Transport integral: A method to calculate the time evolution of phase-space distributions

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An analytical technique using integral equations for the transport of ion-optical intensity distributions through magnetic systems is described. It can serve as an alternative to Monte Carlo simulations to calculate the time evolution of phase-space distributions of any given shape. Under the assumption of linear optics, the solution of the integral equations can be reduced to convolution products. One major application of this approach is the fast calculation of the transmission and purification of radioactive nuclear beams produced by projectile fragmentation.

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I. INTRODUCTION

The time evolution of a phase-space distribution under a given set of constraints is often needed in a broad variety of simulation problems. We describe in this paper a transport integral which analytically defines such an evolution between initial and final phase-space distributions. It can be evaluated directly in some simple cases, but most of the time an analytical solution is not possible, and a sampling simulation of the system has to be performed using Monte Carlo techniques.

One application of the transport integral is related to beam optics, where the knowledge of the evolution of the phase-space distribution is needed at any time or, which is equivalent, at any position on the beam line. For example, the uniform irradiation of a tumor requires a flat-shaped distribution as a function of position, whereas typical beam profiles are usually closer to a Gaussian shape. The transport integral was used to calculate the conditions under which a Gaussian distribution could be transformed into a square one [1]. For that particular problem, the intensity distribution at the final position x is assumed to depend solely on the initial angle distribution $I_0(\theta)$ and the transport integral can be written

$$I(x)=\int I_0(\theta)\delta(x-f(\theta))d\theta\ , \tag{1}$$

where the function $f(\theta)$ describes how the optical system transforms the initial coordinate (θ) into the final one (x). Using the identify $\delta(x-f(\theta))=\sum_i 1/[(\partial f/\partial\theta)\delta(\theta-\theta_i)]$, where the θ_i are the zeros of the function $(x-f(\theta))$, Eq. (1) becomes

$$I(x)=\sum_i \int I_0(\theta)/[(\partial f/\partial\theta)\delta(\theta-\theta_i)]d\theta\ . \tag{2}$$

Equation (2) tells us that in order to have $I(x)$ constant, the function $f(\theta)$ has to be chosen to keep the ratio $I_0(\theta)/(\partial f/\partial\theta)$ constant. Assuming a Gaussian shape for the initial distribution $I_0(\theta)$ and expanding it into a Taylor series, we see that the most important term to be matched by $\partial f/\partial\theta$ is of order θ^2, therefore of order θ^3 in $f(\theta)$, which is accomplished by octupole magnets. These results were confirmed by a TURTLE [2] Monte Carlo computer calculation. In the case where $f(\theta)$ is proportional to θ, its derivative becomes constant and the shape of the distribution is not changed by the system, but merely scaled.

If in some cases the primary phase-space distribution is simple enough to deduce the result analytically for linear optics, as, for instance, with a Gaussian shape, in the case of an arbitrary or more complicated shape the mathematical form of the integral cannot be disentangled. This is the case when considering the phase-space distribution of secondary beams produced by projectile fragmentation where the nuclear reaction mechanism as well as the electron slowing down in the target are responsible for its shape.

In the following we shall derive a first-order reduction of the transport integral which leads to an elegant and fast way to perform the calculation for any given shape of the initial phase-space distribution. This method has proven to be very efficient when many simulations are needed in a short time and under various initial conditions such as the one encountered during the tuning of an experiment.

In its general form the transport integral is written as

$$D'(q_1',\ldots,q_n')=\int_1\cdots\int_n dq_1'\cdots dq_n' D(q_1,\ldots,q_n)\times\prod_{i=1}^{n}\delta(q_i'-f_i(q_1,\ldots,q_n))\ , \tag{3}$$

where D is the initial phase-space distribution at time t and D' is the resulting phase-space distribution at time t'. The $q_1,\ldots,q_n$ and $q_1',\ldots,q_n'$ represent the phase-space coordinates at t and t', respectively. The core of this integral is the set of functions $f_i(q_1,\ldots,q_n)$, which describe how each of the final coordinates depends on the initial ones. The Dirac δ function merely selects the combinations of initial coordinates, which give a contribution at the final coordinate q_i'.

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For calculation purposes it is more practical to consider the projections of the final phase-space distribution. Such a projection is obtained by summing all contributions of the phase-space distribution for each point on the projection axis:

$$P'_j(q'_j)]\int_{i\neq j}\cdots\int_{i\neq j}\prod_{i\neq j}dq'_i\int_1\cdots\int_n dq_1\cdots dq_n D(q_1,\ldots,q_n)\prod_{k=1}^{n}\delta(q'_k-f_k(q_1,\ldots,q_n))$$

and rearranging the integrals

$$P'_j(q'_j)=\int_1\cdots\int_n dq_1\cdots dq_n D(q_1,\ldots,q_n)\times\delta(q'_j-f_j(q_1,\ldots,q_n))\times\prod_{i\neq j}^{n}\int_i dq'_i\delta(q'_i-f_i(q_1,\ldots,q_n))\ .$$

The integration of the δ functions for each q'_i coordinate except q'_j all give a result equal to unity

$$\prod_{i\neq j}^{n}\int_i dq'_i\delta(q'_i-f_i(q_1,\ldots,q_n))=1$$

and one is therefore left with the following n-dimensional integral:

$$P'_i(q'_i)=\int_1\cdots\int_n D(q_1,\ldots,q_n)\times\delta(q'_i-f_i(q_1,\ldots,q_n))dq_1\cdots dq_n\ . \tag{5}$$

A schematic view illustrating this integral is shown in Fig. 1. The projections $P'_i(q'_i)$ of the phase-space distribution $D'(q_1,\ldots,q_n)$ at time t' on the q'_i axis is the weighted sum of the points of the distribution $D(q_1,\ldots,q_n)$ at time t which transform into q'_i through the function $f_i(q_1,\ldots,q_n)$. The δ function ensures that only those points which transform into q'_i are taken in the integral.

When the shape of the initial phase-space distribution $D(q_1,\ldots,q_n)$ is not known analytically, the calculations cannot be performed by means other than the usual sampling methods such as Monte Carlo, where the accuracy of its determination depends on the statistical errors due to the sampling of the primary distribution. However, given two simplifying assumptions on the primary phase-space distribution and the coordinate transformation functions, this integral can be reduced to convolution products, which in turn can be easily calculated using Fourier transform techniques.

An alternative method [3] also uses convolution products to calculate the transformation of phase-space distributions. It is based on the concept of generating functions that describe the system and are successively convoluted to the primary distribution. In this formulation, a generating function must be constructed for each element in the direction of the phase space where it modifies the distributions.

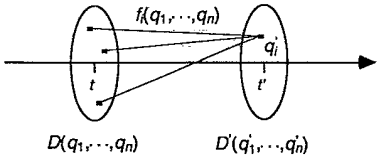

FIG. 1. Schematic representation of the transport integral.

$$P'_j(q'_j)=\int_{i\neq j}\cdots\int_{i\neq j}\prod_{i\neq j}^{n}dq'_i D'(q'_1,\ldots,q'_n)\ , \tag{4}$$

where the integrals run for every coordinate except q'_j, where the projection takes place. Injecting the definition of the transport integral gives

II. SIMPLIFYING ASSUMPTIONS

We first assume that the initial phase-space distribution $D(q_1,\ldots,q_n)$ at time t can be decomposed into its projections on the q_i axis. This means that the variables $q_1,\ldots,q_n$ are noncoupled and the distribution can be written as the product of its projections

$$D(q_1,\ldots,q_n)=\prod_{j=1}^{n}P_j(q_j)\ . \tag{6}$$

In the second assumption we take a first-order approximation for the transport function $f_i(q_1,\ldots,q_n)$. Hence it can be written as a linear combination of the q_i

$$f_i(q_1,\ldots,q_n)=\sum_{k=1}^{n}R_{ik}q_k\ . \tag{7}$$

Therefore, Eq. (5) becomes

$$P'_i(q'_i)=\int_1\cdots\int_n\prod_{j=1}^{n}P_j(q_j)\delta\left[q'_i-\sum_{k=1}^{n}R_{ik}q_k\right]\times dq_1\cdots dq_n\ , \tag{8}$$

where the R_{ik} coefficients are the elements of the first-order transport matrix

$$\mathbf{R}\equiv\begin{bmatrix}R_{11}&\cdots&R_{1n}\\ \vdots&\ddots&\vdots\\ R_{n1}&\cdots&R_{nn}\end{bmatrix}\ .$$

In the following section, we show that with those two assumptions Eq. (8) can be reduced to convolution products.

III. REDUCTION TO CONVOLUTION PRODUCTS

Given the variable changes $p_k=R_{ik}q_k\rightarrow dp_k=R_{ik}dq_k$ and $P_j(q_j)=P_j(p_j/R_{ij})=\bar{P}_j(p_j)$, Eq. (8) can be written

$$P'_i(q'_i)=\frac{1}{\prod_{k=1}^{n}R_{ik}}\int_1\cdots\int_n\prod_{j=1}^{n}\bar{P}_j(p_j)\delta\left[q'_i-\sum_{k=1}^{n}p_k\right]\times dp_1\cdots dp_n\ .$$

Writing $t_1=\sum_{k=1}^{n}p_k\rightarrow p_1=t_1-\sum_{k=2}^{n}p_k$ and $dp_1=dt_1$,

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}\int_1\cdots\int_n \bar{P}_1\left[t_1-\sum_{k=2}^{n} p_k\right]\times\prod_{j=2}^{n}\bar{P}_j(p_j)\delta(q_i'-t_1)\times dt_1 dp_2\cdots dp_n .$$

The δ function is nonzero only for $t_1=q_i'$; therefore

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}\int_2\cdots\int_n \bar{P}_1\left[q_i'-\sum_{k=2}^{n} p_k\right]\times\bar{P}_2(p_2)\cdots\bar{P}_n(p_n)dp_2\cdots dp_n .$$

We then perform the same kind of variable change

$$t_2=\sum_{k=2}^{n} p_k\rightarrow p_2=t_2-\sum_{k=3}^{n} p_k\ ,\quad dp_2=dt_2\ ,$$

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}\int_2\cdots\int_n \bar{P}_1(q_i'-t_2)\times\bar{P}_2\left[t_2-\sum_{k-3}^{n} p_k\right]\cdots\times\bar{P}_n(p_n)dt_2\cdots dp_n\ ,$$

and so forth, one finally ends with the formula

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}\int_2\cdots\int_n \bar{P}_1(q_i'-t_2)\bar{P}_2(t_2-t_3)\cdots\times\bar{P}_{n-1}(t_{n-1}-t_n)\times\bar{P}_n(t_n)dt_2\cdots dt_n . \quad (9)$$

Each integral is now independent and corresponds to a convolution product

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}\int_2\cdots\int_{n-1} \bar{P}_1(q_i'-t_2)\bar{P}_2(t_2-t_3)\cdots\times[\bar{P}_{n-1}\otimes\bar{P}_n](t_{n-1})\times dt_2\cdots dt_{n-1} .$$

Finally, the result is given by the convolution product of all $\bar{P}_j$ functions

$$P_i'(q_i')=\frac{1}{\prod_{k=1}^{n} R_{ik}}[\bar{P}_1\otimes\bar{P}_2\otimes\cdots\otimes\bar{P}_n](q_i') . \quad (10)$$

The convolution products are calculated using Fourier and inverse Fourier transforms. Fast Fourier transform algorithms can increase greatly the speed of the calculations, the best results being obtained when the number of points in the distributions is a power of 2.

IV. GENERAL ALGORITHM

The implementation of an algorithm to calculate the time evolution of a given phase-space distribution can be described as the succession of the following steps (see Fig. 2). Given the projections of the initial phase-space distribution and the first-order transport matrix, the calculation simply consists of convoluting those projections after they have been scaled by the matrix coefficients. The convolution products are performed using the Fourier and inverse Fourier transforms, which reduce the calculations to a multiplication of distributions.

A simple example may illustrate this algorithm. Consider the first-order matrix of a drift space in two dimensions $\mathbf{R}=\begin{bmatrix}1 & L\\ 0 & 1\end{bmatrix}$, where L is the length of the drift space and the coordinates are the position x and angle θ. For any initial phase-space distribution of light rays, for instance, we can calculate the effect of the drift space on the final phase-space distribution using the transport integral. Naming the two initial projections $P_x(x)$ and $P_\theta(\theta)$, we scale the latter to $\bar{P}_\theta(x)$ by interpolation: $\bar{P}_\theta(x)=P_\theta(x/L)$, and obviously $\bar{P}_x(x)=P_x(x)$. The projection of the final phase-space distribution on the x coordinate is then given by the convolution product $P_x'(x)=[1/(1+L)][\bar{P}_x\otimes\bar{P}_\theta](x)$. If, for instance, the two

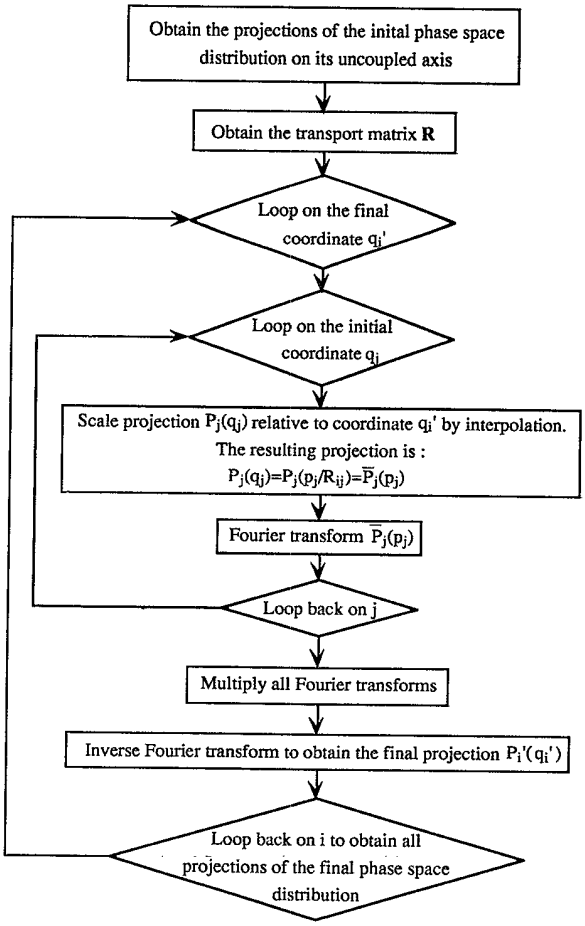

FIG. 2. Algorithm of the transport integral calculation. See text for details.

initial projections were assumed to be Gaussian with widths σ_x and σ_θ, respectively, we see that the resulting position distribution would have the width $\sigma_x+\sigma_\theta L$, which shows, as expected, that the size of the position distribution increases linearly with the length L. The angular projection of the final phase-space distribution remains unchanged, as can be seen from the coefficients on the second line of the matrix $\mathbf{R}(P'_\theta(\theta)=P_\theta(\theta))$. This very simple example illustrates the power of the algorithm since the amount of calculations does not depend on the shape of the initial projections and only linearly on the number of dimensions and the complexity of the first-order matrix describing the system.

V. APPLICATION TO BEAM OPTICS

One application of the result obtained in Sec. III is the first-order calculation of secondary radioactive beam transmission and purification through a recoil spectrometer. The fragmentation of intermediate and relativistic energy heavy ion beams has recently become one of the major methods used to produce radioactive beams [4]. In this method, the projectilelike fragments are emitted in a forward cone centered on 0°. The radioactive beam is produced by collecting these fragments in a 0° magnetic spectrometer.

Because of the reaction mechanism by which the fragments are produced, their spacial and energy distributions cannot be reproduced by simple mathematical formula. Furthermore, in most cases the acceptances of the spectrometer are not big enough to transmit all the fragments produced and the distributions have cuts. Finally, the use of thick targets to optimize the production rate and wedges to improve the purification broadens the energy distributions and produces angular and energy stragglings which have to be accounted for.

The commonly used variables for beam optics are (x,θ,y,φ,dp), where (x,θ) and (y,φ) are the positions and angles in horizontal and vertical planes, respectively, and dp the momentum variation. The first condition for using the reduction of the transport integral is fulfilled at the target position, which is an achromatic focal point, which means that the variables (x,θ,y,φ,dp) are not coupled. The initial phase-space distributions of the fragments emerging from the target can be calculated using a fragmentation model and energy loss and straggling formula. Then, given the first-order transport matrix at any position on the beam line, their phase-space distribution can be deduced via the transport integral. This method is applied in a computer program called LISE [from the LISE spectrometer at Grand Accélérateur National d'Ions Lourds (GANIL) [5]], which simulates the performance of any magnetic spectrometer set in a doubly achromatic mode in order to produce high energy radioactive beams.

Among the various experimental results which have been compared to this program, one was particularly testing the transmission of phase-space distribution with abnormal shape. The aim of this experiment was to study the possibility to produce a 5-MeV/u ^{11}Be beam from an incoming ^{18}O beam at 63 MeV/u, in order to study the dependence of sub-Coulomb barrier fusion reactions cross section on uranium as a function of the isospin of the projectile [6]. Because of such a tremendous difference between the incoming and outgoing energies, very thick targets had to be used to slow down the fragments. Increasing the target thickness has two opposite effects on the final rate of fragments collected in a recoil spectrometer. On the one hand, it increases the number of nuclear reactions in the target and therefore the number of fragments produced; but, on the other hand, their energy and spacial distributions are broadened by electron slowing down, as well as angular and energy stragglings. Those last effects tend to reduce the transmission of the spectrometer which is limited by its acceptances. As a result, there is an optimum target thickness for which the compromise between the two tendencies gives the best rate. The determination of this optimum for the production of ^{11}Be on the LISE spectrometer is shown in Fig. 3.

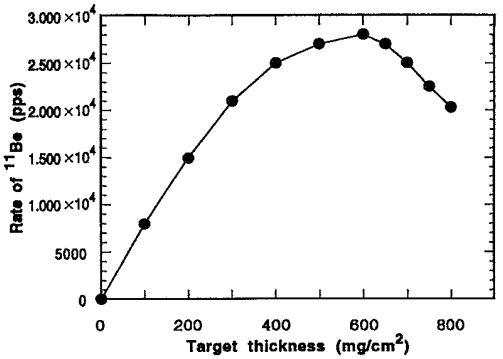

FIG. 3. Calculated rate of ^{11}Be (in particles per second) transmitted through LISE as a function of the Be target thickness for an incoming beam intensity of 2 μAe and a momentum acceptance of 0.12%. The optimum thickness is found around 600 mg/cm^2.

When the target gets even thicker, the energy of the projectiles becomes too low and the reaction cross section begins to drop until it finally vanishes. It is not possible to take this effect into account in the calculations since the energy dependence of fragmentation cross sections is not known. As a rough approximation, one can assume that it drops sharply to zero at a given energy, which still remains to be determined. In the following simulation, we have supposed that the only active thickness, i.e., where nuclear reactions actually take place, is equal to the optimum thickness. The remainder of the target is passive and only slows down the fragments. We have compared the calculations for the five target thicknesses used in the experiment: 370, 740, 1100, 1480 and 1850 mg/cm^2 of Be. The second target corresponds roughly to the calculated optimum thickness and it is indeed for this one that the highest rate of ^{11}Be has been observed. The comparison is shown in Fig. 4, where the points correspond to the data taken from [6] and the lines to the calculations performed by LISE. The five calculated energy distributions have been normalized to the data by a single

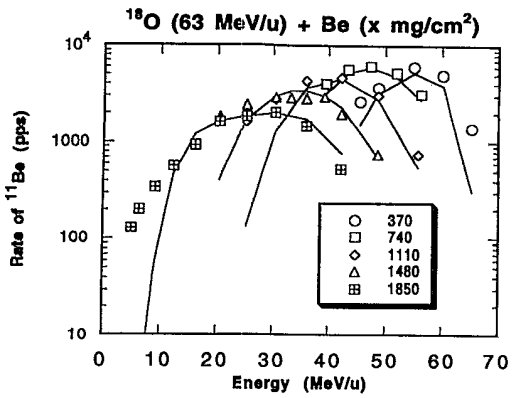

FIG. 4. Comparison between measured and calculated ^{11}Be rates with different target thicknesses x as a function of energy. The points represent the data and the lines the renormalized calculations.

coefficient, which indicates that the transmission of the spectrometer is fairly well simulated by the calculation and the disagreement is due to a bad determination of the total reaction cross section. This cross section has been calculated using the empirical parametrization of Sümmerer *et al.* [7], which gives 1.77 mb. The renormalization of the calculation by a factor of 4.4 allows one to determine the total cross section $\sigma_{\text{tot}}(^{18}\text{O}+\text{Be} \rightarrow ^{11}\text{Be}) = 0.4$ mb. The discrepancy observed at the low energy part of the distributions for the three thickest targets is a clear indication that our assumption on the behavior of the cross section at low energy is not realistic and it indeed decreases smoothly towards zero.

VI. CONCLUSION

In the first part of this paper, we have presented an analytical way to calculate the time evolution of phase-space distributions. However, the number of cases where the transport integral can be solved analytically is very limited, due to its mathematical form, and only when simple configurations are considered can it be disentangled. Two numerical ways to directly calculate this integral are first using numerical integration algorithms and second by sampling methods such as Monte Carlo, but those are either time consuming or imprecise and therefore not well suited when fast calculations are needed. Under the assumption of noncoupled variables in the initial phase-space distribution, and taking a first-order approximation of the transport functions, we have shown that the transport integral can be reduced to convolution products, which in turn are easy and fast to calculate using fast Fourier transform algorithms.

This result has been applied to the simulation of secondary radioactive beam production using the technique which combines projectile fragmentation reactions and a recoil spectrometer to collect and purify the beam. The calculations produced by the program called LISE have been compared to experimental data taken on the spectrometer of the same name at GANIL, on the production of a ^{11}Be beam from the fragmentation of ^{18}O. The transmission of the spectrometer is indeed well reproduced by the calculation, with some discrepancies due to the assumptions made on the cross section energy dependence. The full description of this program will be the subject of a future publication.

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