Quantum Monte Carlo Simulation of High-Field Electron Transport: An Application to Silicon Dioxide

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A new approach to the Monte Carlo simulation of electron transport is presented. The Monte Carlo technique is regarded as a stochastic evaluation of the Green's function expressed as a Feynman path integral. By a proper weighting of the randomly generated trajectories, conventional Monte Carlo simulations can be used to obtain the correct quantum solution. This technique is applied to silicon dioxide by employment of the scattering rates obtained from the Dyson equation, thus extending the validity of the solution beyond the quasiclassical and perturbation approximations.

The problem of electron transport in semiconductors and insulators is commonly tackled by the assumption that the electrons interact only weakly with the scatterers—phonons, impurities, valence or conduction electrons, etc.—so that first-order perturbation theory can be employed to compute the scattering rates. Moreover, in this weak-coupling limit the electron mean free path is large compared to the electron wavelength, so that the collision processes can be treated as independent, occurring instantaneously, and the electrons become quasiclassical particles. These approximations result in the Boltzmann transport equation (BTE)[1] and in the equivalent classical Monte Carlo (CMC) simulation scheme[2] which assigns definite positions and momenta to the electrons, as allowed by classical mechanics.

The presence of very high fields and hot electrons in the small devices of the present technology requires a revision of the semiclassical picture associated with the BTE. Several attempts have been already made in this direction. Some particular problems, such as the calculation of the mass[3] and drift velocity[4] of polarons in polar insulators or the effect of the finite duration of the collision processes,[5,6] have been successfully treated. However, we are still missing a general technique which enables us to treat at a full quantum level the transport problem in realistic instances.

In this Letter we present a new technique which goes beyond the semiclassical and perturbation limits in computing the energy distribution and drift velocity of hot electrons in nondegenerate semiconductors and insulators. First, the scattering rates are obtained from the direct solution of the Dyson equation—thus at all orders in the perturbation series—as previously suggested by Chang et al.[7] Then these are used as input in a quantum Monte Carlo (QMC) scheme which is viewed as a sampling technique to evaluate stochastically the electron Green's function expressed as a Feynman integral over paths,[8] rather than as a simple random generation of classical trajectories. The major difference between the CMC and our QMC technique

consists in the weighting procedure for the various electron paths: The CMC assigns unit weight to all electron trajectories and adds them without interference. On the contrary, the QMC assigns a phase to every path and accounts for the interference of different trajectories ending with the same classical parameters (energy, momentum, position, or time). We exemplify this technique by considering the problem of high-field electron transport in SiO_2, which recently has received significant attention.[9,10]

To illustrate the technique, we shall deal, for simplicity, with independent, nondegenerate electrons which interact with phonons—assumed to remain always at thermal equilibrium—labeled by a branch (transverse or longitudinal) and type (optical or acoustic) index λ. We consider the Fourier-transformed electron Green's function $G(\mathbf{k},w)$ with the electron-phonon interaction turned on, but in the absence of the external field. With vertex corrections and renormalization of the phonon propagator ignored,[11] $G(\mathbf{k},w)$ can be evaluated from the Dyson equation[12]:

$$G(\mathbf{k},w) = G_0(\mathbf{k},w)/[1 - G_0(\mathbf{k},w)\Sigma(\mathbf{k},w)], \quad (1)$$

$$\Sigma(\mathbf{k},w) = \sum_{\lambda,\pm} \int d^3k' |V^{(\lambda)}_{\mathbf{k}-\mathbf{k}'}|^2 (n^{(\lambda)}_{\mathbf{k}-\mathbf{k}'} + \tfrac{1}{2} \pm \tfrac{1}{2})$$

$$\times G(\mathbf{k}',w \mp \hbar\omega^{(\lambda)}_{\mathbf{k}-\mathbf{k}'}), \quad (2)$$

where $G_0(\mathbf{k},w) = (w - w_\mathbf{k} + i\delta)^{-1}$ $(\delta \to 0^+)$ is the free-electron Green's function, $\Sigma(\mathbf{k},w)$ is the proper electron self-energy, $w_\mathbf{k}$ is the bare energy of an electron of wave vector $\mathbf{k}$, $V^{(\lambda)}_\mathbf{q}$ is the matrix element for emission or absorption of a phonon of type λ, wave vector $\mathbf{q}$, and energy $\hbar\omega^{(\lambda)}_\mathbf{q}$, and $n^{(\lambda)}_\mathbf{q}$ is the phonon Bose factor at lattice temperature T.

The integral equation for Σ can be solved iteratively. In the weak-coupling limit Σ reduces to the usual "golden rule" expression in terms of the first-order scattering rate $1/\tau_1(\mathbf{k})$:

$$\text{Re}[\Sigma(\mathbf{k},w_\mathbf{k})] = 0, \quad \text{Im}[\Sigma(\mathbf{k},w_\mathbf{k})] = -\hbar/2\tau_1(\mathbf{k}). \quad (3)$$

This can be employed as a zero-order iteration of

Eq. (2).

Having obtained the self-energy Σ, we obtain the renormalized energy of the quasiparticle, ϵ_k, by solving the equation[12] $\epsilon_k = w_k + \Sigma(k, \epsilon_k)$, which gives the pole of the Green's function closest to the real axis (quasiparticle approximation). The renormalized energy ϵ_k can be found even if Eq. (2) provides $\Sigma(k, w)$ only on the real axis, since we can use the analytic properties of the self-energy[13] and the Cauchy theorem to obtain $\Sigma(k, z)$ on the entire complex plane. The total scattering rate is finally given by

$$1/\tau(k) = -(2/\hbar)\text{Im}[\Sigma(k, \epsilon_k)]$$
$$= -(2/\hbar)\text{Im}(\epsilon_k). \qquad (4)$$

As a final and major step, we have to consider the electron Green's function in the presence of both electron-phonon interaction and a uniform external electric field F. Rather than following again the Dyson-equation approach, we find it convenient to express the amplitude $G_F(r', r'; r, t)$ for an electron at position r at time t to be found at r' at time t' as a sum over all possible paths $\{r(\tau), k(\tau)\}$ in phase space:

$$G_F(r', t'; r, t) = \int \delta[r(\tau)]\delta[k(\tau)]e^{iS(r', t'; r, t)/\hbar}, \qquad (5)$$

where the *effective action* S is given by

$$S(r', t'; r, t) = \int_{(r, t)}^{(r', t')} d\tau[\hbar k(\tau) \cdot \dot{r}(\tau) - \epsilon_{k(\tau)}$$
$$- eF \cdot r(\tau)]. \qquad (6)$$

Here the dot over a symbol denotes the time derivative, and e is the charge of the electron. This expression can be obtained from the procedure outlined, for instance, by Abers and Lee,[14] within the quasiparticle approximation.[15] Notice that *intracollisional field effects*[5,6] as well as all virtual and real phonon emission and absorption processes entering ϵ_k are accounted for by Eq. (5). Moreover, the complete quantum description of the system is implicit in the functional integral, so that quantum reflections, quantum size effects, or quantization in inversion layers (subbands) would be correctly included in simulation of realistic devices described by a nonuniform external potential.

The path integral given by Eq. (5) could be evaluated by techniques such as the *simulated annealing*,[16] molecular dynamics,[17] or the Monte Carlo importance sampling (the Metropolis algorithm[18]). The last technique requires the random generation of a collection of paths with distribution $\exp(\text{Im}S/\hbar)$: The total time interval $t' - t$ is divided into smaller intervals, thus justifying the quasiparticle approximation in Eq. (6). Only (real) classical trajectories and second-order deviations away from them are assumed to contribute to the amplitude of the electron wave function in each elementary path. Then, the problem of generating the paths can be solved by generation of configurations

$\{k_\mu, t_\mu\}$ with distribution

$$\prod_\mu |\Delta_{VM}(k_{\mu, f}, k_\mu)|^{-1}\exp[\text{Im}S^{cl}(\{k_\mu, t_\mu\})/\hbar], \qquad (7)$$

where S^{cl} is the action evaluated along the classical path of duration $t_{\mu+1} - t_\mu$ with initial wave vector k_μ and final wave vector $k_{\mu, f}$, Δ_{VM} is the Van Vleck–Morette normalization factor,[19] while the r_μ's are fixed by the classical solution. Finally, the evaluation of the functional integral can be performed by addition of the phases of the configurations so generated.

Viewed from this perspective, the CMC solution of the BTE and the Monte Carlo importance sampling are actually *almost* equivalent algorithms. The main difference is that the CMC technique provides only an approximate evaluation of the path integral given by Eq. (5), as each path is assigned a *probability* of occurrence, rather than an *amplitude*,[20] and paths are generated according to the probability distribution $\exp(2\,\text{Im}S/\hbar)$. In practice, this is done by approximation of the squared magnitude of the factors of Eq. (7) with the golden-rule transition rates (thus considering *completed* and independent collisions at zero field[21]), and by generation of a Markov chain which is equivalent to the Chambers integral formulation of the BTE.[2] Finally, classical mechanics is used to extract the physical information. For example, in order to obtain the energy distribution of the particles, the paths ending at r' with classical energy[8] $\text{Re}(\epsilon_k)$ $= \text{Re}[\partial S^{cl}(r', t'; r, t)/\partial t']$ are all counted with the same unit weight, independent of their phases (in other words, amplitudes are squared and later added, as required by the classical composition of probabilities).

The Monte Carlo scheme can be converted to a quantum solution by the weighting of each stochastically generated path by its action, thus recovering the correct stochastical evaluation of the Green's function. In order to obtain the correct quantum energy distribution of the renormalized electrons, we generate piecewise classical trajectories with probability-amplitude distribution $\exp[\text{Im}S(\text{path})/\hbar]$, as prescribed by Eq. (7). Simultaneously, we evaluate the real part of the action along each path, obtaining its phase $\exp[i\,\text{Re}(S(\text{path}))/\hbar]$. Finally, having defined small energy intervals Δw_{final}, we consider all paths ending with classical energy $\text{Re}(\epsilon_k)$ within a given interval, add their phases, and square the absolute value of the result, thus obtaining the correct quantum mechanical probability for that particular final energy to occur. A similar procedure can be employed for the average drift time, yielding the drift velocity, or for any other observable whose expectation value is desired. This averaging procedure correctly accounts for the possibility that different paths may destructively interfere or be damped by the exponential of the action. The price that we must pay is the need for a larger statistics (a factor between 10 and 100 with respect to the
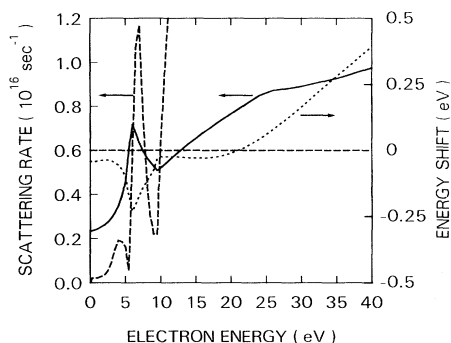
FIG. 1. Total electron-phonon scattering rate and energy shift obtained from the Dyson equation. The golden-rule scattering rate (dashed curve) is shown for comparison.
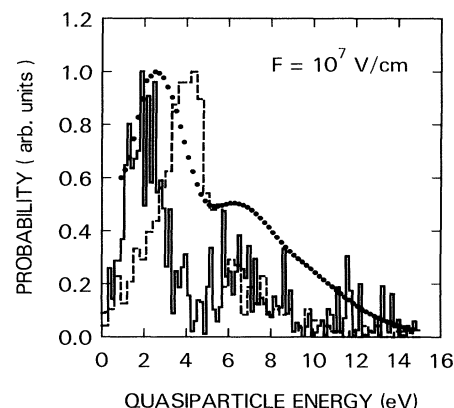

FIG. 2. Electron energy distributions at a field of 10^7 V/cm obtained from the CMC (dashed line) and QMC (solid line) simulations and from the experimental data of Ref. 27 (dots). The simulations have been performed over a distance of 60 nm (CMC) and 100 nm (QMC) of SiO_2 with the scattering rates and band structure described in the text. The minima of the distributions coincide with the minima of the DOS employed in the simulation.

CMC), as many paths per given energy interval are needed to stabilize the oscillations of the phases.

We have applied the QMC technique to the problem of high-field transport in SiO_2. We have assumed essentially the same types of interactions (Fröhlich and nonpolar) with longitudinal optical and acoustic phonons as employed in our previous simulations.[9] Two major modifications have been introduced. (1) The conduction band has been assumed to be spherical, but nonparabolic, in order to reproduce the calculated density of states (DOS) characterized by a conduction band peaked at about 3 and 7 eV above its bottom at the Γ point.[22] We have taken for the electron effective mass at this point one-half of the free-electron mass and used a free-electron dispersion at energies above 10 eV. Notice that we include a minimum of the DOS at about 9 eV which has been observed experimentally.[23] This contrasts with the choice of a much higher DOS made by Porod and Ferry.[10] (2) We have assumed that at very high electron energy a rigid-ion approximation[24] better represents the matrix element for the nonpolar electron-phonon interaction. This amounts to a decrease of the momentum-transfer cross section of the ions as the conduction electron acquires enough velocity to prevent the valence electrons from following its motion adiabatically. This behavior is observed in the collisions between electrons and nonpolar molecules.[25] The critical energy that we have assumed for the transition between the (isotropic scattering) umklapp-dominated and the (forward scattering) rigid-ion response is 25 eV (Ref. 25).

We have solved the Dyson equation iteratively starting from the first-order scattering rates. The assumption of spherical bands allows us to convert the triple integral in Eq. (2) into a single integral. Typically, convergence was reached after about thirty iterations with a relative numerical accuracy of 10^{-6}. The resulting scattering rate and energy shift are shown in Fig. 1.

The average electron energy as a function of the

external electric field obtained from our quantum simulation is very close to the results of our previous semiclassical simulations.[9] This will be discussed in detail in a forthcoming publication.[26] The major difference between quantum and semiclassical results concerns the actual electron energy distribution. In Fig. 2 we show the quantum and semiclassical (no broadening) distributions at a field of 10^7 V/cm. A comparison between the quantum distribution and the experimental data of Brorson et al.[27] indicates that a satisfactory agreement is now obtained not only in terms of average energies, but also in terms of the distribution of electrons at the high energies at which quantum effects must be included. In particular, the results of the QMC technique differ from those obtained from the CMC because of the two somewhat competing effects: Firstly, the peak of the distribution is shifted to lower energies, an effect already known to be due to the collisional broadening.[9,10] Secondly, the high-energy tails are more pronounced, since the low-energy paths—farther away from the stationary-action trajectory—are most likely to interfere destructively. This second effect is typical of the present QMC technique and can be attributed to both intracollisional field effects and interference among partial waves in multiple-collision events.

In conclusion, we have shown that the standard Monte Carlo method can simulate quantum transport, provided each stochastically generated path is properly assigned its phase and quantum-mechanical statistical weight. Thus quantum transport can be dealt with while preserving the conceptual simplicity of the Monte Carlo technique in the handling of realistic

scattering rates and band structures. We have considered the simple case of independent, first-quantized electrons in a spherical band. Extensions to systems involving multiband phenomena, second-quantized interacting electrons, and off-equilibrium phonon population, while straightforward in principle, require numerical algorithms significantly "smarter" than those that we have presented.

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mally decoupled from the lattice, so that the sum over the lattice degrees of freedom factors out of Eq. (5). Without this factorization, our statistical ignorance about the lattice (impure) configurations would enter the problem via the *influence functional* of Refs. 4 and 8. On the contrary, in Eq. (5) only a sum over quantum mechanical amplitudes is involved, dissipation entering the problem only via the Bose factors occurring in the quasiparticle energy ϵ_k.

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can be obtained following Cécile Morette, Phys. Rev. **81**, 848 (1951), by expanding the action to second order in $\mathbf{k}$ around the classical value and performing the Gaussian integral over $\mathbf{k}$. This integration takes care of the many phase cancellations of nonclassical paths. The convergence of the Metropolis algorithm based on piecewise classical paths, rather than on the straight-line paths considered by Claude Garrod, Rev. Mod. Phys. **38**, 483 (1966), is greatly improved. This approach resembles the "smart Monte Carlo" method of P. J. Rossky, J. D. Doll, and H. L. Friedman, J. Chem. Phys. **69**, 4628 (1978).

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