal{M}^o(q,k-k')\right] \\
&+ \frac{\hbar}{\pi}\int dk'\, k'^2 f(q,k')\mathcal{M}^o(q,k-k') \\
&+ \frac{2}{\pi\hbar}\int dk'\, f(q,k')\mathcal{V}(q,k-k') \\
&+ \frac{\hbar}{4\pi}\int dk'\, f(q,k')\frac{\partial^2}{\partial q^2}\mathcal{M}^o(q,k-k'). \qquad \text{(A.4)}
\end{aligned}$$

All terms in the equation, except the last are identical to Eq. 3.20.

Following the discussion in chapter 4, the discrete Liouville superoperator corresponding to Eq. A.4 is

$$\begin{aligned}
\mathcal{L}_{jn;j'n'} &= \mathcal{T}_{jn;j'n'} - \frac{k_{n'}\mathcal{M}^{e}_{j'n-n'}}{N_k}\left(\frac{\delta_{j'j+1}-\delta_{j'j-1}}{2\Delta}\right) \\
&\quad - \frac{\mathcal{M}^{o}_{j'n-n'}}{4N_k}\left(\frac{\delta_{j'j+1}-2\delta_{j'j}+\delta_{j'j-1}}{\Delta^2}\right) \\
&\quad + \frac{(k^2_{n'}\mathcal{M}^{o}_{j'n-n'}+2\mathcal{V}_{j'n-n'}}{N_k}\delta_{j'j} \\
&\quad + \frac{\mathcal{M}^{o}_{j'+1,n-n'}-2\mathcal{M}^{o}_{j',n-n'}+\mathcal{M}^{o}_{j'-1,n-n'}}{4N_k\Delta^2}\delta_{j'j} \qquad \text{(A.5)}
\end{aligned}$$

yielding a much more accurate numerical model. Compare this with Eqs. 24–29 of (Tsuchiya et al., 1991). To yield a form that is closest to Eq. 4.13, we rearrange the above equation to obtain:

$$\begin{aligned}
\mathcal{L}_{jn;j'n'} &= \mathcal{T}_{jn;j'n'} - \frac{k_{n'}\mathcal{M}^{e}_{j'n-n'}}{N_k}\left(\frac{\delta_{j'j+1}-\delta_{j'j-1}}{2\Delta}\right) \\
&\quad - \frac{\mathcal{M}^{o}_{j'n-n'}}{4N_k}\left(\frac{\delta_{j'j+1}+\delta_{j'j-1}}{\Delta^2}\right) + \frac{\mathcal{M}^{o}_{j'+1,n-n'}+\mathcal{M}^{o}_{j'-1,n-n'}}{4N_k\Delta^2}\delta_{j'j} \\
&\quad + \frac{k^2_{n'}\mathcal{M}^{o}_{j'n-n'}+2\mathcal{V}_{j'n-n'}}{N_k}\delta_{j'j} \qquad \text{(A.6)}
\end{aligned}$$

Comparing this to 4.13, the only difference is that the $2\mathcal{M}^{o}_{j',n-n'}\delta_{j'j}$ term in Eq. 4.13 is replaced with $(\mathcal{M}^{o}_{j'+1n-n'}+\mathcal{M}^{o}_{j'-1n-n'})\delta_{j'j}$ This is fairly accurate when effective mass variations are not large.

Using the numerical model presented here, Fig. A.1 shows that Eq. A.2 correctly predicts the decrease in peak current with increasing barrier effective-mass. In contrast, the numerical model of Tsuchiya et al. (1991), for the same equation, predicts that the current increases with increasing barrier effective-mass (as shown in chapter 4). Also compared are the uniform effective-mass case and the predictions of Eq. 3.20.

The care required in developing a numerical model cannot be overemphasized. The first step of course, is to have the correct equation. In addition,

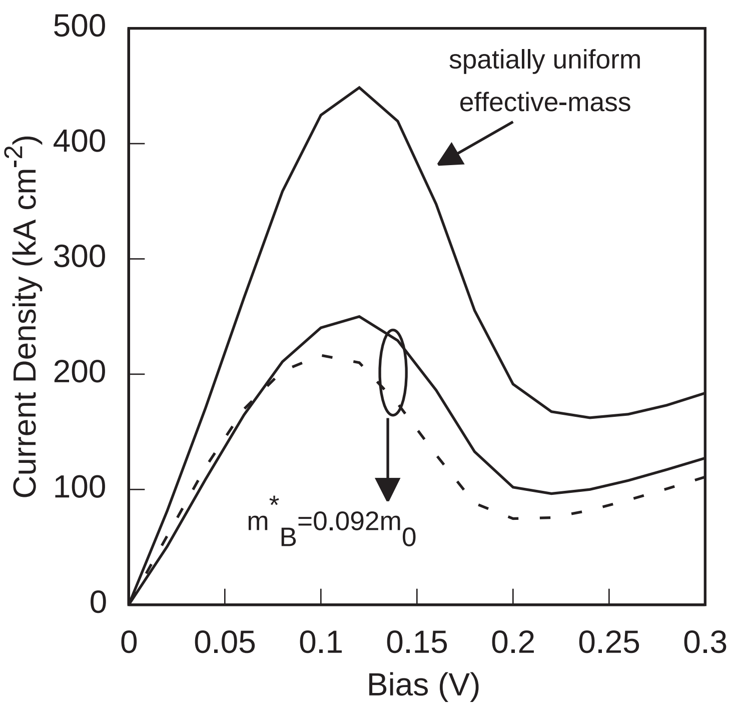

Figure A.1: The predictions of our numerical treatment of the equation of Tsuchiya *et al.* (dashed line), for the AlGaAs/GaAs diode discussed in chapter 4. The constant effective-mass curve is also shown. The proper numerical treatment leads to the expected result that the current falls as the barrier effective-mass increases. The prediction of the equation derived in this work is also shown. A temperature of 77K is assumed and collisions are ignored. First-order upwind differencing is used. $N_q = 200$, $\Delta = a$, and $N_k = 64$.

it is also necessary to have the equation in a form that is suitable for numerical treatment. Finally, as discussed in chapter 4, during the discretization process, care must be taken to retain the essential nature of the underlying problem.