Stochastic Algorithm for Solving the Wigner-Boltzmann Correction Equation

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Abstract. The quantum-kinetics of current carriers in modern nanoscale semiconductor devices is determined by the interplay between coherent phenomena and processes which destroy the quantum phase correlations. The carrier behavior has been recently described with a two-stage Wigner function model, where the phase-breaking effects are considered as a correction to the coherent counterpart. The correction function satisfies a Boltzmann-like equation.
A stochastic method for solving the equation for the correction function is developed in this work, under the condition for an a-priori knowledge of the coherent Wigner function. The steps of an almost optimal algorithm for a stepwise evaluation of the correction function are presented. The algorithm conforms the well established Monte Carlo device simulation methods, and thus allows an easy implementation.

1 Introduction

Modeling and simulation of electronic transport in semiconductor devices is challenged by the nanometer and picosecond scale processes which determine the functionality of modern integrated circuits. Quantum transport models are explored to correctly describe coherent processes, such as tunneling, in conjunction with de-coherence processes of scattering, which try to recover the classical behavior of the current carriers.

The Wigner-Boltzmann (WB) equation gives a comprehensive quantum-kinetic description of these phenomena, and has been recently applied for sumulation of a variety of nanometer devices and involved transport phenomena [1]. Stochastic approaches to the WB equation efficiently describe the scattering processes, however, the coherent part of the transport is obtained at significant numerical costs. A scheme which uses coherent data obtained by alternative approaches has been developed recently. The scattering-induced correction to the coherent Wigner function satisfies a Fredholm integral equation of the second kind, with a free term determined by the coherent data.

Particle methods have been developed and used to calculate the free term. We have successfully applied these methods for very small devices, where this term can be regarded as a zeroth order correction. Here we utilize the numerical

Monte Carlo theory to derive a stochastic algorithm for solving the equation for the WB correction.

An important peculiarity is that the problem is comprised by two models with different dimensions: while the coherent transport involves two variables - the position and wave vector x, k_x, the scattering occurs in the three dimensional wave vector space, thus involving the transversal components $k_y, k_z = \mathbf{k}_\perp$. The two models are combined into a four dimensional space formulation by merely physical considerations. In this respect the sequel does not stick to the formal Monte Carlo schemes for solving integral equations, and in particular the adjoint equation, which proved as an already established approach to carrier transport problems [2], [3]. The adjoint equation remains rather implicit in the derivations, which refers to core schemes for solving integrals in favor of an emphasis on the physical aspects.

2 The model

The time-independent Wigner-Boltzmann equation:

$$\frac{\hbar k_x}{m}\frac{\partial}{\partial x}f_w(x,k_x,\mathbf{k}_\perp) = \int dk_x{}' V_w(x,k_x{}'-k_x)f_w(x,k_x',\mathbf{k}_\perp) + \int d\mathbf{k}' f_w(x,\mathbf{k}')S(\mathbf{k}',\mathbf{k}) - f_w(x,\mathbf{k})\lambda(\mathbf{k}) \tag{1}$$

describes the coherent part of the carrier transport at a rigorous quantum level, accomplished by the Boltzmann scattering model of the phase-breaking processes. Here V_w is the Wigner potential, the Boltzmann scattering operator $S(\mathbf{k},\mathbf{k}')$ presents the scattering rate for a transition from $\mathbf{k}$ to $\mathbf{k}'$. $\lambda(\mathbf{k}) = \int d\mathbf{k}' S(\mathbf{k}.\mathbf{k}')$ is the total out-scattering rate, so that the quantity S/λ is the probability density for scattering from the initial to the final state. The solution of (1) in the region D of a given device determines the physical characteristics of the current carriers and thus the circuit behavior of the device. The external factors which determine the solution are the applied bias, which controls the electric potential profile in the device, and the boundary conditions. The latter are assumed to satisfy the equilibrium distribution function deep inside the device leads. It is the Maxwell-Boltzmann distribution f_{MB}, which is the only function turning the second row in (1) to zero independently of the physical origin of the scattering processes.

The coherent problem is obtained from (1) by switching off all scattering processes. In this case the solution $f_w^c(x,k_x)$ does not depend on the transversal wave vector components. A proper alignment of the variables with the genuine problem must be such that f_w^c is recovered after an integration over the transversal ones. A consistent with the boundary condition assumption is the appearance of the equilibrium with respect to the transversal variables function $f_{MB}(\mathbf{k}_\perp)$:

$$f_w^c(x,\mathbf{k}) = f_w^c(x,k_x)\frac{\hbar^2}{2\pi mkT}e^{-\frac{\hbar^2\mathbf{k}_\perp^2}{2mkT}} \tag{2}$$

This allows to define the function

$$f_w^{\Delta}(x,\mathbf{k}) = f_w(x,\mathbf{k}) - f_w^c(x,\mathbf{k}), \tag{3}$$

which is the scattering induced correction to the coherent Wigner function. The equation for the correction f_w^{Δ} is obtained by subtracting the coherent counterpart from (1). An immediate property of (3) is that the correction is zero at the device boundaries, where the same boundary conditions are assumed for both cases.

The Wigner potential is approximated by its classical limit valid for slowly varying potentials at a next step:

$$\int \mathrm{d}k_x{}' V_w(x,k_x{}'-k_x) f_w^{\Delta}(x,k_x',\mathbf{k}_\perp) = -\frac{eE(x)}{\hbar}\frac{\partial f_w^{\Delta}(x,k_x,\mathbf{k}_\perp)}{\partial k_x} \tag{4}$$

This means that the force $F(x) = eE(x)$, given by the derivative of the potential, can be only a linear function within the spatial support of f_w^{Δ}, related to the spatial width of the electrons. Such an assumption in the general equation (1) precludes the quantum-mechanical description of the transport. The latter, however, has a different physical meaning in the equation for the correction. The width of the electron has been already accounted by the coherent solution, so that the limit precludes only correlations between the electric potential and the scattering processes.

The obtained model for the correction function can be written as a Fredholm integral equation of the second kind with a free term determined by f_w^c:

$$f_w^{\Delta}(x,\mathbf{k}) = \int_{t_b}^{0} dt \int \mathrm{d}\mathbf{k}' f_w^{\Delta}(X(t),\mathbf{k}') S(\mathbf{k}',\mathbf{k}(t)) e^{-\int_t^0 \lambda(\mathbf{k}(\tau))d\tau} + f_w^{\Delta,0}(x,\mathbf{k})$$

$$f_w^{\Delta,0} = \int_{t_b}^{0} dt \left\{ \int \mathrm{d}\mathbf{k}' f_w^c(X(t),\mathbf{k}') S(\mathbf{k}',\mathbf{k}(t)) e^{-\int_t^0 \lambda(\mathbf{k}(\tau))d\tau} \right. \tag{5}$$

$$\left. - f_w^c(X(t),\mathbf{k}(t))\lambda(\mathbf{k}(t)) e^{-\int_t^0 \lambda(\mathbf{k}(\tau))d\tau} \right\}$$

Here

$$X(t) = x - \int_t^0 \frac{\hbar K_x(\tau)}{m} d\tau \qquad K_x(t) = k_x - \int_t^0 \frac{F(X(\tau))}{\hbar} d\tau \tag{6}$$

are classical Newton trajectories initialized by $x, k_x, 0$, $t < 0$, and $\mathbf{k}(t)$ stands for $K_x(t), \mathbf{k}_\perp$. The trajectory crosses the boundary of the device at a certain time t_b, where $f_w^{\Delta}(X(t_b),\mathbf{k}(t_b)) = 0$.

3 Computational Problem

The general task is to compute the averaged value of f_w^{Δ} in the given domain Ω of the two dimensional phase space. The averaged value can be expressed as:

$$I(\Omega) = \int dx \int dk_x f_w^{\Delta}(x,k_x)\theta_\Omega(x,k_x) = \int dx \int dk_x \int d\mathbf{k}_\perp f_w^{\Delta}(x,\mathbf{k})\theta_\Omega(x,k_x) \tag{7}$$

by introducing the domain indicator $\theta_\Omega(x, k_x)$, which is unity if the arguments belong to Ω, and 0 otherwise. The solution of equation (5) can be expressed as consecutive iterations of the kernel on the free term: $f_w^\Delta = \sum_{p=0}^\infty f_w^{\Delta,p}$:

$$f_w^{\Delta,(p+1)} = \int_{-\infty}^0 dt \int \mathrm{d}\mathbf{k}' \theta_D(X(t)) f_w^{\Delta,p}(X(t), \mathbf{k}') S(\mathbf{k}', \mathbf{k}(t)) e^{-\int_t^0 \lambda(\mathbf{k}(\tau))d\tau} \quad (8)$$

The lower bound of the time integral has been extended to $-\infty$, since the introduced device domain indicator θ_D takes care for it's correct value t_b. We consider the contributions to (7) of the consecutive terms of (8). In this way we reduce the general task (7) to a problem of evaluation of the consecutive contributions:

$$I(\Omega) = \int dx \int dk_x \int d\mathbf{k}_\perp f_w^\Delta(x, \mathbf{k}) \theta_\Omega(x, k_x) = \sum_{p=0}^\infty \int d\mathbf{k}_\perp I_\Omega^{(p+1)}(\mathbf{k}_\perp)$$

$$\begin{aligned} I_\Omega^{(p+1)}(\mathbf{k}_\perp) = & \int_{-\infty}^0 dt \int dx \int dk_x \int \mathrm{d}\mathbf{k}' \theta_D(X(t)) \\ & f_w^{\Delta,p}(X(t), \mathbf{k}') S(\mathbf{k}', \mathbf{k}(t)) e^{-\int_t^0 \lambda(\mathbf{k}(\tau))d\tau} \theta_\Omega(x, k_x) \end{aligned} \quad (9)$$

The trajectory $X(t), \mathbf{k}(t) = (K_x(t), \mathbf{k}_\perp)$ is initialized by x, k_x at time 0, and the parameterization is backward: $t < 0$.

3.1 Stochastic Analysis

The aim of the following analysis is twofold: to devise a Monte Carlo method for evaluation of $I(\Omega)$; the method to be compatible with the established algorithms for device simulations and thus to allow an easy implementation. These algorithms emulate the natural processes of the evolution of Boltzmann carriers, which follow an incrementing in time succession. Thus equation (9) must be reformulated in a forward in time, $t > 0$, parameterization. According to (6) the trajectory is initialized by x, k_x at 0, which can be written as: $X(t) = X(t; x, k_x, 0) = x^t \quad K_x(t) = K_x(t; x, k_x, 0) = k_x^t$. Two basic properties of the Newton trajectories are utilized. A trajectory, being a unique solution of a first order differential equations, can be initialized by any of its points x^t, k_x^t associated to given time t. Furthermore, in stationary conditions trajectories are invariant with respect to a shift of both, the time origin and the parameterization time:

$$X(\tau) = X(\tau - t; x^t, k_x^t, 0) = X^t(\tau - t); \quad K_x(\tau) = K_x(\tau - t; x^t, k_x^t, 0) = K_x^t(\tau - t)$$

Here the initialization point/time have been changed accordingly, followed by a shift in time by $-t$. The short notations X^t, K^t recall for the novel initialization by $x^t, k_x^t, 0$. It follows that $x = X^t(-t)$, $k_x = K_x^t(-t)$. The Liouville theorem

$dxdk_x = dx^t dk_x^t$ is finally utilized to reformulate (9) as follows:

$$I_\Omega^{(p+1)}(\mathbf{k}_\perp) = \int_0^\infty dt \int dx^t \int dk_x^t \int \mathrm{d}\mathbf{k}' \theta_D(x^t) f_w^{\Delta,p}(x^t, \mathbf{k}') \left\{ \frac{S(\mathbf{k}', k_x^t, \mathbf{k}_\perp)}{\lambda(\mathbf{k}')} \right\}$$
$$\left\{ \lambda(K_x^t(t), \mathbf{k}_\perp) e^{-\int_0^t \lambda(K_x^t(\tau), \mathbf{k}_\perp) d\tau} \right\} \frac{\lambda(\mathbf{k}')}{\lambda(K_x^t(t), k_\perp)} \theta_\Omega(X^t(t), K_x^t(t)) \quad (10)$$

where, now, the trajectory $X^t(t), K_x^t(t)$, $t > 0$ is initialized by x^t, k_x^t at the time origin, and the equation has been augmented to obtain the (enclosed in curly brackets) well known Monte Carlo probability densities for scattering, $\mathcal{S}$, and drift, $\mathcal{D}$, processes. Indeed these densities associate to an initial point a final point within the scheme:

$$\mathcal{SD}\left\{x^t, \mathbf{k}' \to x^t, k_x^t, \mathbf{k}_\perp \Rightarrow X^t(t), K_x^t(t), \mathbf{k}_\perp\right\}, \quad (11)$$

where $\to$ corresponds to a scattering event, while $\Rightarrow$ to a drift, called also free flight. The scheme defines a segment of a numerical trajectory obtained by the consecutive iterations of (10). To analyze the physical aspects behind such a trajectory, it is sufficient to consider the second iteration $I_\Omega^{(2)}$. The following property will be used: in the limiting case, when the domain Ω shrinks to a point so that the domain indicator becomes a delta function: $\delta(x - X^t(t))\delta(k_x - K_x^t(t))$, equation (10) obtains a recursive form, due to the fact that $I_\delta^{(p+1)}(\mathbf{k}_\perp) = f_w^{\Delta,(p+1)}(x, k_x, \mathbf{k}_\perp)$ A convention to mark the variables by the number of the corresponding iteration is followed, for convenience the superscript ^{t} is omitted along with the subscript of k_x. Finally, the notation (11), which provides a convenient abbreviation for the product of the two probability densities in (10) is utilized:

$$\int_0^\infty dt_2 \int dx_2 \int dk_2 \int \mathrm{d}\mathbf{k}_2' \theta_D(x_2) \int_0^\infty dt_1 \int dx_1 \int dk_1 \int \mathrm{d}\mathbf{k}_1' \theta_D(x_1) f_w^{\Delta,0}(x_1, \mathbf{k}_1') \quad (12)$$
$$\mathcal{SD}\left\{x_1, \mathbf{k}_1' \to x_1, k_1, \mathbf{k}_{\perp 2}' \Rightarrow X_1(t_1), K_1(t_1), \mathbf{k}_{\perp 2}'\right\} \frac{\lambda(\mathbf{k}_1')}{\lambda(\mathbf{k}_2')} \delta(x_2, k_2'; X_1 K_1, t_1)$$
$$\mathcal{SD}\left\{x_2, \mathbf{k}_2' \to x_2, k_2, \mathbf{k}_{\perp 3}' \Rightarrow X_2(t_2), K_2(t_2), \mathbf{k}_{\perp 3}'\right\} \frac{\lambda(\mathbf{k}_2')}{\lambda(\mathbf{k}_3')} \theta_\Omega(X_2(t_2), K_2(t_2))$$

with

$$\delta(x_{s+1}, k_{s+1}'; X_s, K_s, t_s) = \delta(x_{s+1} - X_s(t_s))\delta(k_{s+1}' - K_s(t_s))$$

The zeroth order is given by the free term which, according to (5) has two components denoted by $f_w^{\Delta,0A}$ and $f_w^{\Delta,0B}$. The former is expressed in a forward in time parameterization [4] as follows:

$$f_w^{\Delta,0A}(x_1, \mathbf{k}_1') = \int_0^\infty dt_0 \int dx_0 \int dk_0 \int \mathrm{d}\mathbf{k}_0' \theta_D(x_0) \left\{ \frac{\hbar^2 e^{-\frac{\hbar^2 \mathbf{k}_{\perp 0}'^2}{2mkT}}}{2\pi mkT} \right\} f_w^c(x_0, k_0') \quad (13)$$
$$\left\{ \frac{S(\mathbf{k}_0', k_0, \mathbf{k}_{\perp 1}')}{\lambda(\mathbf{k}_0')} \right\} \left\{ \lambda(K_0(t_0), \mathbf{k}_{\perp 1}') e^{-\int_0^{t_0} \lambda(K_0(\tau), \mathbf{k}_{\perp 1}') d\tau} \right\} \frac{\lambda(\mathbf{k}_0')}{\lambda(\mathbf{k}_1')} \delta(x_1, k_1'; X_0 K_0, t_0)$$

The terms in the curly brackets in (12) and (13) correspond to a sequence of conditional probabilities giving rise to free-flight and scattering events. The final point of each free flight becomes the initial point for the next scattering event:

$$\begin{array}{lll} x_0, k_0', \mathbf{k}_{\perp 0}' \rightarrow x_0, k_0, \mathbf{k}_{\perp 1}' \Rightarrow X_0(t_0) = x_1, K_0(t_0) = k_1', \mathbf{k}_{\perp 1}' & | & f_w^{\Delta,0A}(x_1, \mathbf{k}_1') \\ x_1, k_1', \mathbf{k}_{\perp 1}' \rightarrow x_1, k_1, \mathbf{k}_{\perp 2}' \Rightarrow X_1(t_1) = x_2, K_1(t_1) = k_2', \mathbf{k}_{\perp 2}' & | & f_w^{\Delta,1A}(x_2, \mathbf{k}_2') \\ x_2, k_2', \mathbf{k}_{\perp 2}' \rightarrow x_2, k_2, \mathbf{k}_{\perp 3}' \Rightarrow X_2(t_2), K_2(t_2), \mathbf{k}_{\perp 3}' & | & I_\Omega^{(2)}(\mathbf{k}_{\perp 3}') \end{array}$$

The sequence of events resembles the evolution of a Boltzmann particle and thus enables the implementation of the standard algorithm for trajectory construction utilized in the device Monte Carlo simulators.

3.2 Numerical Aspects

We now return to the general task, the computation of $I(\Omega)$, and analyze what happens from a numerical point of view during the particle evolution. The basic notions from the Monte Carlo evaluation of integrals are assumed to be well known, and will be applied in the following. A general result is that a stochastic approach is optimal provided that the sampling probability density is proportional to the integrand function. In this respect the choice of the initial point $x_0, k_0', \mathbf{k}_{\perp 0}'$ in (13) is according to the Gaussian in the first curly brackets for the transversal variables, and according to:

$$\frac{|f_w^c(x_0, k_0')|}{F_1}; \qquad F_1 = \int dx \int dk_x |f_w^c(x, k_x)|;$$

for the longitudinal ones. Thus the initial weight of the particle is F_1 times the sign of f_w^c in the chosen point. The multiplication by F_1 can be done at the final stage of evaluation of the estimators, so that the initialized particle carries the sign only. The particle evolves to $x_1, k_1', \mathbf{k}_{\perp 1}'$ as a result of a scattering and a drift event, and the weight is updated by the ratio of the two λ values. We note that at this stage the above procedure can be regarded as a legitimate experiment for evaluation of $I(\Omega)^{(0)} = \int d\mathbf{k}_{\perp 1} I_\Omega^{(0)}(\mathbf{k}_{\perp 1})$. An estimator $\xi_\Omega(0)$ is introduced, whose value is updated by adding of $sign(f_w^c)\lambda(\mathbf{k}_0')/\lambda(\mathbf{k}_1')$. The integral over the transverse variables means that the update of the estimator is independent of the concrete value of $\mathbf{k}_{\perp 1}$. The trajectory continues by a second scattering and free flight, and the weight is updated by the next fraction $\lambda(\mathbf{k}_0')/\lambda(\mathbf{k}_1')$. The obtained two-segment trajectory is a legitimate experiment for evaluation of $I(\Omega)^{(1)}$: the weight $sign(f_w^c)\lambda(\mathbf{k}_0')\lambda(\mathbf{k}_1')/\lambda(\mathbf{k}_1')\lambda(\mathbf{k}_2')$ is added to an estimator $\xi_\Omega(1)$. A third step follows in the same fashion, etc. The consecutive steps give rise to a weight $sign(f_w^c)\lambda(\mathbf{k}_0')/\lambda(\mathbf{k}_p')$ used to evaluate the consecutive values of $I(\Omega)^{(p)}$, stored by the corresponding estimators $\xi_\Omega(p)$. The procedure continues, until the trajectory abandons the device domain for the first time: In this case the device domain indicator becomes zero, which resets the value of the accumulated

weight of all further steps to 0. The contributions to the higher order terms in the sum for $I(\Omega)$ become zero and the further evolution of such a trajectory becomes obsolete. In this way one trajectory represents one independent experiment for a direct evaluation of I_Ω: all estimators can be merged into one, ξ_Ω. Finally, the arithmetic mean of the accumulated due to N independent trajectories value of ξ_Ω, multiplied by F_1 is a Monte Carlo estimate of I_Ω.

The contribution of the second component $f_w^{\Delta,0B}$ is a subject of similar analysis. The only difference is that the trajectory begins with a free flight, determined by the initialization point. This can be formally accounted by replacement of the first S/λ term in (13) by a delta function.

Different strategies may be considered: the two contributions can be evaluated separately, or $f_w^{\Delta,0}$ can be evaluated at a first stage and then used for a direct evaluation of the iteration series. As the efficiency of these strategies can be estimated by numerical experiments only, we continue by adopting the 'separate simulation' approach.

3.3 Pointwise Evaluation

It is further assumed that the coherent solution is known only pointwise. The following decomposition can be utilized in (10):

$$\int dx^t \int dk'_x f_w^{\Delta,(p)}(x^t, k'_x, \mathbf{k}'_\perp) = \sum_{mn} f_w^{\Delta,(p)}(x^t_m, k'_{xn}, \mathbf{k}'_\perp)\Delta \tag{14}$$

introduced by the interval $\Delta = \Delta_{kx}\Delta_x$. The computational task is further focused on the evaluation of the averaged value of $f_w^{\Delta,(p+1)}$ in the domain Ω_{ij} specified by Δ around (x_i, k_{xj}). In particular (10) reduces to the recursive relation:

$$f_w^{\Delta,(p+1)}(x_i, k_{xj}, \mathbf{k}_\perp) = \sum_{mn} \int dk^t_x \int_0^\infty dt \int d\mathbf{k}'_\perp f_w^{\Delta,p}(x^t_m, k'_{xn}, \mathbf{k}'_\perp) \left\{ \frac{S(\mathbf{k}', k^t_x, \mathbf{k}_\perp)}{\lambda(\mathbf{k}')} \right\}$$
$$\left\{ \lambda(K^t_x(t), \mathbf{k}_\perp) e^{-\int_0^t \lambda(K^t_x(\tau), \mathbf{k}_\perp) d\tau} \right\} \frac{\lambda(\mathbf{k}')}{\lambda(K^t_x(t), \mathbf{k}_\perp)} \theta_D(x^t_m) \theta_{\Omega_{ij}}(X^t(t), K^t_x(t)), \tag{15}$$

where the trajectory is initialized by x_m, k^t_x, and gives rise to the following algorithm:

- The phase space simulation domain is decomposed into sub-domains Ω_{mn} around x_m, k_{xn} nodes; The estimators ξ_{mn} are initialized to zero. Evaluated are the probabilities:

$$P_{mn} = \frac{|f^c_w(x_m, k_{xm})|}{F_1}; \qquad F_1 = \sum_{mn} |f^c_w(x_m, k_{xm})|;$$

  The number of independent Monte Carlo experiments is specified to N_l.

- Within a loop over $l = 1, \ldots, N_l$: the initial point $x_m, k_{xn}, \mathbf{k}_\perp$ of the l-th trajectory is chosen randomly by using P_{mn} and the Gaussian distribution function of the transversal wave vectors. The product of the sign of f_w^c and λ, both evaluated at the initial point, is assigned to a variable w_l.
- The construction of the trajectory begins by a scattering event for the iteration series A corresponding the first component of the free term, followed by a free flight. For the second component, B, only the free flight remains. In both cases the events are realized by the standard scheme for device Monte Carlo simulators.
- After each free flight: if the trajectory belongs to the device domain, the estimator of the nearest to the end point node is updated by adding w_l/λ where λ is determined by the free flight end point; otherwise the construction of the trajectory is stopped and another trajectory begins.
- At the end of the loop the values of the estimators are divided by N_l It holds:

$$f_w^{\Delta A,B}(x_i, k_{xj}) \simeq \xi_{ij}^{A,B}/N_l.$$

Finally

$$f_w^{\Delta}(x_i, k_{xj}) = f_w^{\Delta A}(x_i, k_{xj}) - f_w^{\Delta B}(x_i, k_{xj}).$$

4 Conclusions

The presented approach aims at an estimation of the effect of scattering to the coherent transport in nanoscale devices. It offers high computational efficiency at the expense of neglecting the correlations between electrical potential and scattering events. The devised Monte Carlo algorithm calculates pointwise the values of the scattering-induced Wigner function correction. It is compatible with the established methods for Monte Carlo device simulations and thus allows an easy implementation.

Acknowledgment

This work has been supported by the Austrian Science Fund Project FWF-P21685.

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