The stationary Monte Carlo method for device simulation. I. Theory

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A theoretical analysis of the Monte Carlo method for steady-state semiconductor device simulation, also known as the single-particle Monte Carlo method, is presented. At the outset of the formal treatment is the stationary Boltzmann equation supplemented by boundary conditions, which is transformed into an integral equation. The conjugate equation has been formulated in order to develop forward Monte Carlo algorithms. The elements of the conjugate Neumann series are evaluated by means of Monte Carlo integration. Using this mathematically-based approach, the single-particle Monte Carlo method is derived in a formal way. In particular, the following are recovered: the probability densities for trajectory construction, both the time averaging and the synchronous ensemble methods for mean value calculation, and the rule that the initial points of the trajectories have to be generated from the velocity weighted boundary distribution. Furthermore, the independent, identically distributed random variables of the simulated process are identified. [DOI: 10.1063/1.1544654]

I. INTRODUCTION

The Monte Carlo (MC) method is known to be a versatile tool for the study of carrier transport phenomena in a large variety of semiconductor materials and devices. The method simulates the motion of charge carriers in the six-dimensional phase space formed by position and momentum. Subjected to the action of an external force field, the point-like carriers follow trajectories governed by Newton's law and the carrier's dispersion relation. These drift processes are interrupted by scattering events that are assumed to occur locally in space and instantaneously in time. The duration of a drift process, the type of scattering mechanism, and the state after scattering are selected randomly according to given probabilities that are characteristic to the microscopic process. In principle, such a procedure yields a carrier distribution that satisfies a Boltzmann equation (BE). The method of generating sequences of drift processes and scattering events appears so obvious from a physical point of view, that it is frequently interpreted as a direct emulation of the physical process rather than as a numerical method. The main MC algorithms used to date were originally devised from merely physical considerations, viewing a MC simulation as a simulated experiment. The proof that the used algorithms implicitly solve the BE was carried out later.[1–3]

In the field of semiconductor transport, the alternative way to use the BE as a starting point and to formulate MC algorithms for its solution was reported end of the 1980s.[4,5] This mathematically based approach lead to the development of algorithms such as the weighted ensemble MC method[6,7] and the backward MC method.[4,5] These early works focused on the transient problem.

In the present work, the theoretical background of the single-particle MC method is investigated, in order to prove this method for the calculation of steady-state device characteristics.

In Sec. II, the mathematical method used, including some basics of integral equations, the iteration series, and MC integration, are outlined. In Sec. III, the integral form of the stationary BE is derived. From the corresponding conjugate equation, the iteration terms of the Neumann series are obtained. Particular emphasis is put on the treatment of boundary conditions in the integral equation and the iteration terms. The evaluation of the iteration terms by means of Monte Carlo integration, which leads to the single-particle MC algorithm, is discussed in Sec. IV.

II. THE MATHEMATICAL METHOD

In semiclassical transport theory, the general problem to be considered is that of finding f to satisfy a Fredholm integral equation of the second kind:

$$f(x)=\int f(x')K(x',x)\mathrm{d}x'+f_0(x). \tag{1}$$

The kernel K describes the propagation of the particles in phase space, while the free term f_0 accounts for boundary and initial conditions. The variable x stands for $(\mathbf{k},\mathbf{r},t)$ in the transient case and for $(\mathbf{k},\mathbf{r})$ in steady state. Often one is more interested in statistical averages rather than in a point-wise evaluation of f. An average represents a linear functional of f, expressible in terms of an inner product:

$$(f,A)=\int f(x)A(x)\mathrm{d}x. \tag{2}$$

Substituting Eq. (1) recursively into itself gives an iteration series, known as the Neumann series, which is a formal solution to the integral equation[8]

$$f=f^{(0)}+f^{(1)}+f^{(2)}+\cdots. \tag{3}$$

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The iteration terms are defined recursively beginning with $f^{(0)}(x)=f_0(x)$:

$$f^{(n+1)}(x)=\int f^{(n)}(x')K(x',x)\,\mathrm{d}x'. \tag{4}$$

Since the integral form of the BE is a backward equation, the corresponding forward equation, that is the conjugate equation, needs to be derived. Its kernel is given by $K^{\dagger}(x,x')=K(x',x)$.

$$g(x')=\int g(x)K(x,x')\,\mathrm{d}x+A(x'). \tag{5}$$

Multiplying Eq. (1) by $g(x)$ and Eq. (5) by $f(x')$, and integrating over x and x', respectively, results in the equality

$$(f,A)=(g,f_0). \tag{6}$$

By means of Eq. (6), one can calculate a statistical average not only from *f*, but also from *g*, the solution of the conjugate equation. The given function *A* has to be used as the free term of the conjugate equation. Note that usage of Eq. (6) precludes a point-wise evaluation of the distribution function using a forward algorithm, because in this case $A(x)=\delta(x)$.

The link with the MC method is established by approaching the terms of the Neumann series by MC integration, the basic idea of which is briefly reviewed as follows.

A way of computing the integral

$$I=\int_a^b \phi(x)\,\mathrm{d}x=\int_a^b p(x)\,\psi(x)\,\mathrm{d}x, \tag{7}$$

is to represent it as an expected value of some random variable. Consider a factorization $\phi=p\psi$, where *p* is a density function; thus, *p* is non-negative and satisfies $\int_a^b p(x)\,\mathrm{d}x=1$. Integral (7) denotes the expected value of the random variable $\Psi: I=E\{\Psi\}$. In a MC simulation, a sample $x_1,\ldots x_N$ of the random variable *X* is generated from the density *p*, and the sample mean is computed which is an estimate of the expected value:

$$I\simeq\overline{\psi}=\frac{1}{N}\sum_{i=1}^{N}\psi(x_i). \tag{8}$$

In addition to the result *I*, the MC method gives an estimate of the error, which is obtained via the sample variance. Since the factorization of the integrand is not unique, different random variables can be introduced depending on the choice of the density *p*. All of them have the same expected value, but different variance.

III. THE BOLTZMANN EQUATION

Aiming at steady-state device simulation, the position-dependent and time-invariant BE is to be considered. The applied field and all material properties are independent of time.

$$[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}+\mathbf{F}(\mathbf{r})\cdot\nabla_{\mathbf{k}}]\,f(\mathbf{k},\mathbf{r})=Q[f]\,(\mathbf{k},\mathbf{r}),\quad \mathbf{r}\in D. \tag{9}$$

This equation, which is posed in the simulation domain *D*, is supplemented by boundary conditions modeling the interaction of the device with the environment. In semiconductor transport, the distribution function is commonly normalized as

$$\frac{1}{4\pi^3}\int_D \mathrm{d}\mathbf{r}\int \mathrm{d}\mathbf{k}\,f(\mathbf{k},\mathbf{r})=N_D, \tag{10}$$

where N_D denotes the number of carriers contained in the semiconductor domain of volume V_D. This normalization is based on the notion of discrete states in **k**-space, having a of density $2V_D/(2\pi)^3$, such that *f* can be viewed both as an occupation probability of the discrete state **k** and a density function in the continuous **k**-space. In both cases, however, *f* is to be interpreted as a density function with respect to **r**.

The force field **F** in Eq. (9) takes into account electric and magnetic fields. If the electric field **E** is dominant and the magnetic field can be neglected, the force field is approximated by $\mathbf{F}=q\mathbf{E}/\hbar$, where *q* is the charge of the carrier. The scattering operator $Q=Q_g-Q_l$ consists of a gain and a loss term, respectively. If many-body effects, such as carrier–carrier scattering and degeneracy, are neglected, the scattering operator will be linear, an assumption that is crucial for the presented approach. The two components of *Q* are

$$Q_g[f]\,(\mathbf{k},\mathbf{r})=\int f(\mathbf{k}',\mathbf{r})S(\mathbf{k}',\mathbf{k},\mathbf{r})\mathrm{d}\mathbf{k}', \tag{11}$$

$$Q_l[f]\,(\mathbf{k},\mathbf{r})=\lambda(\mathbf{k},\mathbf{r})f(\mathbf{k},\mathbf{r}), \tag{12}$$

with $\lambda(\mathbf{k},\mathbf{r})=\int S(\mathbf{k},\mathbf{k}',\mathbf{r})\,\mathrm{d}\mathbf{k}'$ denoting the total scattering rate.

A. Time invariance of the system

To describe a time-invariant system, an absolute time scale is obviously not needed. Only the time difference between two consecutive events is significant. The equations of motion in phase space are given by Newton's law (13) and the carrier's group velocity (14):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{K}(t)=\mathbf{F}[\mathbf{R}(t)], \tag{13}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{R}(t)=\mathbf{v}[\mathbf{K}(t)]. \tag{14}$$

A phase-space trajectory with the initial condition $\mathbf{K}(t_0)=\mathbf{k}_0$ and $\mathbf{R}(t_0)=\mathbf{r}_0$ is obtained by formal integration:

$$\mathbf{K}(t;t_0,\mathbf{k}_0,\mathbf{r}_0)=\mathbf{k}_0+\int_{t_0}^{t}\mathbf{F}[\mathbf{R}(y;t_0,\mathbf{k}_0,\mathbf{r}_0)]\,\mathrm{d}y,$$

$$\mathbf{R}(t;t_0,\mathbf{k}_0,\mathbf{r}_0)=\mathbf{r}_0+\int_{t_0}^{t}\mathbf{v}[\mathbf{K}(y;t_0,\mathbf{k}_0,\mathbf{r}_0)]\,\mathrm{d}y. \tag{15}$$

In addition to the time argument of the functions **K** and **R**, the parameters t_0, $\mathbf{k}_0$, $\mathbf{r}_0$ describing the initial condition of the phase-space trajectory are stated explicitly. Expressions (15) can be read as the phase-space position of a particle at time *t* that passes through $\mathbf{k}_0$ and $\mathbf{r}_0$ at time t_0. In this regard, the order of t_0 and *t* is irrelevant. For $t\leqslant t_0$, $\mathbf{k}_0$ and $\mathbf{r}_0$ denote a final condition.

Invariance under time translation can be proven, provided that **F** does not depend explicitly on time:

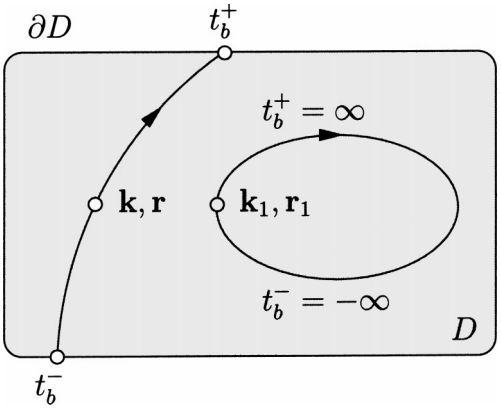

FIG. 1. Illustration of the functions $t_b^-(\mathbf{k},\mathbf{r})$ and $t_b^+(\mathbf{k},\mathbf{r})$ which give the time at a trajectory's entry point and exit point, respectively. If $\mathbf{k}_1$, $\mathbf{r}_1$ is the initial point of a closed trajectory, the times are infinite, $t_b^\pm(\mathbf{k}_1,\mathbf{r}_1)=\pm\infty$.

$$\mathbf{K}(t+\tau;\, t_0+\tau,\mathbf{k}_0,\mathbf{r}_0)=\mathbf{K}(t;\, t_0,\mathbf{k}_0,\mathbf{r}_0), \tag{16}$$

$$\mathbf{R}(t+\tau;\, t_0+\tau,\mathbf{k}_0,\mathbf{r}_0)=\mathbf{R}(t;\, t_0,\mathbf{k}_0,\mathbf{r}_0). \tag{17}$$

This property will be used repeatedly in the following to adjust conveniently the time reference for each free flight.

B. Integral form of the steady-state Boltzmann equation

In this section, the BE is transformed from integrodifferential form into integral form. Particular care is taken to account for the boundary conditions.

Assume a given phase-space point $\mathbf{k}$, $\mathbf{r}$. This point determines uniquely a phase-space trajectory, for which the notation $\mathbf{K}(t)=\mathbf{K}(t;\,0,\mathbf{k},\mathbf{r})$ and $\mathbf{R}(t)=\mathbf{R}(t;\,0,\mathbf{k},\mathbf{r})$ is used. The arbitrary initial time is set to $t_0=0$. The left-hand side of Eq. (9) represents the total time derivative of $\hat{f}(t)=f[\mathbf{K}(t),\mathbf{R}(t)]$, which allows the BE to be rewritten as an ordinary differential equation of first order:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}(t)+\hat{\lambda}(t)\hat{f}(t)=\hat{Q}_g[f](t). \tag{18}$$

The structure of the BE is more compact if multiplied by an integrating factor of the form $\exp[\int_0^t\hat{\lambda}(y)\mathrm{d}y]$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp\left[\int_0^t\hat{\lambda}(y)\mathrm{d}y\right]\hat{f}(t)=\exp\left[\int_0^t\hat{\lambda}(y)\mathrm{d}y\right]\hat{Q}_g[f](t). \tag{19}$$

This equation can be integrated straightforwardly. The upper bound of integration should be $t=0$ to obtain $\hat{f}(0)=f(\mathbf{k},\mathbf{r})$, the value of f at the given phase-space point. The lower-time bound has to be chosen such that the functions $\mathbf{K}(t)$ and $\mathbf{R}(t)$ take on values at which the distribution function is known. In the steady state, the distribution function is known only at the domain boundary. An appropriate lower time bound is therefore the time, say t_b^-, at which the trajectory enters the simulation domain (see Fig. 1). Apparently, this time depends on the point $\mathbf{k}$, $\mathbf{r}$ under consideration.

If the real-space trajectory $\mathbf{R}(t;\,0,\mathbf{k},\mathbf{r})$ never intersects the domain boundary, that is, when the trajectory forms a closed loop, then $t_b^-=-\infty$ is an appropriate choice. This means that a particle found at $t=0$ on such a closed trajectory must have been scattered onto this trajectory at some time $t\in(-\infty,0)$ in the past.

Integration of Eq. (19) in the time bounds discussed earlier results in the integral form of the stationary BE,

$$f(\mathbf{k},\mathbf{r})=\int_{t_b^-(\mathbf{k},\mathbf{r})}^0\mathrm{d}t'\int\mathrm{d}\mathbf{k}'\,f[\mathbf{k}',\mathbf{R}(t')]S[\mathbf{k}',\mathbf{K}(t'),\mathbf{R}(t')]\times\exp\left\{-\int_{t'}^0\lambda[\mathbf{K}(y),\mathbf{R}(y)]\mathrm{d}y\right\}+f_0(\mathbf{k},\mathbf{r}), \tag{20}$$

$$f_0(\mathbf{k},\mathbf{r})=f_b\{\mathbf{K}[t_b^-(\mathbf{k},\mathbf{r})],\mathbf{R}[t_b^-(\mathbf{k},\mathbf{r})]\}\times\exp\left\{-\int_{t_b^-(\mathbf{k},\mathbf{r})}^0\lambda[\mathbf{K}(y),\mathbf{R}(y)]\mathrm{d}y\right\}, \tag{21}$$

where f_b denotes the boundary distribution. The integral form is a bookkeeping equation for the probability $f(\mathbf{k},\mathbf{r})\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{r}$ of finding a carrier in the volume element $\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{r}$ of $\mathbf{k}$ and $\mathbf{r}$. The first summand in Eq. (20) describes the contribution of carriers that are scattered onto the considered trajectory at some time $t'\in(t_b^-,0)$ and stay on it until time 0, whereas the second summand gives the contribution of carriers that stay from the time of entry t_b^- on the trajectory and have a collisionless free flight until time 0, reaching the point of interest $\mathbf{k}$, $\mathbf{r}$.

In Eq. (20), the term $S(\mathbf{k}',\mathbf{k}_f)\mathrm{d}\mathbf{k}'\,\mathrm{d}t'$ denotes the probability of a transition from an initial state within the volume element $\mathrm{d}\mathbf{k}'$ to the final state $\mathbf{k}_f$ during the interval $\mathrm{d}t'$. This probability will in general be different from the forward transition probability $S(\mathbf{k}',\mathbf{k}_f)\mathrm{d}\mathbf{k}_f\mathrm{d}t'$, where the initial state is fixed and the final state is within some volume element $\mathrm{d}\mathbf{k}_f$. To obtain a forward MC algorithm, one has to change from integration over initial states to integration over final states, a task calling for the introduction of the conjugate equation.

C. The conjugate equation

Using the notation of Sec. II, the conjugate equation has the same kernel as the integral equation, but integration is carried out over the unprimed variables. To apply this rule, the integral form of the BE first has to be transformed into the standard form (1):

$$f(\mathbf{k},\mathbf{r})=\int\mathrm{d}\mathbf{k}'\int\mathrm{d}\mathbf{r}'\,f(\mathbf{k}',\mathbf{r}')K(\mathbf{k}',\mathbf{r}',\mathbf{k},\mathbf{r})+f_0(\mathbf{k},\mathbf{r})\,. \tag{22}$$

The required $\mathbf{r}'$ integration is introduced by augmenting the kernel by a δ-function.

$$K(\mathbf{k}',\mathbf{r}',\mathbf{k},\mathbf{r})=\int_{t_b^-(\mathbf{k},\mathbf{r})}^0\mathrm{d}t'\,S[\mathbf{k}',\mathbf{K}(t'),\mathbf{r}']\times\exp\left\{-\int_{t'}^0\lambda[\mathbf{K}(y),\mathbf{R}(y)]\mathrm{d}y\right\}\times\delta[\mathbf{r}'-\mathbf{R}(t')]\theta_D(\mathbf{r}'), \tag{23}$$

where θ_D is the indicator function of the simulation domain. Since the integral equation (22) is posed in the six-dimensional phase space, it must contain a sixfold integral.

The time integral in Eq. (20), therefore, cannot stay in Eq. (22), and has to be assigned consequently to the kernel. This means that the kernel of the stationary BE is given by the kernel of the transient BE integrated over time.

After changing variables and reversing time, as shown in Appendix A, the conjugate equation can be stated explicitly:

$$g(\mathbf{k}',\mathbf{r}') = \int \mathrm{d}\mathbf{k}_a \int_0^{t_b^+(\mathbf{k}_a,\mathbf{r}')} \mathrm{d}\tau\, S(\mathbf{k}',\mathbf{k}_a,\mathbf{r}') \times \exp\left\{ -\int_0^{\tau} \lambda[\mathbf{K}(y),\mathbf{R}(y)]\mathrm{d}y \right\} \times g[\mathbf{K}(\tau),\mathbf{R}(\tau)] + A(\mathbf{k}',\mathbf{r}'). \tag{24}$$

This equation has now the desired properties that integration is carried out over final states and that the time variable is positive. The iteration series of Eq. (24) will lead to forward MC algorithms.

D. Expressing mean values

Assume we are interested in the mean value of some quantity $A(\mathbf{k},\mathbf{r})$:

$$\langle\langle \mathrm{A} \rangle\rangle = \int_D \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{k}\, A(\mathbf{k},\mathbf{r}) f(\mathbf{k},\mathbf{r}). \tag{25}$$

A will typically be a product of some $\mathbf{k}$-dependent function and an $\mathbf{r}$-dependent charge assignment function.[9] The mean value per particle is obtained as $\langle \mathrm{A} \rangle = \langle\langle \mathrm{A} \rangle\rangle / \langle\langle 1 \rangle\rangle$.

Equation (25) is an inner product (A,f), which can be transformed into (f_0,g) by means of Eq. (6):

$$\langle\langle \mathrm{A} \rangle\rangle = \int_D \mathrm{d}\mathbf{r}' \int \mathrm{d}\mathbf{k}'\, f_b[\mathbf{K}_b(t_b^-),\mathbf{R}_b(t_b^-)] \times \exp\left\{ -\int_{t_b^-}^0 \lambda[\mathbf{K}_b(y),\mathbf{R}_b(y)]\mathrm{d}y \right\} g(\mathbf{k}',\mathbf{r}'). \tag{26}$$

Here, t_b^- is an abbreviation for $t_b^-(\mathbf{k}',\mathbf{r}')$ and $\mathbf{K}_b$ and $\mathbf{R}_b$ is the phase-space trajectory that passes through $\mathbf{k}'$ and $\mathbf{r}'$ at $t=0$.

In Eq. (26), variables need to be changed such that the arguments of f_b become integration variables. The new variables, $\mathbf{k}_b$ and $\mathbf{r}_b$, represent the initial state of a particle injected at the domain boundary. Since f_b is defined only at the boundary ∂D, the transformation must lead from a volume integral to a boundary integral.

In deriving the transformation first the domains of the involved variables have to be analyzed. The integration domain Φ is the direct product of D and K, the $\mathbf{k}$-space; thus, the following decomposition of Φ can be considered:

$$\Phi = D \otimes K = \Phi_b \cup \overline{\Phi}_b. \tag{27}$$

The subdomain Φ_b is formed by all points for which t_b^- is finite. Each point $\mathbf{k}'$, $\mathbf{r}' \in \Phi_b$ is connected with a boundary point $\mathbf{k}_b$, $\mathbf{r}_b$ by a free-flight trajectory. The complementary subdomain $\overline{\Phi}_b$ contains all points for which $t_b^- = -\infty$, that are those points that lie on closed trajectories. The integrand of Eq. (26) vanishes for all points in $\overline{\Phi}_b$ because of the exponential function, and therefore the integral over $\overline{\Phi}_b$ is zero, and is sufficient to restrict the integration domain to Φ_b.

Another decomposition needed in the following is that of the $\mathbf{k}$-space at a boundary point. If $\mathbf{n}(\mathbf{r}_b)$ denotes the outward directed normal vector in a point $\mathbf{r}_b$ at the domain boundary, the two subspaces are defined by

$$K_+(\mathbf{r}_b) = \{\mathbf{k}:\mathbf{v}(\mathbf{k})\cdot\mathbf{n}(\mathbf{r}_b) < 0\}, \tag{28}$$

$$K_-(\mathbf{r}_b) = \{\mathbf{k}:\mathbf{v}(\mathbf{k})\cdot\mathbf{n}(\mathbf{r}_b) \geqslant 0\}. \tag{29}$$

All $\mathbf{k}$-points in $K_+(\mathbf{r}_b)$ have an inward directed component of the group velocity and are therefore initial points of trajectories entering the domain at $\mathbf{r}_b$. Conversely, points in K_- are endpoints of trajectories leaving the domain.

Each point $(\mathbf{k}',\mathbf{r}') \in \Phi_b$ can now be mapped one-to-one onto a boundary point $(\mathbf{k}_b,\mathbf{r}_b)$ and a positive time t_0, where $\mathbf{k}_b \in K_+(\mathbf{r}_b)$ and $\mathbf{r}_b \in \partial D$. The time $t_0 = -t_b^-(\mathbf{k}',\mathbf{r}')$ is the time necessary for a particle to drift from the boundary point $(\mathbf{k}_b,\mathbf{r}_b)$ to the inner point $(\mathbf{k}',\mathbf{r}')$. This transformation is carried out formally in Appendix B. The volume element transforms as

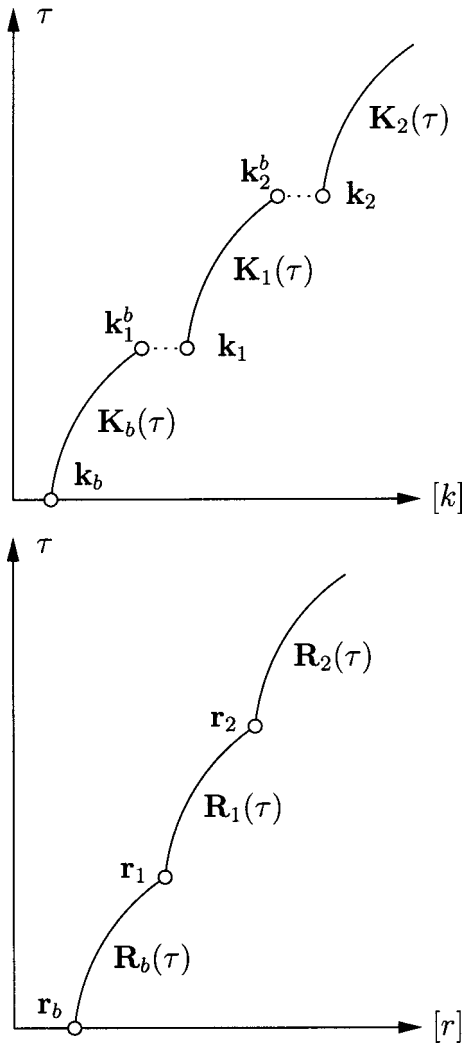

FIG. 2. Sketch of a trajectory which starts at the boundary point $(\mathbf{k}_b,\mathbf{r}_b)$ and evolves until the third free flight. The symbols used in Eq. (35) are shown.

$$d\mathbf{r}'\, d\mathbf{k}' = |v_\perp(\mathbf{k}_b)|\, d\sigma(\mathbf{r}_b)\, d\mathbf{k}_b dt_0, \tag{30}$$

where $d\sigma(\mathbf{r}_b)$ is the surface element at $\mathbf{r}_b$, and Eq. (26) becomes

$$\begin{aligned}\langle\langle A\rangle\rangle = & \oint_{\partial D} d\sigma(\mathbf{r}_b) \int_{K_+(\mathbf{r}_b)} d\mathbf{k}_b \\ & \times \int_0^{t_b^+(\mathbf{k}_b,\mathbf{r}_b)} dt_0 |v_\perp(\mathbf{k}_b)| f_b(\mathbf{k}_b,\mathbf{r}_b) \\ & \times \exp\left\{ -\int_0^{t_0} \lambda[\mathbf{K}_b(y),\mathbf{R}_b(y)]dy \right\} \\ & \times g[\mathbf{K}_b(t_0),\mathbf{R}_b(t_0)].\end{aligned} \tag{31}$$

The accomplished change from volume to boundary integration is a key step in the treatment of the boundary value problem. It proves that knowledge of the boundary distribution is sufficient to determine arbitrary volume integrals defined by Eq. (25) and therefore to determine f uniquely.

Note that from f_b, only the part in K_+ determines the boundary condition, whereas the part in K_- is unknown and is a result of the simulation.

Required for the purpose of normalization are the integrals

$$j_\perp(\mathbf{r}) = \int_{K_+(\mathbf{r})} d\mathbf{k} |v_\perp(\mathbf{k})| f_b(\mathbf{k},\mathbf{r}), \quad \mathbf{r} \in \partial D, \tag{32}$$

$$\Gamma_D = \oint_{\partial D} j_\perp(\mathbf{r}) d\sigma(\mathbf{r}). \tag{33}$$

Taking into account the normalization given in (10), $j_\perp/(4\pi^3)$ represents the normal component of the incident particle current density and $\Gamma_D/(4\pi^3)$ the total incident particle current.

E. The Neumann series

Substituting the Neumann series of the conjugate equation, $g = \Sigma_0^\infty g^{(i)}$, into Eq. (31) results in a series for the mean value, for which the following notation is adopted:

$$\langle\langle A\rangle\rangle = \sum_{i=0}^{\infty} \langle\langle A\rangle\rangle_i. \tag{34}$$

As an instructive example the term of second order is stated explicitly:

$$\begin{aligned}\langle\langle A\rangle\rangle_2 = & \oint_{\partial D} d\sigma(\mathbf{r}_b) \int_{K_+(\mathbf{r}_b)} d\mathbf{k}_b \int_0^{t_b^+(\mathbf{k}_b,\mathbf{r}_b)} dt_0 \int d\mathbf{k}_1 \int_0^{t_b^+(\mathbf{k}_1,\mathbf{r}_1)} dt_1 \int d\mathbf{k}_2 \int_0^{t_b^+(\mathbf{k}_2,\mathbf{r}_2)} dt_2 |v_\perp(\mathbf{k}_b)| f_b(\mathbf{k}_b,\mathbf{r}_b) \\ & \times \exp\left\{ -\int_0^{t_0} \lambda[\mathbf{K}_b(y),\mathbf{R}_b(y)]dy \right\} S[\mathbf{K}_b(t_0),\mathbf{k}_1,\mathbf{R}_b(t_0)] \exp\left\{ -\int_0^{t_1} \lambda[\mathbf{K}_1(y),\mathbf{R}_1(y)]dy \right\} S[\mathbf{K}_1(t_1),\mathbf{k}_2,\mathbf{R}_1(t_1)] \\ & \times \exp\left\{ -\int_0^{t_2} \lambda[\mathbf{K}_2(y),\mathbf{R}_2(y)]dy \right\} A[\mathbf{K}_2(t_2),\mathbf{k}_2,\mathbf{R}_2(t_2)].\end{aligned} \tag{35}$$

Initial conditions for the $\mathbf{k}$-space trajectories are given by $\mathbf{k}_b$ and the after-scattering states $\mathbf{k}_i$, respectively, as shown in Fig. 2:

$$\mathbf{K}_b(0) = \mathbf{k}_b \tag{36}$$

$$\mathbf{K}_i(0) = \mathbf{k}_i, \quad i = 1,2,\ldots. \tag{37}$$

The real space trajectory is continuous at the time of scattering. It holds $\mathbf{R}_b(0) = \mathbf{r}_b$ and $\mathbf{R}_i(t_i) = \mathbf{R}_{i+1}(0)$.

The iteration term (35) describes the contribution of all particles that propagate from the boundary to the interior of the device, having undergone two scattering events and finished the third free flight. Analogously, the ith iteration term, $\langle\langle A\rangle\rangle_i$, represents the contribution of all particles which propagate into the device with i scattering events and $i+1$ free flights.

Furthermore, the symbols $\mathbf{k}_i^b$ and $\mathbf{r}_i$ are introduced, which denote the before-scattering momentum and the particle position for the ith scattering event, respectively. They are related to the trajectories by

$$\mathbf{r}_{i+1} = \mathbf{R}_i(t_i), \tag{38}$$

$$\mathbf{k}_{i+1}^b = \mathbf{K}_i(t_i). \tag{39}$$

IV. THE MONTE CARLO METHOD

As a next step, the integrand of the iteration term (35) must be decomposed into a probability density p and a random variable ψ, as shown in Eq. (7). For this purpose we repeat the well-known probability densities used in MC device simulation, which are the distribution of the free-flight time, p_t, and that of the state after scattering, p_k:

$$p_t(t;\mathbf{k},\mathbf{r}) = \lambda[\mathbf{K}(t),\mathbf{R}(t)] \exp\left\{ -\int_0^t \lambda[\mathbf{K}(y),\mathbf{R}(y)]dy \right\}, \tag{40}$$

$$p_k(\mathbf{k}';\mathbf{k},\mathbf{r}) = \frac{S(\mathbf{k},\mathbf{k}',\mathbf{r})}{\lambda(\mathbf{k},\mathbf{r})}. \tag{41}$$

Both distributions are normalized as they satisfy for all $\mathbf{k}$, $\mathbf{r}$:

$$\int_0^\infty p_t(t;\mathbf{k},\mathbf{r})\,\mathrm{d}t = 1, \tag{42}$$

$$\int p_k(\mathbf{k}';\mathbf{k},\mathbf{r})\,\mathrm{d}\mathbf{k}' = 1. \tag{43}$$

In the integrand of Eq. (35), terms representing an unnormalized probability density are divided by the respective normalization factors. Beginning with the left-most term, the velocity-weighted boundary distribution $v_\perp f_b$, these factors are given by Eqs. (32) and (33). Products of the form $\exp(-\int\lambda)\,S$ are extended by λ/λ in order to obtain the free-flight-time distribution of the form $p_t=\lambda\exp(-\int\lambda)$ and the distribution of the after-scattering states, $p_k=S/\lambda$. The modifications outlined above are applied in such a way that the value of the multiple integral remains unchanged. The remaining product of the form $\exp(-\int\lambda)\,A$ can be treated in two different ways, leading to either the *synchronous ensemble* method or the *time-integration* method of average recording.

A. The synchronous ensemble method

One option is to multiply $\exp(-\int\lambda)A$ again by λ/λ to obtain a product of p_t and A/λ. For the sake of brevity, the position-dependence of the scattering rate is suppressed in the following. Equation (35) becomes:

$$\begin{aligned}\langle\langle \mathrm{A}\rangle\rangle_2 = \Gamma_D \oint_{\partial D}\mathrm{d}\sigma\int_{K_+}\mathrm{d}\mathbf{k}_b\int_0^{t_{b0}^+}\mathrm{d}t_0\int\mathrm{d}\mathbf{k}_1\int_0^{t_{b1}^+}\mathrm{d}t_1\int\mathrm{d}\mathbf{k}_2\int_0^{t_{b2}^+}\mathrm{d}t_2\left\{\frac{j_\perp(\mathbf{r}_b)}{\Gamma_D}\right\}\left\{\frac{|v_\perp(\mathbf{k}_b)|f_b(\mathbf{k}_b,\mathbf{r}_b)}{j_\perp(\mathbf{r}_b)}\right\}\\ \times\left\{\lambda[\mathbf{K}_b(t_0)]\exp\left(-\int_0^{t_0}\lambda[\mathbf{K}_b(y)]\mathrm{d}y\right)\right\}\left\{\frac{S[\mathbf{K}_b(t_0),\mathbf{k}_1]}{\lambda[\mathbf{K}_b(t_0)]}\right\}\left\{\lambda[\mathbf{K}_1(t_1)]\exp\left(-\int_0^{t_1}\lambda[\mathbf{K}_1(y)]\mathrm{d}y\right)\right\}\\ \times\left\{\frac{S[\mathbf{K}_1(t_1),\mathbf{k}_2]}{\lambda[\mathbf{K}_1(t_1)]}\right\}\left\{\lambda[\mathbf{K}_2(t_2)]\exp\left(-\int_0^{t_2}\lambda[\mathbf{K}_2(y)]\mathrm{d}y\right)\right\}\frac{A[\mathbf{K}_2(t_2),\mathbf{R}_2(t_2)]}{\lambda[\mathbf{K}_2(t_2)]}.\end{aligned} \tag{44}$$

Each term representing a probability density is enclosed in curly brackets. In Eq. (44) we designate the multidimensional integration variable as x_2, the probability density as p_2, and a random variable as ψ_2: $\langle\langle \mathrm{A}\rangle\rangle_2 = \int \mathrm{d}x_2\, p_2(x_2)\psi_2(x_2)$, where

$$x_2=(\mathbf{r}_b,\mathbf{k}_b,t_0,\mathbf{k}_1,t_1,\mathbf{k}_2,t_2), \tag{45}$$

$$p_2(x_2)=\{j_\perp/\Gamma_D\}\{v_\perp f_b/j_\perp\}\{p_t\}\{p_k\}\{p_t\}\{p_k\}\{p_t\}, \tag{46}$$

$$\psi_2(x_2)=A/\lambda \tag{47}$$

To evaluate Eq. (44) by MC integration one has to generate a sample $x_{2,1}\ldots x_{2,N}$ from the density p_2. A realization $x_{2,j}$ is referred to as a numerical trajectory, its generation as numerical trajectory construction.

In the following, we consider the construction of the jth numerical trajectory $x_{2,j}$. Since all factors in Eq. (46), except $j_\perp/\Gamma_D$, denote conditional probability densities, one first selects a boundary point $\mathbf{r}_{b,j}$ with the density $j_\perp/\Gamma_D$. We generate $\mathbf{k}_{b,j}$ from the velocity-weighted boundary distribution, we generate $t_{0,j}$ from the free-flight time distribution p_t, we select $\mathbf{k}_{1,j}$ with density p_k, and so forth. Finally, at the end of the third free flight we evaluate A/λ. After construction of N numerical trajectories, the following sample mean is formed:

$$\langle\langle \mathrm{A}\rangle\rangle_2 \simeq \frac{\Gamma_D}{N}\sum_{j=1}^{N}\psi_2(x_{2,j}). \tag{48}$$

This procedure contains all basic steps known from single-particle MC algorithm:

- generation of an initial state from the velocity-weighted boundary distribution, $v_\perp f_b$ (see for example, Ref. 10)
- free-flight time generation from density p_t
- selection of the after scattering state with density p_k
- the synchronous ensemble method of average recording.[11]

In Eq. (44), the bounds of time integration are $(0,t_{bj}^+)$, where t_{bj}^+ can be either finite or infinite. Note that the distribution of the free-flight time (40) is normalized in the bounds $(0,\infty)$. The issue of normalization is related to trajectories that terminate at the domain boundary (cf. Sec. IV C).

B. The time averaging method

A second option is to process the t_2-integral in Eq. (35) by integration by parts:

$$\begin{aligned}&\int_0^\infty\exp\left(-\int_0^{t_2}\lambda[\mathbf{K}_2(y),\mathbf{R}_2(y)]\mathrm{d}y\right)\\ &\times H(t_{b2}^+-t_2)A[\mathbf{K}_2(t_2),\mathbf{R}_2(t_2)]\mathrm{d}t_2\\ &=\int_0^\infty\mathrm{d}t_2\lambda[\mathbf{K}_2(t_2)]\exp\left(-\int_0^{t_2}\lambda[\mathbf{K}_2(y)]\mathrm{d}y\right)\\ &\quad\times\int_0^{t_2}H(t_{b2}^+-\tau)A[\mathbf{K}_2(\tau),\mathbf{R}_2(\tau)]\mathrm{d}\tau,\end{aligned} \tag{49}$$

where H stands for the unit step function. On the left-hand side, $\exp(-\int)$ represents the probability that a particle drifts without scattering from 0 to t_2. Differentiating this probability gives the probability density p_t appearing on the right side. In this way, the density p_2 defined by Eq. (46) is recovered, and the iteration term can be reformulated as

$$\langle\langle \mathrm{A} \rangle\rangle_2 = \Gamma_D \oint_{\partial D} \mathrm{d}\sigma \int_{K_+} \mathrm{d}\mathbf{k}_b \int_0^{t_{b0}^+} \mathrm{d}t_0 \int \mathrm{d}\mathbf{k}_1 \int_0^{t_{b1}^+} \mathrm{d}t_1 \times \int \mathrm{d}\mathbf{k}_2 \int_0^{\infty} \mathrm{d}t_2 p_2(\mathbf{r}_b, \mathbf{k}_b, t_0, \mathbf{k}_1, t_1, \mathbf{k}_2, t_2) \times \int_0^{\tau_2} A[\mathbf{K}_2(\tau), \mathbf{R}_2(\tau)]\, \mathrm{d}\tau, \tag{50}$$

with $\tau_2 = \min(t_{b2}^+, t_2)$. The random variable ψ_2 in this expression is identified as the path integral over τ. As opposed to Eq. (44), the integration domain of t_2 is now $(0,\infty)$, which means that the random variable is nonzero regardless of the selected value for t_2. If $t_2 < t_{b2}^+$, the τ-integration is performed until the next scattering event occurs, otherwise until the boundary is reached.

C. Monte Carlo evaluation of the iteration series

One peculiarity of the single-particle MC method is that the sample for the iteration term of order i is not generated independently from that for the term of order $i-1$. Instead, x_i is generated by adding to x_{i-1} another after-scattering state $\mathbf{k}_i$ and another free-flight time t_i. The aim of this section is to find that random variable whose realizations are independent from each other.

We begin the analysis with the iteration term of order zero. Setting $g^{(0)} = A$ it follows from Eq. (31),

$$\langle\langle \mathrm{A} \rangle\rangle_0 = \Gamma_D \oint_{\partial D} \mathrm{d}\sigma \int_{K_+} \mathrm{d}\mathbf{k}_b \int_0^{t_{b0}^+} \mathrm{d}t_0 p_0(\mathbf{r}_b, \mathbf{k}_b, t_0) \times \frac{A[\mathbf{K}_b(t_0), \mathbf{R}_b(t_0)]}{\lambda[\mathbf{K}_b(t_0)]}, \tag{51}$$

with

$$p_0(\mathbf{r}_b, \mathbf{k}_b, t_0) = \left\{ \frac{j_\perp(\mathbf{r}_b)}{\Gamma_D} \right\} \left\{ \frac{|v_\perp(\mathbf{k}_b)| f_b(\mathbf{k}_b, \mathbf{r}_b)}{j_\perp(\mathbf{r}_b)} \right\} \times \left\{ \lambda[\mathbf{K}_b(t_0)] \exp\left(- \int_0^{t_0} \lambda[\mathbf{K}_b(y)]\, \mathrm{d}y \right) \right\}. \tag{52}$$

The idea is now to add a scattering term and another free-flight term to the density p_0. The formal procedure is to multiply Eq. (51) by

$$\int \mathrm{d}\mathbf{k}_1 \left\{ \frac{S[\mathbf{K}_b(t_0), \mathbf{k}_1]}{\lambda[\mathbf{K}_b(t_0)]} \right\} \int_0^{\infty} \mathrm{d}t_1 \left\{ \lambda[\mathbf{K}_1(t_1)] \times \exp\left(- \int_0^{t_1} \lambda[\mathbf{K}_1(y)]\, \mathrm{d}y \right) \right\} = 1, \tag{53}$$

the product of two normalization integrals. In this way, p_0 is multiplied by two factors such that the product gives p_1. This allows the partial sum of the first two iteration terms to be rewritten as one multiple integral:

$$\langle\langle \mathrm{A} \rangle\rangle_0 + \langle\langle \mathrm{A} \rangle\rangle_1 = \Gamma_D \oint_{\partial D} \mathrm{d}\sigma \int_{K_+} \mathrm{d}\mathbf{k}_b \int_0^{\infty} \mathrm{d}t_0 \int \mathrm{d}\mathbf{k}_1 \times \int_0^{\infty} \mathrm{d}t_1 p_1(\mathbf{r}_b, \mathbf{k}_b, t_0, \mathbf{k}_1, t_1) \times H(t_{b0}^+ - t_0) \left[\frac{A(\mathbf{k}_1^b, \mathbf{r}_1)}{\lambda(\mathbf{k}_1^b)} + H(t_{b1}^+ - t_1) \frac{A(\mathbf{k}_2^b, \mathbf{r}_2)}{\lambda(\mathbf{k}_2^b)} \right]. \tag{54}$$

Here, the electron momentum before scattering, $\mathbf{k}_i^b$, is defined by Eq. (39). Since the integration domain of, for instance, t_1, is different in Eqs. (44) and (54), time integration is generally carried out in $(0,\infty)$, while the integrand is set to zero above the actual time bound using the unit step function. Multiplying Eq. (54) by an integral similar to Eq. (53) and adding $\langle\langle \mathrm{A} \rangle\rangle_2$, gives the partial sum of the first three iteration terms expressed as one multiple integral. This procedure can be repeated to express the partial sum of any order n as one multiple integral

$$\langle\langle \mathrm{A} \rangle\rangle_0 + \langle\langle \mathrm{A} \rangle\rangle_1 + \ldots + \langle\langle \mathrm{A} \rangle\rangle_n = \int p_n(x_n) \psi^{[n]}(x_n) \mathrm{d}x_n, \tag{55}$$

using the recursive definitions

$$x_n = (x_{n-1}, \mathbf{k}_n, t_n), \tag{56}$$

$$p_n = p_{n-1} \times \left\{ \frac{S(\mathbf{k}_n^b, \mathbf{k}_n)}{\lambda(\mathbf{k}_n^b)} \right\} \left\{ \lambda[\mathbf{K}_n(t_n)] \times \exp\left(- \int_0^{t_n} \lambda[\mathbf{K}_n(y)] \mathrm{d}y \right) \right\}, \tag{57}$$

$$\psi^{[n]} = \psi^{[n-1]} + \prod_{j=0}^{n} H(t_{bj}^+ - t_j) \frac{A(\mathbf{k}_{n+1}^b, \mathbf{r}_{n+1})}{\lambda(\mathbf{k}_{n+1}^b)}. \tag{58}$$

At the beginning of the recursions are $x_0 = (\mathbf{k}_b, \mathbf{r}_b, t_0)$, p_0 given by Eq. (52), and $\psi^{[-1]} = 0$. Clearly, Eqs. (56) and (57) are generalizations for arbitrary n of Eqs. (45) and (46), respectively.

At the moment, it is assumed that the series given by Eq. (55) is convergent, which means that there exists always some n such that the series of the truncated elements is below a desired limit. To evaluate Eq. (55) by MC integration, one has to generate N realizations of the random variable x_n. As described in Sec. III E first the initial state at the boundary, $\mathbf{r}_b$, $\mathbf{k}_b$, and the first free-flight time, t_0, have to be generated from p_0. If t_0 is less than t_{b0}^+ the unit step function in Eq. (58) evaluates to one and hence $\psi^{[0]} = A(\mathbf{k}_1^b, \mathbf{r}_1)/\lambda(\mathbf{k}_1^b)$. In this case, numerical trajectory construction is continued by realizing a scattering event from $\mathbf{k}_1^b$ to $\mathbf{k}_1$ and by choosing t_1. Again, if $t_1 < t_{b1}^+$, one must compute $\psi^{[1]} = \psi^{[0]} + A(\mathbf{k}_2^b, \mathbf{r}_2)/\lambda(\mathbf{k}_2^b)$. In principle, this process should be continued until $\psi^{[n]}$ is obtained. However, if in the course of numerical trajectory construction a time $t_l > t_{bl}^+$ is generated, the unit step function in Eq. (58) evaluates to zero, such that the recursion terminates and the random vari-

able keeps the value $\psi^{[l-1]}$. This is the realization of a numerical trajectory terminating at the boundary during the lth free flight.

For a numerical trajectory of arbitrary ordering number $i \leqslant N$, which terminates after $l+1$ free-flight segments, the random variable takes the value

$$\psi_i = \frac{A(\mathbf{k}_1^b, \mathbf{r}_1)}{\lambda(\mathbf{k}_1^b)} + \cdots + \frac{A(\mathbf{k}_l^b, \mathbf{r}_l)}{\lambda(\mathbf{k}_l^b)}. \tag{59}$$

The ψ_i given by Eq. (59) are summed up in the sample mean (8). This gives a double sum that can be replaced by one sum over all generated before-scattering states:

$$\langle\langle \mathrm{A} \rangle\rangle \simeq \Gamma_D \frac{1}{N} \sum_{i=1}^{N} \psi_i = \Gamma_D \frac{1}{N} \sum_b \frac{A(\mathbf{k}^b, \mathbf{r}^b)}{\lambda(\mathbf{k}^b)}. \tag{60}$$

Choosing *n a priori* implies that a numerical trajectory cannot contain more than $n+1$ free-flight segments. This restriction can be omitted by always following a numerical trajectory until it terminates at the boundary, permitting numerical trajectories with arbitrary many free-flight segments. In this case the infinite series representing $\langle\langle \mathrm{A} \rangle\rangle$ is evaluated exactly rather than the partial sum given by Eq. (55).

There exists another representation for the series (55) in which all possible realizations of the random variable ψ appear explicitly. At the outset of this expansion is again Eq. (51); however, in the multipliers of the form (53) the time integral is split at the boundary time:

$$\int \mathrm{d}\mathbf{k}_i \int_0^{t_{bi}^+} \mathrm{d}t_i + \int \mathrm{d}\mathbf{k}_i \int_{t_{bi}^+}^{\infty} \mathrm{d}t_i = 1. \tag{61}$$

Following the same steps that have led to the series (55) one obtains

$$\langle\langle \mathrm{A} \rangle\rangle = I_1(A) + I_2(A) + \cdots. \tag{62}$$

As examples, the lowest-order elements are shown:

$$I_1(A) = \Gamma_D \int \mathrm{d}\sigma \, \mathrm{d}\mathbf{k}_b \, \mathrm{d}\mathbf{k}_1 \int_0^{t_{b0}^+} \mathrm{d}t_0 \int_{t_{b1}^+}^{\infty} \mathrm{d}t_1 \, p_1 \times \frac{A(\mathbf{k}_1^b, \mathbf{r}_1)}{\lambda(\mathbf{k}_1^b)}, \tag{63}$$

$$I_2(A) = \Gamma_D \int \mathrm{d}\sigma \, \mathrm{d}\mathbf{k}_b \, \mathrm{d}\mathbf{k}_1 \, \mathrm{d}\mathbf{k}_2 \int_0^{t_{b0}^+} \mathrm{d}t_0 \int_0^{t_{b1}^+} \mathrm{d}t_1 \int_{t_{b2}^+}^{\infty} \mathrm{d}t_2 \, p_2 \times \left[\frac{A(\mathbf{k}_1^b, \mathbf{r}_1)}{\lambda(\mathbf{k}_1^b)} + \frac{A(\mathbf{k}_2^b, \mathbf{r}_2)}{\lambda(\mathbf{k}_2^b)} \right]. \tag{64}$$

After augmentation of the time integration domains to $(0,\infty)$, one finds that the integrand of $I_n(A)$ is the product of p_n and $\hat{\psi}^{[n]}$, defined by

$$\hat{\psi}^{[n]} = \prod_{j=0}^{n-1} H(t_{bj}^+ - t_j) H(t_n - t_{bn}) \sum_{j=1}^{n} \frac{A(\mathbf{k}_j^b, \mathbf{r}_j)}{\lambda(\mathbf{k}_j^b)}. \tag{65}$$

The task is to evaluate an infinite number of integrals. By construction of one numerical trajectory, a realization of the infinite set of random variables $\psi^{[0]}, \psi^{[1]} \ldots$ is obtained simultaneously. If the sequence of generated free-flight times, $t_0, \ldots, t_n$ satisfies the conditions $t_i < t_{bi}^+$ for $i < n$ and $t_n > t_{bn}^+$, then the nth random variable is nonzero, with a value given by Eq. (59), while all the other ones evaluate identically to zero.

In the remainder of this section, expressions for the time-recording formalism are summarized. The starting point is the zero order iteration term reformulated as

$$\langle\langle \mathrm{A} \rangle\rangle_0 = \Gamma_D \oint_{\partial D} \mathrm{d}\sigma \int_{K_+} \mathrm{d}\mathbf{k}_b \int_0^{\infty} \mathrm{d}t_0 \, p_0(\mathbf{r}_b, \mathbf{k}_b, t_0) \times \int_0^{\tau_0} A[\mathbf{K}_b(\tau), \mathbf{R}_b(\tau)] \, \mathrm{d}\tau. \tag{66}$$

This expression shows $\psi^{[0]}$ explicitly. The recursive definition of the random variable changes from (58) to

$$\psi^{[0]} = \int_0^{\tau_0} A[\mathbf{K}_b(\tau), \mathbf{R}_b(\tau)] \, \mathrm{d}\tau, \tag{67}$$

$$\psi^{[n]} = \psi^{[n-1]} + \prod_{j=0}^{n-1} H(t_{bj}^+ - t_j) \int_0^{\tau_n} A[\mathbf{K}_n(\tau), \mathbf{R}_n(\tau)] \, \mathrm{d}\tau, \tag{68}$$

where $\tau_j = \min(t_{bj}^+, t_j)$.

For a numerical trajectory comprising $l+1$ free-flight segments, the random variable takes on the value

$$\psi_i = \int_0^{t_0} A \, \mathrm{d}\tau + \ldots \int_0^{t_{l-1}} A \, \mathrm{d}\tau + \int_0^{t_{bl}} A \, \mathrm{d}\tau. \tag{69}$$

This sum is over free flights and contains, therefore, one element more than Eq. (59).

D. Normalization of the distribution function

The normalization constant Γ_D should not be evaluated from the theoretical definition (10). Instead, by setting $A = 1$, a relation between Γ_D and the total number of particles N_D is obtained:

$$4\pi^3 N_D = \Gamma_D \frac{1}{N} \sum_b \lambda(\mathbf{k}^b)^{-1}, \tag{70}$$

where N_D is usually known, for instance, from the constraint of total charge neutrality in the device. N is the number of trajectories constructed. In the special case $A = 1$, the realization (69) represents the total time of the ith numerical trajectory, $\psi_i = T_i$. With $T = \Sigma T_i$ denoting the total time the particle has been followed, one finds from Eq. (70):

$$T = \sum_b \lambda(\mathbf{k}^b)^{-1}. \tag{71}$$

The finite sum recorded during the simulation is an unbiased estimate of the total time the particle path is followed.

E. Convergence of the iteration series

Since the one-particle MC method has been applied successfully to a large variety of materials, systems, and conditions, it can be expected that the series expansion of the BE converges for a wide range of models, such as scattering rate and band structure models. In the following, convergence of the series (62) is proven for the simple case that the subspace

$\overline{\Phi}_b$ (see Sec. III D) is empty. Then, every point in $D\otimes K$ is connected to a boundary point via a free-flight trajectory, and the function $t_b^+(\mathbf{k},\mathbf{r})$ is bounded. Furthermore, it is assumed that the total scattering rate, which is non-negative, has upper and lower bounds and that A has an upper bound. For all $(\mathbf{r},\mathbf{k})\in D\otimes K$ it must hold

$$t_b^+(\mathbf{k},\mathbf{r})\leqslant t_m,\quad \lambda(\mathbf{k},\mathbf{r})\leqslant\lambda_m,$$
$$A(\mathbf{k},\mathbf{r})\leqslant A_m,\quad \lambda(\mathbf{k},\mathbf{r})\geqslant\lambda_{\min}>0. \tag{72}$$

Note that in systems with phonon absorption, λ is nonzero even for zero energy, such that a nonzero $\lambda_{\min}$ does exist. The following proof is similar to that for the transient problem reported in Ref. 12. Using the constants defined earlier, an upper bound for Eq. (64) can be derived:

$$I_2(A)\leqslant\Gamma_D\frac{2A_m}{\lambda_{\min}}\int \mathrm{d}\sigma\,\mathrm{d}\mathbf{k}_b\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2\int_0^{t_{b0}^+}\mathrm{d}t_0\int_0^{t_{b1}^+}\mathrm{d}t_1\int_{t_{b2}^+}^{\infty}\mathrm{d}t_2\,p_2. \tag{73}$$

The integral with respect to t_2 can be evaluated explicitly and estimated by

$$\int_{t_{b2}^+}^{\infty}\mathrm{d}t_2\lambda[\mathbf{K}_2(t_2)]\exp\left\{-\int_0^{t_2}\lambda[\mathbf{K}_2(y)]\mathrm{d}y\right\}$$
$$=\exp\left\{-\int_0^{t_{b2}^+}\lambda[\mathbf{K}_2(y)]\mathrm{d}y\right\}\leqslant 1. \tag{74}$$

After having replaced this integral with its upper bound being 1, in the resulting inequality the $\mathbf{k}_2$ integration of the distribution S/λ can be carried out, giving one. After this step integration over t_1 is possible.

$$\int_{t_{b1}^+}^{\infty}\mathrm{d}t_1\lambda[\mathbf{K}_1(t_1)]\exp\left\{-\int_0^{t_1}\lambda[\mathbf{K}_1(y)]\mathrm{d}y\right\}$$
$$=1-\exp\left\{-\int_0^{t_{b1}^+}\lambda[\mathbf{K}_1(y)]\mathrm{d}y\right\}\leqslant C, \tag{75}$$

where $C=1-\exp(-\lambda_m t_m)$. The described steps are repeated for the integrals over $\mathbf{k}_1$ and t_0. Finally, integration over the normalized boundary distribution gives 1. It is found that I_2 is less than $\Gamma_D(A_m/\lambda_{\min})2C^2$, a result that can be generalized to arbitrary order n:

$$I_n(A)\leqslant\Gamma_D\frac{A_m}{\lambda_{\min}}nC^n. \tag{76}$$

The series $\Sigma_1^{\infty}nC^{n-1}=(1-C)^{-2}$ is convergent since $C<1$, which proofs convergence of the series (62).

$$\sum_{n=1}^{\infty}I_n(A)\leqslant\Gamma_D\frac{A_m}{\lambda_{\min}}\exp(2\lambda_m t_m). \tag{77}$$

V. SUMMARY

The single-particle Monte Carlo algorithm is formulated consistently with the formalism presented in the previous section. Given is a function $A(\mathbf{k},\mathbf{r})$, the number of trajectories N, and N_D, the number of particles inside the simulation domain. As an example, the calculation of the normalized average $\langle\mathrm{A}\rangle=\langle\langle\mathrm{A}\rangle\rangle/\langle\langle 1\rangle\rangle$ is demonstrated, using the time-averaging and the before-scattering estimators.

Begin (single particle MC algorithm using time-averaging estimators)
$\mu_1=0,\ \mu_A=0$ (initialize estimators)
For $i=1$ **to** N **do** (construct N trajectories)
$n=0,\ \psi_1=0,\ \psi_A=0$
generate $x_0=(\mathbf{r}_0,\mathbf{k}_0,t_0)$ from density p_0 [see Eq. (52)]
While $t_n<t_b^+(k_n,r_n)$
[path integrals of 1 and A over free-flight path, see Eq. (69)]
$$\psi_1=\psi_1+t_n,\quad \psi_A=\psi_A+\int_0^{t_n}A[\mathbf{K}(\tau;0,k_n,r_n)]\mathrm{d}\tau$$
(determine end point of free-flight path)
$$\mathbf{r}_{n+1}=\mathbf{R}(t_n;0,\mathbf{k}_n,\mathbf{r}_n),\quad \mathbf{k}_{n+1}^b=\mathbf{K}(t_n;0,\mathbf{k}_n,\mathbf{r}_n)$$
$n=n+1$ [next step in the recursions (56) and (57)]
generate after-scattering state $\mathbf{k}_n$ from density $S(\mathbf{k}_n^b,k_n)/\lambda(\mathbf{k}_n^b)$ [see Eq. (57)]
generate free-flight time t_n from density $\lambda[\mathbf{K}(t_n)]\exp\{-\int_0^{t_n}\lambda[\mathbf{K}(y)]\mathrm{d}y\}$
EndWhile (trajectory terminates at boundary)
$t_n=t_b^+(\mathbf{k}_n,\mathbf{r}_n)$ (time to reach boundary)
$$\psi_1=\psi_1+t_n,\quad \psi_A=\psi_A+\int_0^{t_n}A[\mathbf{K}(\tau;0,\mathbf{k}_n,\mathbf{r}_n)]\mathrm{d}\tau$$
[sum up the realizations of ψ_1 and ψ_A for the sample means, see Eq. (8)]:
$$\mu_1=\mu_1+\psi_1,\quad \mu_A=\mu_A+\psi_A$$
EndFor
$\langle\mathrm{A}\rangle=\mu_A/\mu_1$ (result)
$\Gamma_D=4\pi^3N_DN/\mu_1$ [normalization coefficient, see Eq. (70)]
End

Begin (single particle MC algorithm using before-scattering estimators)
$\mu_1=0,\ \mu_A=0$ (initialize estimators)
For $i=1$ **to** N **do** (construct N trajectories)
$n=0,\ \psi_1=0,\ \psi_A=0$
generate $x_0=(\mathbf{r}_0,\mathbf{k}_0,t_0)$ from density p_0 [see Eq. (52)]
While $t_n<t_b^+(k_n,r_n)$
$$\mathbf{r}_{n+1}=\mathbf{R}(t_n;0,\mathbf{k}_n,\mathbf{r}_n),\quad \mathbf{k}_{n+1}^b=\mathbf{K}(t_n;0,\mathbf{k}_n,\mathbf{r}_n)$$
$n=n+1$
$$\psi_1=\psi_1+1/\lambda(\mathbf{k}_n^b),\quad \psi_A=\psi_A+A(\mathbf{k}_n^b,\mathbf{r}_n)/\lambda(\mathbf{k}_n^b)$$
generate after scattering state $\mathbf{k}_n$ from density $S(\mathbf{k}_n^b,k_n)/\lambda(\mathbf{k}_n^b)$ [see Eq. (57)] generate free-flight time t_n from density $\lambda[\mathbf{K}(t_n)]\exp\{\int_0^{t_n}\lambda[\mathbf{K}(y)]\mathrm{d}y\}$
EndWhile (trajectory terminates at boundary)
$$\mu_1=\mu_1+\psi_1,\quad \mu_A=\mu_A+\psi_A$$
EndFor
$\langle\mathrm{A}\rangle=\mu_A/\mu_1$ (result)

$\Gamma_D = 4\pi^3 N_D N/\mu_1$ [normalization constant, see Eq. (70)]
End

In this example, only the result is estimated, while the stochastic error is not considered. Error estimation is discussed in Part II of this article.

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APPENDIX A: THE CONJUGATE EQUATION

Using the kernel given by Eq. (23) the conjugate equation becomes

$$g(\mathbf{k}',\mathbf{r}') = \int \mathrm{d}\mathbf{k} \int d\mathbf{r}\, g(\mathbf{k},\mathbf{r}) \int_{t_b^-(\mathbf{k},\mathbf{r})}^{0} \mathrm{d}t'\, S(\mathbf{k}',\mathbf{K}(t'),\mathbf{r}') \times \exp\left\{ -\int_{t'}^{0} \lambda[\mathbf{K}(y),\mathbf{R}(y)]\mathrm{d}y \right\} \times \delta[\mathbf{r}'-\mathbf{R}(t')]\theta_D(\mathbf{r}') + g_0(\mathbf{k}',\mathbf{r}'). \quad (78)$$

In this equation, t_b^- and hence t' is negative. The following steps can be formalized by using the extended notation of the free-flight trajectories introduced in Sec. III A. The integration variables are changed from $\mathbf{k}$ and $\mathbf{r}$, denoting the trajectory end point, to $\mathbf{k}^a = \mathbf{K}(t';0,\mathbf{k},\mathbf{r})$ and $\mathbf{r}'' = \mathbf{R}(t';0,\mathbf{k},\mathbf{r})$, denoting the trajectory starting point.

According to the Liouville theorem, the volume element is invariant under this transformation, $\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{r} = \mathrm{d}\mathbf{k}^a\,\mathrm{d}\mathbf{r}''$. The trajectory end point is now expressed as

$$\mathbf{k} = \mathbf{K}(0;t',\mathbf{k}_a,\mathbf{r}'') = \mathbf{K}(-t';0,\mathbf{k}_a,\mathbf{r}''),$$
$$\mathbf{r} = \mathbf{R}(0;t',\mathbf{k}_a,\mathbf{r}'') = \mathbf{R}(-t';0,\mathbf{k}_a,\mathbf{r}''),$$

where the time invariance stated in Sec. III A is used to perform a time-shift by $-t'$. This time-shift affects the path integral in Eq. (78) as follows:

$$\int_{t'}^{0} \lambda[\mathbf{K}(y;t',\mathbf{k}_a,\mathbf{r}''),\mathbf{R}(y;t',\mathbf{k}_a,\mathbf{r}'')]\mathrm{d}y = \int_{0}^{-t'} \lambda[\mathbf{K}(y;0,\mathbf{k}_a,\mathbf{r}''),\mathbf{R}(y;0,\mathbf{k}_a,\mathbf{r}'')]\mathrm{d}y.$$

In the next step, time is reversed by setting $\tau = -t'$. The lower bound of τ is 0 in the trajectory starting point $\mathbf{k}_a$, $\mathbf{r}''$. The domain indicator function is taken into account by the upper bound $t_b^+(\mathbf{k}_a,\mathbf{r}'')$ which is the time of the trajectory exit point on the domain boundary. Finally, the $\mathbf{r}''$ integration is carried out by means of $\delta(\mathbf{r}'-\mathbf{r}'')$, yielding Eq. (24).

APPENDIX B: TRANSFORMATION TO A BOUNDARY INTEGRAL

Augmenting Eq. (26) by a time integral and using the restricted integration domain Φ_b gives

$$\langle\langle \mathrm{A} \rangle\rangle = \int_{\Phi_b}\int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{k}' \int_{-\infty}^{0} \mathrm{d}t'\, \delta(t'-t_b^-) f_b[\mathbf{K}_b(t')\mathbf{R}_b(t')] \times \exp\left\{ -\int_{t'}^{0} \lambda[\mathbf{K}_b(y),\mathbf{R}_b(y)]\,dy \right\} g(\mathbf{k}',\mathbf{r}'). \quad (81)$$

Strictly speaking, the functions $\mathbf{K}$ and $\mathbf{R}$ are defined only inside D, that is for $t' \geqslant t_b^-$. For $t' < t_b^-$ these functions can be thought to be arbitrarily continued in such a way that they do not reenter the domain.

The derivation of the proposed transformation makes use of the following property of the δ-function,

$$\delta[b(t)] = \sum_i \frac{\delta(t-t_i)}{|\dot{b}(t_i)|}, \quad (82)$$

and the three-dimensional counterpart

$$\int_D \delta[B(\mathbf{r})]\phi(\mathbf{r})\mathrm{d}\mathbf{r} = \oint_{\partial D} \frac{\phi(\mathbf{r}_b)}{|(\nabla_{\mathbf{r}} B)(\mathbf{r}_b)|}\mathrm{d}\sigma(\mathbf{r}_b). \quad (83)$$

Here, t_i denote the roots of b, and ϕ is some test function.

Assume the domain boundary is defined implicitly by $B(\mathbf{r}) = 0$. This gives an implicit definition for the boundary time as the root of $B[\mathbf{R}_b(t')] = 0$. In $(-\infty,0)$ the one and only solution is t_b^-. Owing to the definition of Φ_b every considered trajectory will reach the boundary such that a solution exists. Setting $b(t') = B[\mathbf{R}_b(t')]$ one obtains from Eq. (82),

$$\delta(t'-t_b^-) = \delta[b(t')]|\dot{b}(t_b^-)| \quad (84)$$
$$= \delta[b(t')]|(\nabla_{\mathbf{r}} B)[\mathbf{R}_b(t')]\cdot\mathbf{v}[\mathbf{K}_b(t')]|. \quad (85)$$

In the latter equation t_b^- is replaced by t' for convenience. Since $\nabla_{\mathbf{r}} B(\mathbf{r})$ is normal to the surface defined by $B(\mathbf{r}) = 0$, the normal component of the group velocity can be introduced.

$$\delta(t'-t_b^-) = \delta\{B[\mathbf{R}_b(t')]\}|(\nabla_{\mathbf{r}} B)[\mathbf{R}_b(t')]||v_\perp[\mathbf{K}(t')]| \quad (86)$$

This expression is now inserted into Eq. (81). Then the integration variables are changed from $\mathbf{k}'$ and $\mathbf{r}'$, denoting the trajectory end point, to $\mathbf{k}_b = \mathbf{K}_b(t';0,\mathbf{k}',\mathbf{r}')$ and $\mathbf{r}'' = \mathbf{R}_b(t';0,\mathbf{k}',\mathbf{r}')$. The original variables are expressed as

$$\mathbf{k}' = \mathbf{K}'(0;t',\mathbf{k}_b,\mathbf{r}'') = \mathbf{K}'(-t';0,\mathbf{k}_b,\mathbf{r}''),$$
$$\mathbf{r}' = \mathbf{R}'(0;t',\mathbf{k}_b,\mathbf{r}'') = \mathbf{R}'(-t';0,\mathbf{k}_b,\mathbf{r}''). \quad (87)$$

Applying the Liouville theorem, $\mathrm{d}\mathbf{k}'\,\mathrm{d}\mathbf{r}' = \mathrm{d}\mathbf{k}_b\,\mathrm{d}\mathbf{r}''$, and reversing time by setting $t_0 = -t'$, one obtains

$$\langle\langle \mathrm{A} \rangle\rangle = \int_{\Phi_b}\int \mathrm{d}\mathbf{r}''\mathrm{d}\mathbf{k}_b \int_0^{t_b^+(\mathbf{k}_b,\mathbf{r}'')} \mathrm{d}t_0\, \delta[B(\mathbf{r}'')]|(\nabla_{\mathbf{r}} B)(\mathbf{r}'')| \times |v_\perp(\mathbf{k}_b)|\, f_b(\mathbf{k}_b,\mathbf{r}'') \times \exp\left\{ -\int_0^{t_0} \lambda[\mathbf{K}_b(y),\mathbf{R}_b(y)]\mathrm{d}y \right\} \times g[\mathbf{K}_b(t_0),\mathbf{R}_b(t_0)]. \quad (88)$$

Using Eq. (83), the volume integral over $\mathbf{r}''$ is transformed into a boundary integral leading to Eq. (31).

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