Split-operator technique and solution of Liouville propagation equations

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We use the split-operator technique (SOT) to solve evolution equations of the Liouville type. The method we propose is based on an iterative application of the evolution operator, associated with the equation under study, on the initial distribution. The SOT approximation of the evolution operator leads to analytical expressions that can be easily programmed. We discuss the validity of the method, solving the Liouville equation governing the longitudinal phase-space dynamics of an e beam undergoing free-electron-laser interaction and the phase-space evolution of a quartic anharmonic oscillator.

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The use of a symmetrically split propagation operator technique has been successfully applied by Feit, Fleck, and Steiger [1] for the solution of Schrödinger equations in the coordinate representation. The same method was successively exploited by Torres-Vega and Frederick [2] to study the phase-space evolution of wave functions.

In this paper we will start from the split-operator technique (SOT) to solve the classical evolution of a phase-space distribution of particles subject to a given potential. The method we propose differs from that exploited in Refs. [1,2] because we mostly employ analytical methods and avoid using the Fourier transform as an intermediate step. Here, we outline the basic features of the procedure and a more general analysis will be presented elsewhere.

The Liouville equation describing the evolution of the phase-space distribution of an ensemble of noninteracting particles subject to the potential $V(q)$ is specified by [3]

$$\frac{\partial}{\partial\tau}\rho(q,p;\tau)=\left\{-p\frac{\partial}{\partial q}+V'(q)\frac{\partial}{\partial p}\right\}\rho(q,p;\tau)\ , \tag{1}$$

with q and p being canonically conjugate variables and

$$V'(q)=\frac{\partial}{\partial q}V(q)\ .$$

If we assume that the initial phase-space distribution is continuous and infinitely differentiable in the (q,p) variables, we can write the formal solution of (1) as

$$\rho(q,p;\tau)=\exp\left\{\tau\left[-p\frac{\partial}{\partial q}+V'(q)\frac{\partial}{\partial p}\right]\right\}\rho(q,p;0)\ . \tag{2}$$

Let us now define the differential operators

$$\hat{A}=-p\frac{\partial}{\partial q}\ ,\quad \hat{B}=V'(q)\frac{\partial}{\partial p}\ , \tag{3}$$

whose commutation is provided by

$$\hat{C}=[\hat{A},\hat{B}]=-p\left\{V''(q)\frac{\partial}{\partial p}-V'(q)\frac{\partial}{\partial q}\right\}\ . \tag{4}$$

For a few specific cases of $V(q)$, $\hat{A}$, $\hat{B}$, and $\hat{C}$ provide a closed group and thus the exponential operator on the right-hand side of (2) can be written as the following ordered product [4]:

$$\exp\left\{\tau\left[-p\frac{\partial}{\partial x}+V'(q)\frac{\partial}{\partial p}\right]\right\}=e^{a(\tau)\hat{A}}e^{b(t)\hat{B}}e^{c(\tau)\hat{C}}\ , \tag{5}$$

where (a,b,c) are τ-dependent functions satisfying a set of nonlinear equations specified by the particular type of group spanned by $\hat{A}$, $\hat{B}$, and $\hat{C}$. For the case where one is able to disentangle the evolution operator in the ordered form (5), the time evolution of $\rho(q,p;\tau)$ can be easily obtained using standard operational rules [4].

The problem arises when $\hat{A}$, $\hat{B}$, and $\hat{C}$ do not provide any closed group; in this case, one should use approximate but efficient methods, such as the SOT approximation, according to which the evolution operator can be written as

$$e^{\delta\tau(\hat{A}+\hat{B})}\cong e^{(1/2)\delta\tau\hat{A}}e^{\hat{B}\delta\tau}e^{(1/2)\delta\tau\hat{A}}\ . \tag{6}$$

The difference between the two sides of the above relation is [1,2]

$$e^{\delta\tau(\hat{A}+\hat{B})}-e^{(1/2)\delta\tau\hat{A}}e^{\hat{B}\delta\tau}e^{(1/2)\delta\tau\hat{A}}\cong\tfrac{1}{24}(\delta\tau)^3[(\hat{A}+2\hat{B}),[\hat{A},\hat{B}]]+0((\delta\tau)^4)\ . \tag{7}$$

The representation (6) is valid for short interval times, and the solution $\rho\,(q,p;\delta\tau)$ makes sense if

$$\left|\tfrac{1}{24}(\delta\tau)^3[\hat{A}+2\hat{B},[\hat{A},\hat{B}]]\rho(q,p;0)\right|\ll\rho(q,p;\delta\tau)\ . \tag{8}$$

The extension to longer interval times can be obtained applying the evolution operator (6) n times to the initial distribution. The problem is now how to effectively apply the operator (6) to the phase-space distribution. The Fourier transform method can be adopted as suggested in Refs. [1,2]; however, in the present case, we can skip this intermediate step, noting that

$$[\hat{U}(\delta\tau)]^n f(q,p)=f(q_n,p_n)\ , \tag{9}$$

where there are n factors of $\hat{U}(\delta\tau)$ and

$$\hat{U}(\delta\tau)=\exp\left\{-\frac{\delta\tau}{2}p\frac{\partial}{\partial q}\right\}\exp\left[\delta\tau V'(q)\frac{\partial}{\partial p}\right]\times\exp\left[-\frac{\delta\tau}{2}p\frac{\partial}{\partial q}\right]\ ,$$
$$f(q,p)=\rho(q,p;0)\ . \tag{10}$$

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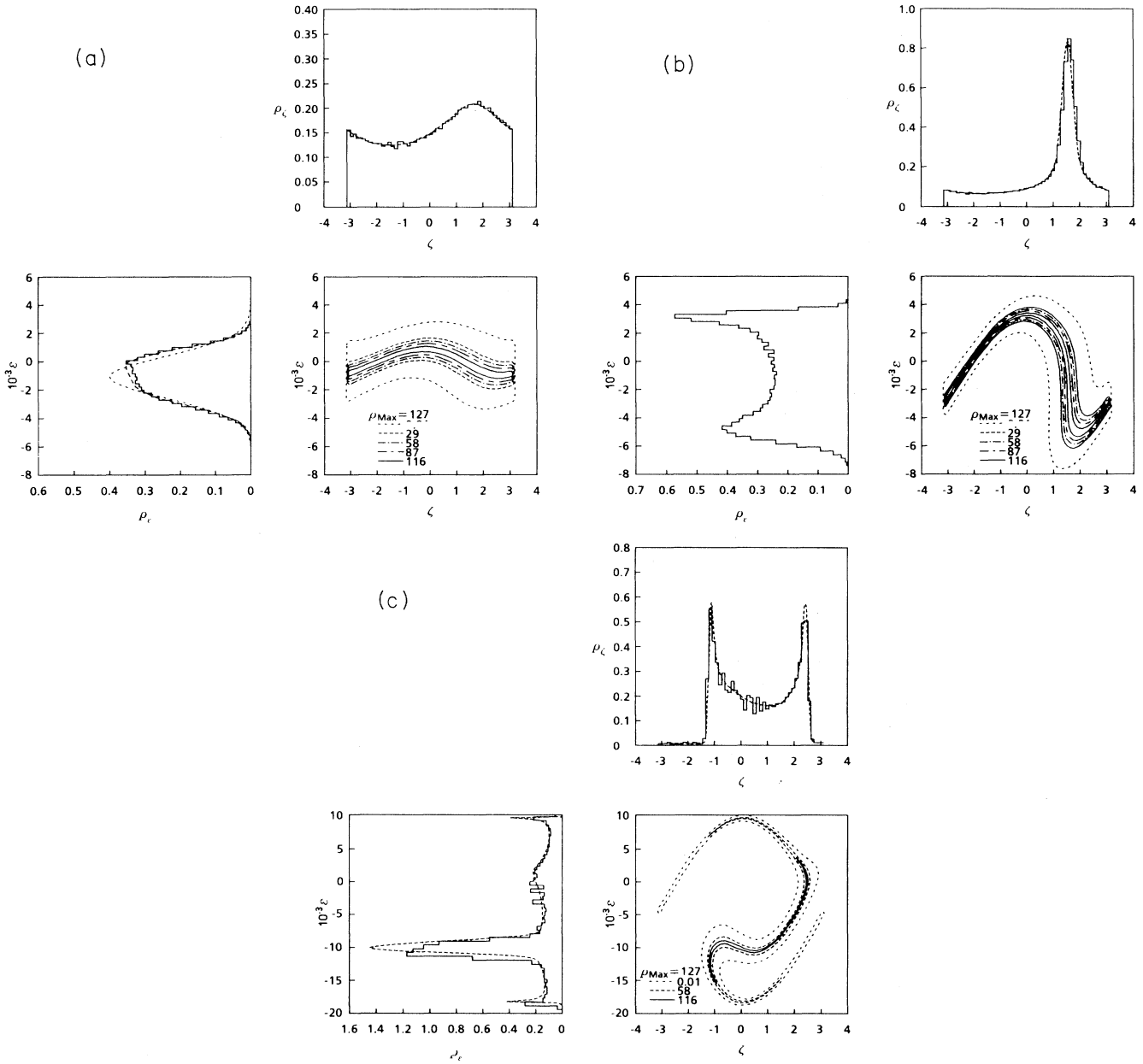

FIG. 1 (a) Integration of the FEL Liouville equation $\rho_\nu\rho_\xi$ and phase-space distribution contour plots at $\tau=1$. The histogram refers to the results of the simulation code. Parameters: $N=40$, $\sigma_\varepsilon(0)=5\times10^{-4}$, $\mu_\varepsilon(0)=4N\sigma_\varepsilon(0)$, $\xi=0.624$. (b) Same as (a), $\xi=2.79$. (c) same as (a), $\xi=12.48$.

Using the well-known relation

$$\exp\left[\lambda\frac{d}{dx}\right]f(x)=f(x+\lambda)\ ,$$

we find that q_n and p_n satisfy the recurrence relations

$$q_n=q_{n-1}-\delta\tau p_{n-1}-\tfrac{1}{2}(\delta\tau)^2V'\left[q_{n-1}-\frac{\delta\tau}{2}p_{n-1}\right],\quad p_n=p_{n-1}\delta\tau V'\left[q_{n-1}-p_{n-1}\frac{\delta\tau}{2}\right],$$
$$q_1=q-p\delta\tau-\tfrac{1}{2}(\delta\tau^2)V'\left[q-\frac{\delta\tau}{2}p\right],\quad p_1=p+\delta\tau V'\left[q-\tfrac{1}{2}p\delta\tau\right]. \tag{11}$$

The above relations provide the solution of the problem. We will illustrate two examples to prove the usefulness of

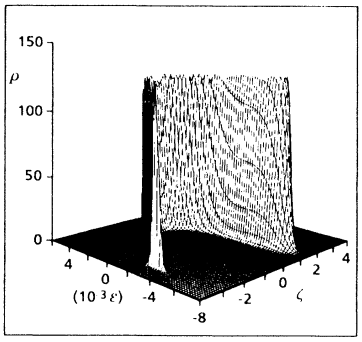

FIG. 2. Longitudinal phase-space distribution. Same parameters as Fig. 1(b) (SOT integration).

the technique described.

The Liouville equation associated with the one-dimensional treatment of free-electron-laser (FEL) dynamics is [5]

$$\frac{\partial}{\partial\tau}\rho(\nu,\zeta;\tau)=\left\{-\nu\frac{\partial}{\partial\zeta}+\xi\sin(\zeta)\frac{\partial}{\partial\nu}\right\}\rho(\nu,\zeta;\tau)\ , \tag{12}$$

where ν and ζ are longitudinal phase-space canonically conjugate variables, τ is a dimensionless time ranging from 0 to 1, and ξ plays the role of coupling strength. The evolution operator associated with Eq. (12) writes

$$\hat{U}(\delta\tau)\cong\exp\left[-\tfrac{1}{2}(\nu\delta\tau)\frac{\partial}{\partial\zeta}\right]\exp\left[\xi\delta\tau(\sin\zeta)\frac{\partial}{\partial\nu}\right]\times\exp\left[-\tfrac{1}{2}(\nu\delta\tau)\frac{\partial}{\partial\zeta}\right]\ . \tag{13}$$

In the case of the FEL, the initial distribution is usually independent of ζ and, therefore,

$$[\hat{U}(\delta\tau)]^n f(\nu)=f(\nu_n)\ ,$$
$$\nu_n=\nu_{n-1}+\xi\delta\tau\sin\left[\zeta_{n-1}-\frac{\delta\tau}{2}\nu_{n-1}\right]\ , \tag{14}$$
$$\zeta_n=\zeta_{n-1}-\delta\tau\nu_{n-1}-\tfrac{1}{2}(\delta\tau)^2\sin\left[\zeta_{n-1}-\frac{\delta\tau}{2}\nu_{n-1}\right]\ .$$

In the first equation, there are n factors of $\hat{U}(\delta\tau)$. The last equation should be able to provide the solution of the Liouville equation (13) with initial condition $f(\nu)$. The results of the integration are shown in Fig. 1. We have assumed a Gaussian initial distribution, namely [6],

$$f(\nu)=\frac{1}{2\pi}\frac{1}{\sqrt{2\pi}[\pi\mu_\varepsilon(0)]}\exp\left[-\frac{(\nu-\nu_0)^2}{2[\pi\mu_\varepsilon(0)]^2}\right]\ . \tag{15}$$

The parameter $\mu_\varepsilon(0)$ is linked to the rms value of the initial distribution. In Fig. 1 we have plotted the quantities

$$\rho_\nu=\frac{\mu_\varepsilon(0)}{4N}\int_{-\pi}^{\pi}\rho(\nu,\zeta;1)d\zeta\ ,$$
$$\rho_\zeta=\int_{-\infty}^{+\infty}\rho(\varepsilon,\zeta;1)d\varepsilon\ ,\quad \varepsilon=\frac{\nu-\nu_0}{4\pi N}\ , \tag{16}$$

and the contour plots of $\rho(\varepsilon,\zeta;1)$, for different values of the coupling strength ξ. The choice of the normalizations is due to the fact that we have confronted the analytical results with those from a macroparticle simulation code requiring the number of undulator periods (N), the relative electron energy ε, etc. The quantity $\mu_\varepsilon(1)$ is the rms of the ν distribution at $\tau=1$. The agreement between the solution (14) and the fully numerical procedure is good. The advantage of the SOT is that the relevant results are obtained at an almost negligible computer cost. An idea of the distribution $\rho(\nu,\zeta;1)$ is offered by Fig. 2.

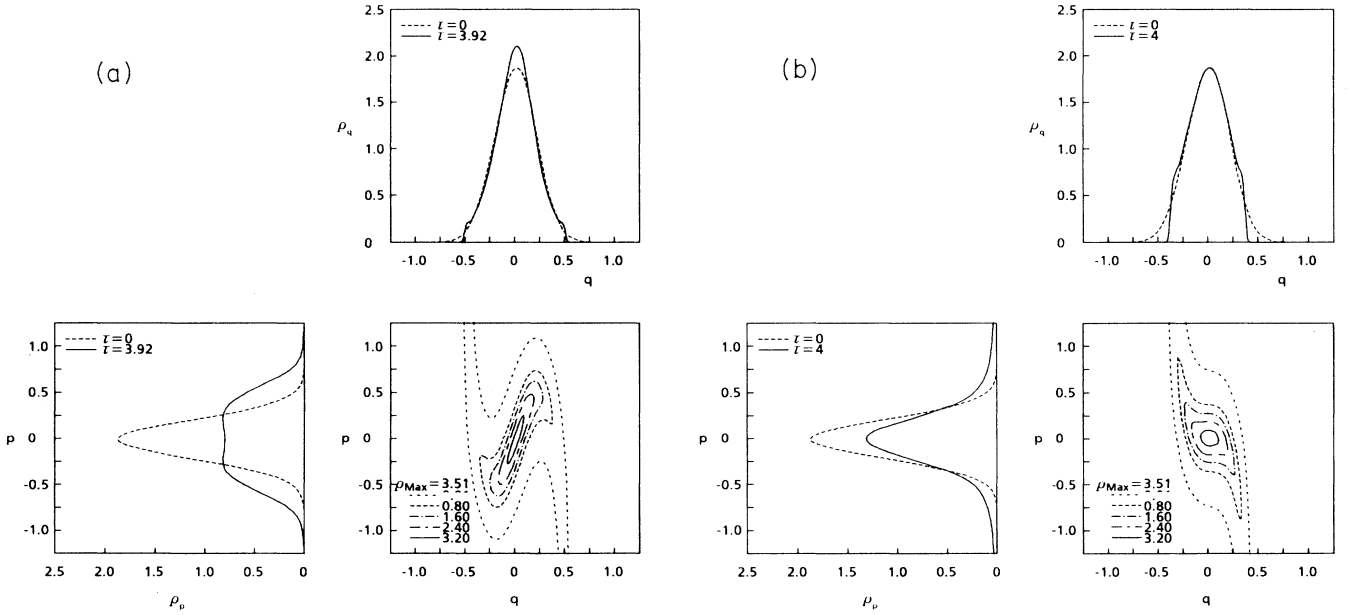

FIG. 3. (a) Quartic harmonic oscillator phase-space evolution: ρ_q,ρ_p and $\rho(q,p)$ contour plots at $\tau=3.92$ ($\beta=\gamma=1,\alpha=0,\sigma=4.536\times10^{-2}$, $\omega=2\pi$). (b) Same as (a), $\tau=4$.

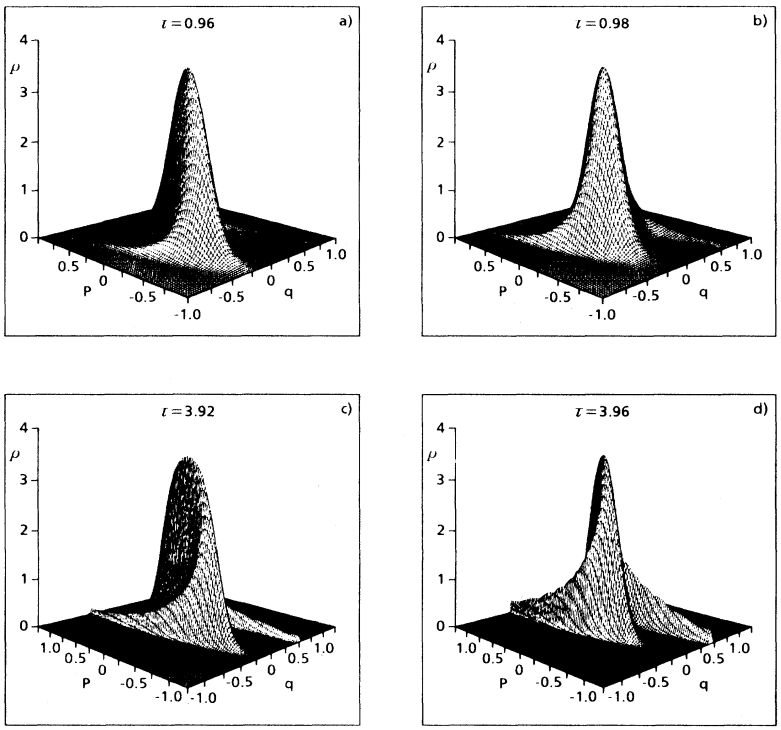

FIG. 4. Evolution of $\rho(q,p)$; same parameters as Fig. 3(a). (a) $\tau=0.96$; (b) $\tau=0.98$; (c) $\tau=3.92$; (d) $\tau=3.96$.

Let us now return to Eq. (1) and assume the initial distribution

$$f(q,p)=\frac{1}{(2\pi)\sigma}\exp\left[-\frac{1}{2\sigma}(\gamma q^2-2\alpha qp+\beta p^2)\right], \quad (17)$$

where (γ,β,α) are the Twiss coefficients satisfying the condition [6]

$$\gamma\beta=1+\alpha^2 . \quad (18)$$

The potential $V(q)$ is further assumed to be of the form

$$V(q)=\frac{\omega^2}{2}\left[q^2+\tfrac{1}{6}q^4\right] . \quad (19)$$

The solution of Eq. (1) has been obtained using the method discussed in the paper, and the results of the integration are shown in Fig. 3 where we have plotted the quantities

$$\rho_q=\int_{-\infty}^{+\infty}\rho(q,p;\tau)dp ,$$
$$\rho_p=\int_{-\infty}^{+\infty}\rho(q,p;\tau)dq , \quad (20)$$

and the contour plots of $\rho(q,p;\tau)$ for different values of τ. In Fig. 4 we also provide a three-dimensional view of the phase-space distribution. The accuracy of the results has been checked with a standard ray-tracing procedure.

The pictures clearly display the phase-space distortion due to the anharmonic contribution of the potential (19).

In a forthcoming paper, we will extend the method to the multidimensional case and discuss more thoroughly the procedure outlined. Finally, it is worth stressing that the SOT algorithm naturally leads to an area-preserving mapping [7]. In fact, the Jacobian determinant

$$J=\begin{vmatrix} \dfrac{\partial q_n}{\partial q_{n-1}} & \dfrac{\partial p_n}{\partial q_{n-1}} \\ \dfrac{\partial q_n}{\partial p_{n-1}} & \dfrac{\partial p_n}{\partial p_{n-1}} \end{vmatrix} \quad (21)$$

is easily shown [see Eq. (11)] to be equal to unity. This also ensures that the SOT form of the evolution operator provides, at each step n, a canonical transformation. This last point and the link with Lie algebraic methods will be discussed elsewhere.

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