A generalized Ramo–Shockley theorem for classical to quantum transport at arbitrary frequencies

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We present a generalized Ramo–Shockley theorem to evaluate particle currents and energy currents at device contacts, in classical drift-diffusion or hydrodynamic simulation techniques as well as for semiclassical Monte Carlo and quantum mechanical transport simulation. In contrast to the Ramo–Shockley theorem, our technique (1) is derived for conditions of extreme time dependence in the charge carriers and forces (including particle-induced radiation), (2) explicitly accounts for particle generation and recombination processes such as photoexcitation, forward and inverse Auger processes, or Shockley–Read–Hall recombination, and (3) distinguishes clearly between the contributions of electrons, holes, and the displacement current. The resulting simple new formalism reduces to the standard Ramo–Shockley theorem as a special case. © *1996 American Institute of Physics.* [S0021-8979(96)03603-X]

I. INTRODUCTION

Using the method of Green functions, Shockley[1] and Ramo[2] independently derived a highly useful domain integration formula for terminal currents induced by charge motion in an arbitrary multidimensional structure with multiple contacts:

$$I^{(k)}=\sum_j q_j \mathbf{E}_j^{(k)}\cdot \mathbf{v}_j\,, \tag{1}$$

where the summation j runs over all particles within the volume, q_j and $\mathbf{v}_j$ represent particle charge and velocity, respectively, and the index k indicates the contact number for which the current is to be evaluated. The variable $\mathbf{E}_j^{(k)}$ is the electric field evaluated at the position of particle j which would result if all charges were removed from the volume and all contacts except for contact k were grounded, and contact k were set to 1 V. Its application has been widespread, ranging from hot carrier noise in bulk semiconductors[3] and submicron semiconductor structures[4,5] to generators and detectors of electromagnetic radiation (typically microwave),[6,7] to terminal currents in Monte Carlo device transport simulation.[8] Recent work on the Ramo–Shockley (RS) theorem has led to its reconfirmation using an energy balance approach,[9] and its generalization to inhomogeneous media and quasielectrostatic applications.[10,11]

That the RS theorem, in spite of its apparent simplicity, holds in both the classical and quantum limits, and under physical conditions not considered in the theory, hints at a more general, unifying feature of charge transport. In this article, we argue that this general feature is the familiar current continuity equation, and use this equation in conjunction with Maxwell's equations as the starting point for the derivation of a set of generalized RS formulas. Our technique, related to the mathematical concept of weak solutions, and quite similar to that of Mock[12] and Gajewski,[13] results in domain integration formulas for all three components of the contact current. From these general time-dependent equations with generation/recombination sources, valid also in inhomogeneous media, one may extract the original RS equations as a limiting case.

II. GENERALIZED TERMINAL CURRENT CALCULATION

We begin with the two inhomogeneous Maxwell equations which, with the usual definitions of electric field and magnetic flux density in terms of the scalar electric potential ϕ and magnetic vector potential $\mathbf{A}$, yield the following well-known equations:

$$\boldsymbol{\nabla}\cdot\epsilon\boldsymbol{\nabla}\phi+\frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot\epsilon\mathbf{A}=-\rho, \tag{2}$$

$$\boldsymbol{\nabla}^2\mathbf{A}-\mu\epsilon\frac{\partial^2 A}{\partial t^2}-\mu\epsilon\frac{\partial}{\partial t}\boldsymbol{\nabla}\phi-\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot A)-\mu\boldsymbol{\nabla}\frac{1}{\mu}\times\boldsymbol{\nabla}\times\mathbf{A}$$
$$=-\mu\mathbf{J}. \tag{3}$$

Here the symbols ϵ, μ, ρ, and $\mathbf{J}$ $(=\mathbf{j}_n+\mathbf{j}_p)$ represent electrical permittivity, magnetic susceptibility, total charge density, and total conduction current, respectively. Without loss of generality, we may choose to work in the radiation gauge for inhomogeneous media, in which $\boldsymbol{\nabla}\cdot\epsilon\mathbf{A}=0$, and Eq. (2) reduces to

$$\boldsymbol{\nabla}\cdot\epsilon\boldsymbol{\nabla}\phi=-\rho, \tag{4}$$

where now ϕ may be interpreted as the usual electrostatic potential due to the instantaneous charge configuration. Using the relationship

$$\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\times\mathbf{H}=\boldsymbol{\nabla}\cdot\mathbf{J}+\boldsymbol{\nabla}\cdot\epsilon\frac{\partial\mathbf{E}}{\partial t}$$
$$=\boldsymbol{\nabla}\cdot\mathbf{J}+\boldsymbol{\nabla}\cdot\epsilon\frac{\partial(-\boldsymbol{\nabla}\phi)}{\partial t}+\boldsymbol{\nabla}\cdot\epsilon\left(-\frac{\partial^2\mathbf{A}}{\partial t^2}\right)=0, \tag{5}$$

in the chosen gauge yields

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$$\nabla \cdot \epsilon \nabla \frac{\partial \phi}{\partial t} = \nabla \cdot \mathbf{J}. \tag{6}$$

Similarly, the time derivative of the homogeneous Maxwell equation for the electric flux density yields

$$\nabla \cdot \epsilon \dot{\mathbf{E}} = -\nabla \cdot \epsilon \nabla \dot{\phi} - \nabla \cdot \epsilon \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\nabla \cdot \epsilon \nabla \dot{\phi} = \dot{\rho}. \tag{7}$$

Alternatively, Eqs. (6) and (7) may, using the definition $\mathbf{j}_d = \epsilon \dot{\mathbf{E}}$ for the displacement current, be rewritten in the following form:

$$-\nabla \cdot \mathbf{j}_d = \nabla \cdot \epsilon \nabla \dot{\phi} = \nabla \cdot (\mathbf{j}_n + \mathbf{j}_p) = -\dot{\rho} = -e(\dot{p} - \dot{n}), \tag{8}$$

where the quantities p and n are the free carrier densities of holes and electrons, respectively.

Continuity equations are one of the most fundamental properties of all types of transport, and are easily derived by taking moments of the appropriate transport equations. For classical or semiclassical systems, one most often takes moments of the Boltzmann transport equation,[14] and for quantum systems it is typically either the Wigner–Boltzmann equation[15] or the quantum Liouville equation.[16] We are at first only interested in the 0th moment equations, expressing the spatial variation of particle current flux density in terms of particle density time variation and particle generation/recombination rates. For electrons and holes, these equations have the general form;

$$-\nabla \cdot \mathbf{j}_n = eG_n(\mathbf{r}) - e\dot{n}, \tag{9}$$

$$-\nabla \cdot \mathbf{j}_p = -eG_p(\mathbf{r}) + e\dot{p}. \tag{10}$$

From Eq. (8), we have the additional relation

$$-\nabla \cdot \mathbf{j}_t = -\nabla \cdot (\mathbf{j}_n + \mathbf{j}_p + \mathbf{j}_d) = 0. \tag{11}$$

We now have an equation of the form

$$-\nabla \cdot \mathbf{j}_k = R_k, \quad k = n,p,d,t \tag{12}$$

for electron, hole, displacement, and total current. We work on a Lipschitzian domain Ω with an appropriate set of test functions h_{kl} satisfying

$$h_{kl}|_{\Gamma_l} = 1, \quad h_{kl}|_{\Gamma_j} = 0, \quad j \neq l, \quad h \in H^1, \quad k = n,p,d,t, \tag{13}$$

where $H^1(\Omega)$ and $H_0^1(\Omega)$ are the usual Sobolev spaces,[17] and assuming all variables $\in H^1$. Here Γ denotes the boundary, which consists of both Dirichlet (Γ_D) and Neumann (Γ_N) parts, with $\Gamma_D = \cup_i \Gamma_i$. Multiplying each of the four equations of type (12) with the corresponding test function h_{kl}, and then integrating by parts over the entire domain Ω, results in

$$(-\nabla \cdot \mathbf{j}_k, h_{kl}) = (R_k, h_{kl}),$$

$$-\int_\Omega h_{kl} \nabla \cdot \mathbf{j}_k \, dV = -\int_\Gamma h_{kl} \mathbf{j}_k \cdot d\mathbf{S} + \int_\Omega \nabla h_{kl} \cdot \mathbf{j}_k \, dV. \tag{14}$$

Equation (13) ensures that the surface integral in Eq. (14) is exactly equal to the particle current at contact l, since $h_k|_{\Gamma_l} = 0$, 1, and $(\mathbf{j}_k \cdot \hat{\mathbf{n}})|_{\Gamma_N} = 0$. The surface integral in Eq. (14) also gives the displacement current at contact l plus a contribution from the radiation term along Γ_N, which must be subtracted at high frequencies. The final results for the generalized Ramo–Shockley theorem terminal currents at an arbitrary contact l follow from Eqs. (8), (9), (10), (11), and (14):

$$I_{nl} = \int \nabla h_{nl}(\mathbf{r}) \cdot \mathbf{j}_n \, dV + e \int \dot{n} h_{nl}(\mathbf{r}) dV - e \int G_n(\mathbf{r}) h_{nl}(\mathbf{r}) dV, \tag{15}$$

$$I_{pl} = \int \nabla h_{pl}(\mathbf{r}) \cdot \mathbf{j}_p \, dV - e \int \dot{p} h_{pl}(\mathbf{r}) dV + e \int G_p(\mathbf{r}) h_{pl}(\mathbf{r}) dV, \tag{16}$$

$$\begin{aligned} I_{dl} &= \int \nabla h_{dl}(\mathbf{r}) \cdot \mathbf{j}_d \, dV - \int h_{dl}(\mathbf{r}) \nabla \cdot (\mathbf{j}_n + \mathbf{j}_p) dV + \int_{\Gamma_N} \epsilon h_{dl}(\mathbf{r}) \ddot{\mathbf{A}} \cdot d\mathbf{S} = \int \nabla h_{dl}(\mathbf{r}) \cdot \mathbf{j}_d \, dV \\ &\quad + e \int (\dot{p} - \dot{n}) h_{dl}(\mathbf{r}) dV + \int_{\Gamma_N} \epsilon h_{dl}(\mathbf{r}) \ddot{\mathbf{A}} \cdot d\mathbf{S}, \end{aligned} \tag{17}$$

$$I_{tl} = \int \nabla h_{tl}(\mathbf{r}) \cdot (\mathbf{j}_n + \mathbf{j}_p + \mathbf{j}_d) dV + \int_{\Gamma_N} \epsilon h_{tl}(\mathbf{r}) \ddot{\mathbf{A}} \cdot d\mathbf{S}. \tag{18}$$

Analogously, this technique may also be applied to higher moments of the transport equations, for example to the energy continuity equations, of which one of the many possible realizations is the following:

$$-\nabla \cdot \mathbf{S}_n = \frac{\partial n\langle w_n \rangle}{\partial t} - \mathbf{j}_n \cdot \mathbf{E} - \left.\frac{\partial n\langle w_n \rangle}{\partial t}\right|_{\text{coll}}, \tag{19}$$

$$-\nabla \cdot \mathbf{S}_p = \frac{\partial p\langle w_p \rangle}{\partial t} - \mathbf{j}_p \cdot \mathbf{E} - \left.\frac{\partial p\langle w_p \rangle}{\partial t}\right|_{\text{coll}}, \tag{20}$$

$$-\nabla \cdot \mathbf{S}_f = \frac{\partial u_f}{\partial t} + (\mathbf{j}_n + \mathbf{j}_p) \cdot \mathbf{E}, \tag{21}$$

$$-\nabla \cdot \mathbf{S}_c = \frac{\partial u_c}{\partial t} + \frac{\partial}{\partial t} [n\langle w_n \rangle + p\langle w_p \rangle]\Big|_{\text{coll}}, \tag{22}$$

$$-\nabla \cdot \mathbf{S}_t = 0. \tag{23}$$

In this case, one additional equation appears, since charge carriers may also exchange energy with the medium. The symbol $\mathbf{S}_k$, $k \in \{n,p,f,c,t\}$, stands for the electron, hole, electromagnetic, lattice, and total $(= n+p+f+c)$ energy flux densities. For the electromagnetic case, this is simply the familiar Poynting vector. The position-dependent energy densities stored in the electromagnetic field and the crystal are designated by u_f and u_c, respectively. The symbol $\partial/\partial t(n\langle w_n \rangle)|_{\text{coll}}$ stands for the (usually negative) rate at which energy is gained by the electrons from the crystal lattice, and is often approximated by

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$$\frac{\partial}{\partial t}\,(n\langle w_n\rangle)\bigg|_{\mathrm{coll}} \approx \langle w_n\rangle G_{\mathrm{SRH}}(\mathbf{r}) + \frac{\partial}{\partial t}\,(n\langle w_n\rangle)\bigg|_{\mathrm{phonons}}. \tag{24}$$

The corresponding definition of this quantity for holes is fully analogous. Using the technique developed in the preceeding paragraphs, the energy currents at an arbitrary contact l may be written as

$$I_{nl}^E = \int \nabla h_{nl}(\mathbf{r})\cdot\mathbf{S}_n\,dV - \int h_{nl}(\mathbf{r}) \times\left(\frac{\partial n\langle w_n\rangle}{\partial t} - \mathbf{j}_n\cdot\mathbf{E} - \frac{\partial n\langle w_n\rangle}{\partial t}\bigg|_{\mathrm{coll}}\right)dV, \tag{25}$$

$$I_{pl}^E = \int \nabla h_{pl}(\mathbf{r})\cdot\mathbf{S}_p\,dV - \int h_{pl}(\mathbf{r}) \times\left(\frac{\partial p\langle w_p\rangle}{\partial t} - \mathbf{j}_p\cdot\mathbf{E} - \frac{\partial p\langle w_p\rangle}{\partial t}\bigg|_{\mathrm{coll}}\right)dV, \tag{26}$$

$$I_{fl}^E = \int \nabla h_{fl}(\mathbf{r})\cdot\mathbf{S}_f\,dV - \int h_{fl}(\mathbf{r})\left(\frac{\partial u_f}{\partial t} + (\mathbf{j}_n+\mathbf{j}_p)\cdot\mathbf{E}\right)dV + \int_{\Gamma_N} h_{fl}(\mathbf{r})\dot{\mathbf{A}}\times\frac{1}{\mu}\nabla\times\mathbf{A}\cdot d\mathbf{S}, \tag{27}$$

$$I_{cl}^E = \int \nabla h_{cl}(\mathbf{r})\cdot\mathbf{S}_c\,dV - \int h_{cl}(\mathbf{r}) \times\left(\frac{\partial u_c}{\partial t} + \frac{\partial}{\partial t}\,[p\langle w_p\rangle + n\langle w_n\rangle]\bigg|_{\mathrm{coll}}\right)dV, \tag{28}$$

$$I_{tl}^E = \int \nabla h_{tl}(\mathbf{r})\cdot(\mathbf{S}_n+\mathbf{S}_p+\mathbf{S}_f+\mathbf{S}_c)\,dV + \int_{\Gamma_N} h_{tl}(\mathbf{r})\dot{\mathbf{A}}\times\frac{1}{\mu}\nabla\times\mathbf{A}\cdot d\mathbf{S}. \tag{29}$$

These simple but general equations, with the flexibility afforded by the choice of h_{kl}, should provide a useful method for calculating time-dependent or steady-state particle and energy currents at the contacts of complex multidimensional domains. An application of this technique involving the optimization of the test functions $h_{kl}(\mathbf{r})$ for statistically best estimators of contact currents in particle-based charge transport simulation may be found in Ref. 18.

III. DISCUSSION

The quasi-electrostatic limit of Eq. (18) for the total contact current has previously been derived by Mock[12] and Gajewski.[13] As we have shown, it is in fact valid at all frequencies, provided the scalar and vector potentials are evaluated properly. If all time dependence is eliminated, and additionally h_{tl} is the solution to Poisson's equation with all charges removed from the domain, then Eq. (18) is identical to the original RS formulation. Note, however, that in situations with time-dependence or generation/recombination processes, the electron (or hole) contribution to the total terminal current is not simply equal to sum of the electron (or hole) terms in the RS (or Mock) total current formula. One perhaps important disadvantage of using the RS theory instead of Eq. (18) is that the RS theory always results in global current conservation,

$$\sum_l I_{tl} = 0 \tag{30}$$

regardless of any gross inaccuracies in the calculation of the current densities $\mathbf{j}_k$; as long as $\Sigma_l h_{kl}(\mathbf{r}) \neq c$—whose equality is a sufficient condition for unconditional global current conservation in the absence of radiation—Eq. (18) only yields this physical result if the current densities $\mathbf{j}_k$ are also physically meaningful. (Note: functions h_{kl} which satisfy the Poisson-like equation $[\nabla\cdot\gamma(\mathbf{r})\nabla + \beta(\mathbf{r})\cdot\nabla]h_{kl} = 0$ with the previously specified boundary conditions automatically satisfy $\Sigma_l h_{kl}(\mathbf{r}) = c$. However, application of a simple continuous nonlinear transformation with $f(0)=0$ and $f(1)=1$ destroys this property.)

It is immediately noticed that the total current I_{tl} has a form different from that of the sum of its components, $I_{nl}+I_{pl}+I_{tl}$, for arbitrary choices of h_{kl}. The general equivalence of these two expressions is in fact a property of the solutions to the defining transport equations. This is, of course, also the case for terminal currents of higher-order moment quantities.

In contrast to the low-frequency situation where the particle force is simply $q\mathbf{E} = -q\nabla\phi$, particle motion at high frequencies is governed by the new forces $-q\nabla\phi - q\,d\mathbf{A}/dt$ and $q\mathbf{v}\times\nabla\times\mathbf{A}$, which include the effect of radiation fields generated from other particles. Therefore, the effect of the radiation is already implicitly accounted for in the particle velocities, energies, and number densities used in the GRST. The only complication which arises for purposes of analytical calculation or numerical simulation is the necessary burden of solving the additional Eq. (3), in order to obtain the proper electric and magnetic fields which determine the forces acting on the particles. Similarly, use of the GRST (or even RS) equations at high carrier densities must in principle be preceeded by calculations of carrier density and velocity profiles which incorporate highly complicated many-body effects such as the exchange and correlation forces.

IV. CONCLUSIONS

We have demonstrated the validity of a new GRST for classical, semiclassical, and quantum systems, from 0 Hz up to arbitrary frequencies, based upon Maxwell's equations and continuity equations arising from moments of transport equations. The resulting formulas retain nearly the same level of simplicity as the original RS equations, and their accuracy is limited only by that of the preceeding calculation of charge density and velocity information, and higher-order moments of the carrier distribution functions as needed.

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