phasons[10] is observed there, and a more complete picture of phasons in potassium would be possible.

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Self-Scattering Path-Variable Formulation of High-Field, Time-Dependent, Quantum Kinetic Equations for Semiconductor Transport in the Finite-Collision-Duration Regime

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Quantum kinetic equations for describing transport in submicron semiconducting devices in the finite collision duration regime are developed which are nonlocal in time and momentum. Utilizing a projected self-scattering formulation, a retarded path-integral equation is obtained. Quantum kinetic equations are usually exceedingly difficult to solve. The formulation found here presents a powerful technique to achieve these solutions even in the case where nonlocal effects are important.

The Boltzmann transport equation (BTE) has long been the basis for semiclassical transport studies in semiconductors and other materials. Its utility also stems from the fact that it is readily transformable into a path variable form which can be adapted to numerical solutions for complicated energy-dependent scattering processes.[1-3] In this form, the BTE is often referred to as the Chambers-Rees path-integral equation, and serves as the basis for Monte Carlo[4-6] and iterative[7-9] calculations of transport. However, the BTE is valid only in the weak-coupling limit under the assumptions that the electric field is weak and slowly varying at most, the collisions are independent, and the collisions occur *instantaneously* in space and time. Each of these approximations can be expected to be violated in future submicron-dimensioned semiconductor devices. We have previously shown that in such devices, the time scales are such that collision durations are no longer negligible when compared to the relevant time scale upon which transport through the device occurs.[10,11] In this situation, even for time-independent fields, the quantum kinetic equations are nonlocal in time and momentum. It may be recalled that the BTE can be rigorously derived from the density-matrix Liouville-equation formulation of quantum transport.[12,13] Here, we draw upon that formulation for a retarded-time kinetic equation, which replaces the BTE, and show that by introducing a projected self-scattering process, a retarded path integral can be developed. The power of this technique allows a single path integral to be used, rather than the expected multiple retarded path integrals.

If the instantaneous collision approximation is relaxed, an additional field contribution appears as a differential superoperator term in the collision integrals evaluated in the momentum repre-

sentation, resulting in an intracollisional field effect.[13-15] This effect is important either when the field is large or when the collision duration is a significant fraction of the mean time between collisions, and has previously been analyzed for steady-state transport in uniform, time-independent fields.[14,16] In the steady-state case, the intracollisional field effect induces a broadening and skewing of the usual energy-conserving δ functions. This leads, e.g., to a lowering of the threshold for phonon emission due to acceleration during the collision and to a reduction of scattering strength at high fields. As we mentioned above, the quantum kinetic equations are then nonlocal in time and momentum. As a consequence, the energy conserving δ functions which appear in the "golden rule" transition rates are replaced by path integrals over the time t into a collision. The earlier analysis, extended to time-varying fields, leads to a high-field quantum kinetic equation, which replaces the BTE, as

$$\partial f(\vec{p},t)/\partial t + e\vec{E}(t)\cdot\nabla_{\vec{p}} f(\vec{p},t) = \int_0^t dt' \sum_{\vec{p}'} \{S(\vec{p},\vec{p}';t,t')f(\vec{p}',t') - S(\vec{p},\vec{p}';t,t')f(\vec{p},t')\}, \tag{1}$$

where the momenta $\vec{p}$ and $\vec{p}'$ are explicit functions of the retarded time t' on the right-hand side through the relationship

$$\vec{p}(t') = \vec{p} - \int_{t'}^{t} e\vec{E}(t'')dt'', \tag{2a}$$

$$\vec{p}'(t') = \vec{p}' - \int_{t'}^{t} e\vec{E}(t'')dt'', \tag{2b}$$

and the transition terms S take the form, for inelastic phonon scattering,

$$S(\vec{p},\vec{p}';t,t') = \mathrm{Re}\,\frac{2\pi}{\hbar}\sum_{\vec{q}}\left(\frac{1}{\pi\hbar}\right)\exp\left(-\frac{t-t'}{\tau_\Gamma}\right)(N_{\vec{q}}+\tfrac{1}{2}+\tfrac{1}{2}\eta)\,|V(\vec{q})|^2\delta_{\vec{p},\vec{p}'+\eta\vec{q}}\exp\left[-i\int_t^{t'}\frac{dt''}{\hbar}\beta(\vec{p},\vec{p}';t'')\right], \tag{3}$$

where

$$\beta(\vec{p},\vec{p}';t'') \equiv \mathcal{E}[\vec{p}(t'')] - \mathcal{E}[\vec{p}'(t'')] + \eta\hbar\omega_{\vec{q}}. \tag{4}$$

The exponential factors in (3) are the joint spectral density function (the term τ_Γ represents the joint collision broadening of states p, p' against all scattering process[13]), which reduces to an energy-conserving δ function in the instantaneous collision, low-field limit,[13,17] and $\mathcal{E}(\vec{p})$ is the quasiparticle renormalized electron energy, and η takes the values $+1$ or -1 for phonon emission or absorpiton, respectively, in the in-scattering term. For the out-scattering term, the roles of $\vec{p}$ and $\vec{p}'$ are interchanged, although this does not upset detailed balance in the equilibrium sense.

The nonlocal equation (1) cannot be immediately written as a Chambers-Rees-type path integral because of the inherent retardation of the out-scattering term.[2,3] Therefore, the numerical evaluation of (1) remains a formidable task. However, by generalizing the concept of the self-scattering process, we can obtain a relatively simple path-integral formulation for the distribution function $f(\vec{p},t)$ which is similar in form to the more usual path-integral formalism for the BTE, and hence is readily amenable to numerical iterative analysis. To accomplish this, we add and subtract identical terms to the right-hand side of (1), so that we can redefine

$$S^*(\vec{p},\vec{p}';t,t') = S(\vec{p},\vec{p}';t,t') + [\Gamma(t,t') - \Gamma_{\mathrm{out}}(t,t')]\delta(\vec{p}-\vec{p}'), \tag{5}$$

where

$$\Gamma_{\mathrm{out}}(t,t') \equiv \sum_{\vec{p}''} S(\vec{p},\vec{p}'';t,t'), \tag{6}$$

and

$$\Gamma(t,t') \equiv \Gamma_0\delta(t-t'), \tag{7}$$

with Γ_0 a positive constant selected by convenience of convergence criteria. The self-scattering terms in the square-brackets of (5) make no contribution to the collision integral, but the term in Γ_{out} plays an important role. This term effectively projects out of Γ the contribution due to uncompleted out-scattering and the retardation in the out-scattering is accounted for here rather than in the term involving $f(\vec{p},t)$. The kinetic equation (1) may then be written

$$[(\partial/\partial t) + e\vec{E}(t)\cdot\nabla_{\vec{p}} + \Gamma_0]f(\vec{p},t) = \sum_{\vec{p}}\int_0^t dt' S^*(\vec{p},\vec{p}';t,t')f[\vec{p}'(t'),t'], \tag{8}$$

which may now be solved by the method of characteristics[18] to obtain the path-variable structure

$$f(\vec{p},t) = \int_0^t dt' \exp[-\Gamma_0(t-t')]G(\vec{p};t,t'), \tag{9}$$

where

$$G(\vec{p}; t, t') = \sum_{\vec{p}'} \int_0^{t'} dt'' \, S^*[\vec{p}(t''), \vec{p}'(t); t', t''] \, f[\vec{p}'(t''), t''] . \quad (10)$$

In the limit of long times $t \gg 0$, instantaneous collisions, and no quasiparticle effects from the field, (9) and (10) reduce to the normal path-integral form of the BTE.

It is worth noting here that although a Feynman path-integral approach has also been developed for quantum transport,[19] its applicability has only been demonstrated for strong-coupled polar optical scattering and is much more difficult to apply. The desirability of Eqs. (9) and (10) lies in their structural similarity to path integrals obtained from the BTE, and thus techniques used for these can readily be adapted to the present quantum transport equations. For example, this pair of equations form the basic set to adopt in iterative solution for $f(\vec{p}, t)$.[1-3] Moreover, nonlinear scattering processes, such as carrier-carrier scattering, are readily incorporated into the iterative approach. Monte Carlo techniques can also be used to find the distribution function, although care must be exercised in treating transient solutions. This latter follows also for the BTE, since the basic times involved are assumed long compared to fluctuation periods, so that the equations are almost deterministic. Monte Carlo reintroduces significant fluctuations into transient calculations, so that such calculations as recently performed,[20] must be carefully interpreted and be averaged over a great many trials.

In summary, our generalization of self-scattering, as contained in Eqs. (6) and (7), to include the time-dependent out-scattering terms through a time-dependent self-scattering effect. As a result, single path-variable equation is obtained that is functionally similar to that obtained from the BTE. Care should be exercised, however. In dealing with quantum kinetic equations and the density matrix, off-diagonal terms can arise, and while these can be handled by projection-operator techniques,[9-11] the detailed nature of $S(\vec{p}, \vec{p}'; t, t')$ can be significantly different from the more normal forms in any but the weak-coupling limit. While it might be though that these effects will only be found in devices many generations away from current-day practice, we show in detailed calculations, to be published elsewhere, the finite-collision-duration modifications are, in fact, important in any situation in which transient dynamics of electrons are important. This means that overshoot-velocity effects, as recently calculated for GaAs field-effect transistors,[20] are strongly affected by the effects discussed here.

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