A REJECTION METHOD FOR
SELECTION OF SCATTERED STATES

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ABSTRACT

A rejection method is presented that sidesteps much of the labor necessary in the usual techniques for choosing a scattered state after an electron-phonon collision with full band structure. The phonon wave number is chosen randomly, then tested to see if the resultant collision will satisfy energy conservation to within some accuracy. If not, the collision is rejected, and if so, then the wave number is adjusted in order to enforce energy conservation more precisely. The price one pays is in a high rejection rate. If the cost of a rejection is small, however, this rejection rate can be tolerated. This method will not compete with analytical models (near valley minima), but may outperform the more usual techniques. Accuracies of a few percent are practical.

I. INTRODUCTION

In Monte Carlo simulations, a time-consuming problem is the calculation of the phonon scattering rate for a given particle, and the selection of the scattered state given that a scatter has occurred. Typically, these two problems are dealt with separately. The scattering rate is usually tabulated in some fashion, and the scattered state is found randomly taking into account the surface within the Brillouin zone on which energy is conserved, and the density of states at each point on that surface.

One advance made early in deciding when to scatter a particle was the invention of the Null-Scatter, or Rejection method. In this method the scattering rate is assumed to be some simple function of the wave number (usually a step function) that is always larger than the true scattering rate. The true scattering rate *at the time of the scatter* can then be applied by rejecting some fraction of the intended scatters, *i.e.,* not scattering the particle. This technique has become almost universal.

Choosing a scattered state for a particle is a more difficult task, since momentum and energy must be conserved, implying that the scattered particle must lie on a complex surface within the Brillouin zone. Furthermore, the local density of states varies over that surface, and the scattering rate is proportional to the density of states. At least two groups have addressed this problem with reasonably accurate band structures. My interpretation of their techniques is the following: Fischetti and Laux [1], divide the Brillouin zone into small cubical cells, locate all the cells through which the energy-conserving surface passes, weight each cell according to the density of states, the scattering rate and the area of the energy-conserving surface contained within the cell, then choose a cell randomly according to these weights. The scattered state is chosen from the plane within the cell that approximates the energy-conserving surface. Yoder *et al.* [2], also choose such cubical cells randomly, and by a similar method. They then choose the scattered state by a rejection method: states are chosen randomly within the cell with a *uniform* distribution; if energy is not conserved within a given tolerance, the state is rejected and another state chosen at random until a suitable state is found. The present technique shares some features with that of Yoder *et al.*, but dispenses with the cells.

II. THE METHOD

The scattering rate from wave number k to wave number k′ can be written in the form

$$S(\mathbf{k},\mathbf{k}') = f(\mathbf{k},\mathbf{k}')g(\mathbf{p})\delta(E - E' \pm E_p)$$

where $p = \pm(k' - k)$, is the phonon wave number, E is the initial particle energy, E' is the final particle energy, and E_p is the phonon energy. Usually f does not vary strongly with k and k', and can be approximated by a constant — if this is not good enough, the rejection method can be used to correct the scattering rate. In the present work it is assumed that f is constant. For Polar optical phonons (most important for Gallium Arsenide), $g(p) \propto 1/p^2$ for small p.

The basis of the present method is to approximate the scattering rate as

$$S(k, k') \approx f(k, k') g(p) \cdot \frac{1}{2\Delta E} H(\Delta E - |E - E' \pm E_p|)$$

where H is the Heavyside step function, and ΔE can be virtually anything, as long as it is small enough to give an accurate measure of the local density of states. States are chosen at random over some domain known to encompass the energy-conserving surface (allowing for the energy mismatch ΔE), and those within the energy tolerance ΔE are accepted, while those that do not are rejected, and treated as null scatters. States that are accepted are then moved onto the energy-conserving surface using a second-order Newton's method (using both the first and second derivatives).

This technique has the advantages that no energies, densities of states, or surface areas must be computed and tabulated within cubical cells, nor need the actual scattering rate be calculated. Furthermore, the method is not tied to a mesh, and so its speed does not suffer when meshes are refined. It has the obvious disadvantage that a high rate of rejection is likely, so that fast evaluation of the energy is critical to minimize the time spent on rejections. (A mesh *is* used in the evaluation of the band energy.)

The accuracy of the method is limited by the value of ΔE. If one is not close to a critical energy (a valley, saddle point or maximum), the density of states is smooth, and it is easy to see that the error in the effective density of states will be of order ΔE^2. If one is close to a critical energy, one must either be sure that the resulting inaccuracy is of little consequence (as for maxima and saddle points, or when $\Delta E << kT$), or ensure that ΔE is small enough. For a parabolic ellipsoidal valley, one can show that as long as $E - \Delta E$ is above the energy of the valley minimum, the density of states is reasonably accurate. This fortuitous fact makes it possible to use this method near valleys, but since an analytic technique can be used near any but the X valleys in GaAs (which are not close to parabolic or ellipsoidal), it would probably not be the method of choice. Nonetheless, it has been implemented here.

Several techniques can be used to increase the speed of the method. For low energies one can reduce the k-space volume to be sampled to the regions around the valleys. This is especially easy when the scattering is independent of p, since then choosing p uniformly is equivalent to choosing k' uniformly, and any shape volume in which a wave number can easily be chosen with uniform probability density can be used; in particular, ellipsoids bounding the valleys can be used, eliminating most of the volume of the Brillouin zone. In this case, acceptance rates of 20%-50% can be achieved near valleys, with ΔE proportional to the energy above the valley minimum. At higher energies (sampling from the entire Brillouin zone), with $\Delta E = 0.2$ eV, acceptance rates of 10%-20% are typical (this is about as large as one can reasonably make ΔE).

When g is not constant, as in polar optical phonons, it is necessary to work in the phonon Brillouin zone. A fair amount of work is necessary to locate and surround the valleys (with a conical section of a spherical shell, in this case), making the method unattractive for low-energy scattering when analytical methods are applicable. This technique was used here as a proof-of-principle, regardless of its attractiveness. Another difficulty in the polar optical case is that for small p, g changes so rapidly that one must limit ΔE to less than about 1/5 of the phonon energy for reasonable accuracy. This would be a fatal restriction if it were necessary for ΔE to be independent of p. By making ΔE a function of p (in this work $\Delta E \propto \sqrt{p}$ for intra-valley and full-band scattering, constant for inter-valley scattering), ΔE can be made small only for small p. The result of this technique is an overall acceptance rate of between 4% and 6%, with the high-energy acceptance rate being on the low end.

The limits on the accuracy of this method might seem to be a drawback, but a fundamental limit exists in the accuracy of the semi-classical model. The source of this limit is in the application of Fermi's Golden Rule in computing the scattering rate. The Golden Rule assumes that a long period of time is available during which the interaction (a scatter in this case) may occur. In fact, the mean

scattering time is itself a limit on the time available for interaction. Heisenberg's uncertainty principle is applicable here, and indicates that the selection rules for momentum conservation and energy conservation will only hold to within limits determined by the mean free path, and the scattering time (and phonon life-time) respectively, according to $\Delta k \geq 1/2\lambda$ and $\Delta E \geq \hbar/2\tau$. This should not be interpreted as non-conservation of energy, of course, but as an indeterminacy in the band energy. For most semiconductors at high fields, the scattering rate implies an uncertainty in the carrier energy of almost 0.1 eV; of course, at low fields the scattering rates are much lower, and the bands are accordingly very narrow. This implies that the accuracy of the semi-classical model is probably limited to a few percent at high fields, and it would be pointless to attempt to reduce simulation errors below this level.

Once a scattered state has been accepted, it must be brought to the energy-conserving surface. To do this quickly requires at least the first derivatives of the energy with respect to the wave number, and preferably the second derivatives. In the present work a cubic interpolation scheme was used to compute the energy as a function of wave number. This scheme required most of those derivatives, and could interpolate them as well. The accuracy of interpolated derivatives used in Newton's method was of some concern, but the scheme has worked extremely well, with only one or two iterations necessary in most cases. If four iterations do not suffice, the state is discarded (this is very rare). One must also specify a direction in which the wave number will be moved in order to bring it to the energy-conserving surface. In general, this direction was taken to be the gradient *at each iteration*, but when the wave number was in a valley, it was constrained to move in a line through the center of the valley.

III. RESULTS

Simulations were performed with the first conduction band of Gallium Arsenide. The band structure was calculated using the pseudopotential method with the form factors of Cohen and Bergstresser [3]. Ten thousand particles were advanced in momentum, but not in space, with a uniform and constant electric field. Only polar optical phonon scattering was allowed, but both absorption and emission were included. The phonon temperature was 0.026 eV, and all phonons were assumed to have an energy of 0.0355 eV. No attempt was made to properly scale the time, electric field, velocity or scattering constant, but the time scale is a consequence of the electric field and the scattering constant, and the velocity is purely a diagnostic, so no arbitrary physical parameters are introduced. The simulation was run on a CRAY-YMP, but was not vectorized (much vectorization should be possible, but was avoided for simplicity).

The drift velocity versus electric field in the 100 direction is shown in Figure 1 (arbitrary units, lines delimit rough statistical error bounds). Acoustic phonon scattering is important for scattering at moderately large energies, so the saturation level should not be taken too seriously, but negative differential resistivity is clearly exhibited.
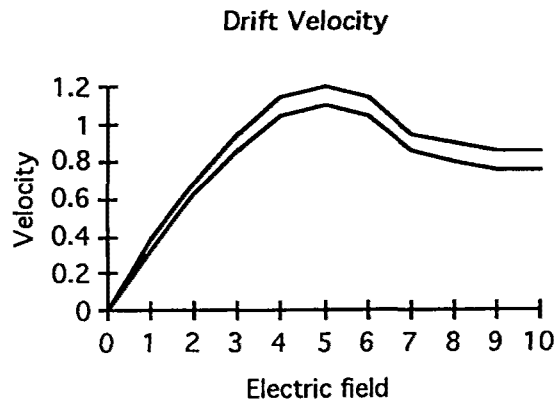
Fig. 1. Drift velocity versus field, polar optical scattering only.

Numerous tests were performed to ensure that the various parts of the test code were performing properly. These included scattering of an ensemble of particles from a single initial state, scatter plots of randomly chosen states from limited regions of the Brillouin zone and zero-field runs at various temperatures, as well as scatter plots of the actual simulation runs. These tests cannot guarantee that the code contains no errors, but serious error is unlikely and no potential errors are likely to affect the timing, which is of the most interest in assessing the usefulness of the scheme.

At low electric fields (with few particles outside the Γ valley) the mean computer time per actual scatter, including the cost of null scatters, is 1.6 ms. At higher electric fields (in the saturated regime), the mean time per scatter is 2.6 ms. The time required for a rejection outside the valleys is 70 μs, while an acceptance requires 140 μs. Within the valleys, a rejection requires 105 μs (an acceptance 175 μs), which is more than compensated by the higher acceptance rate for valley scatters. An evaluation of the electron energy requires 15 μs, and an evaluation of the energy with all its first and second derivatives requires 30 μs. For reference, a scalar multiply on the CRAY YMP requires 50 ns. All these times are for no vectorization at all. Obviously vectorization would improve the performance.

IV. SUMMARY

The rejection scheme for selection of scattered states presented here has been successfully implemented, and may be competitive when analytic methods are not applicable. When the scattering rate does not depend directly on the phonon momentum, the scheme is reasonably efficient. The scheme has a higher rejection rate when the scattering is not uniform in the phonon momentum. The high rejection rate may be compensated by the computational simplicity of the method and the relative speed of rejections.

The scheme can be extended to a complete and realistic scattering model, given the necessary data on band structures, overlap integrals and so on. The possible techniques for increasing the acceptance rate and improving the speed of rejections have not been exhausted.

REFERENCES

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[3] M.L. Cohen and T.K. Bergstresser, "Band structures and pseudopotential form factors for fourteen semiconductors of the diamond and zinc-blende structures", in Physical Review 141, 789 (1966).