We have also studied the effects on the calculated eigendefects of making various approximations to different terms in the potential in the radial Eqs. (6) and (7). For example, even though the contribution $y_3(3d, 3d|r)$ from the nonspherical charge density is relatively small compared with V_2, and even though the potentials for different atomic configurations differ only slightly from each other, it is very important to take these differences into account. Similarly, we find that the use of the Herman-Skillman potential[10] instead of the Hedin-Lundqvist approximation (with self-consistent, self-energy correction) gives significant errors [(10–30)%] in quantum defects (modulo 1) even for weakly interacting triplet channels.

The relatively simple method used here may be useful for calculating accurate photoionization cross sections as well as for calculating excited bound-state energies for open-shell atoms.

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Calculation of Turbulent Diffusion for the Chirikov-Taylor Model

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A probabilistic method for the solution of the Vlasov equation has been applied to the Chirikov-Taylor model. The analytical solutions for the probability function and its second velocity moment have been obtained. Good agreement between the theory and numerical computations has been found.

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The purpose of this Letter is to present an analytical solution for the Chirikov-Taylor model.[1,2] This model has been studied extensively in the last ten years in reference to many different plasma physics problems.[1-6] Such an interest is due to the fact that this simple model exhibits chaotic or turbulent dynamics manifested in the region above the so-called stochastic transition.[1,2] We will introduce the method of solution and the underlying physical arguments through the differential equation which describes the motion of charged particles in a field of electrostatic plane waves. The equation of motion is

$$\mu\, d^2x/dt^2 = eE(x,t), \tag{1}$$

where μ is the mass, e is the charge of the particle, and the electric field is given by the equation

$$E(x, t) = \sum_{m,n} E_{mn} \exp[i(k_m x - \omega_n t)] + \text{c.c.} \tag{2}$$

We assume here periodic boundary conditions in the interval $0 \leq x \leq a$, $k_m = 2\pi m/a$, m integer, and a discrete spectrum in ω. Consider the case

$$k_m = (2\pi/a)\,\delta_{1m}\; \omega_n = \omega_0 n \tag{3}$$

with $n = 0, \pm 1, \pm 2, \ldots, \pm N$, and $E_{1,n} = E_0/2i$ is constant. The symbol δ_{mn} is a Kronecker function. With use of dimensionless variables by rescaling distance with $a/2\pi$ and time with $2\pi/\omega$, Eq. (1) takes the form

$$dx/dt = v \tag{4}$$

$$\frac{dv}{dt} = \epsilon \sin x \frac{\sin[\pi t(2N+1)]}{\sin \pi t} \tag{5}$$

and $\epsilon = (2\pi)^3 E_0 e/a\omega_0^{\,2}\mu$, $N \gg 1$.

Consider the phase space (x, v) and introduce the initial distribution of phase-space points $f(x, v, t=0)$. The time evolution of f is described by a Vlasov equation

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{dv}{dt}\frac{\partial f}{\partial v} = 0. \tag{6}$$

This is just a continuity equation of phase-space flow. This flow is deterministic, that is, the position of every point can be predicted uniquely for an arbitrary large time t. Because of the complicated nonlinear character of Eq. (5), some phase-space points which are initially separated can come arbitrarily close to each other if the time of evolution is long enough. This implies that ∇f can become arbitrarily large because phase-space density is conserved along the orbits (Liouville theorem). We may say that long-time solutions are intrinsically singular. This is why it is impossible to find an analytic solution of the Vlasov equation even for the simple motion described by Eqs. (4) and (5). On the other hand, there are always some processes which are not included in these equations, including small errors introduced in a numerical solution. In spite of being very small they do play an important role in the limit of large times as we will see later. A simple way of modeling such effects is to introduce a random velocity term in Eq. (4) or a random force term in Eq. (5). We have done these numerically. From the analytic point of view, it is more convenient to treat these as additional spatial or velocity diffusion terms in the Vlasov equation. The analysis happens to be much easier for the case of spatial diffusion. The Vlasov equation in this case takes the form:

$$\frac{\partial P}{\partial t} + v\frac{\partial P}{\partial x} + \frac{dv}{dt}\frac{\partial P}{\partial v} - \frac{\sigma}{2}\frac{\partial^2 P}{\partial x^2} = 0. \tag{7}$$

Thus the deterministic description given by the Vlasov equation is substituted by a probabilistic one with probability function $P(x, v, t)$, which we normalize to unity. We consider $\sigma \ll 1$. As we will see later it is the diffusion which resolves the singular nature of the long-time solutions of the Vlasov equation. The effect of weak diffusion has been discussed qualitatively for the similar problem of electron heat transport in tokamaks with destroyed magnetic surfaces.[7] The initial condition for P we take of the form

$$P(x, v, 0) = (2\pi)^{-1}\,\delta(v - v_0). \tag{8}$$

The Chirikov-Taylor model corresponds to the limit $N \to \infty$. Then $\sin[\pi t(2N+1)]/\sin(\pi t)$ can be approximated by $\sum_{i=-\infty}^{\infty}(t - i)$.

Consider now the time evolution of the probability function P. In the interval $i - 0 < t < i + 0$ it can be written as

$$P(x, v, i+0) = P(x, v + \epsilon \sin x, i - 0). \tag{9}$$

Here i is an integer and $+0$ is an arbitrary small number. Evolution in the interval $i + 0 < t < i + 1 - 0$ is given by the formula

$$P(x, v, t) = \int_{-\infty}^{+\infty} dv_1 \int_0^{2\pi} G(x - x_1, v, v_1, t - t_1) P(x_1, v_1, t_1)\, dx_1, \tag{10}$$

where G is a solution of the equation

$$\frac{\partial G}{\partial t} + v\frac{\partial G}{\partial x} - \frac{\sigma}{2}\frac{\partial^2 G}{\partial x^2} = \delta(x - x_1)\,\delta(v - v_1)\,\delta(t - t_1), \tag{11}$$

$$G = \frac{\theta(t - t_1)\,\delta(v - v_1)}{[2\pi\sigma(t - t_1)]^{1/2}} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{[x - x_1 - v(t - t_1) + 2\pi n]^2}{2\sigma(t - t_1)}\right). \tag{12}$$

Here $\theta(t)$ is the Heaviside function.

The summation appears because of the periodic boundary conditions in the interval $0 \leq x \leq 2\pi$. We can now write a formal solution to Eq. (7) for initial probability given by Eq. (8) for arbitrary time t (for simplicity, we consider $t=T$, a large integer):

$$P(x_T, v, T) = \sum_{n_T=-\infty}^{\infty} \cdots \sum_{n_1=-\infty}^{\infty} \prod_{i=0}^{T-1} \int_0^{2\pi} \frac{dx_i}{(2\pi\sigma)^{1/2}} \frac{1}{2\pi} \delta(v - v_0 - S_T) \exp\left[-2\sigma^{-1} \sum_{j=1}^{T} (x_j - x_{j-1} - v_0 - S_{j-1} + 2\pi n_j)^2\right],$$

$$S_j = \epsilon \sum_{p=0}^{j} \sin x_p. \tag{13}$$

It is easy to check by direct integration that $P(x, v, T)$ is correctly normalized,

$$\int_{-\infty}^{\infty} dv \int_0^{2\pi} dx\, P(x, v, T) = 1. \tag{14}$$

To calculate the diffusion rate we use the formula

$$D = \lim_{T\to\infty} \left[(2T)^{-1} \int_{-\infty}^{\infty} \int_0^{2\pi} (v - v_0)^2 P(x, v, T) dx\, dv\right]. \tag{15}$$

With the use of the identity

$$(2\pi\sigma)^{1/2} \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(y+2\pi n)^2}{2\sigma}\right] = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \exp(-\tfrac{1}{2}\sigma m^2 + imy) \tag{16}$$

we can write Eq. (15) as

$$D = \lim_{T\to\infty} \frac{1}{2T} \sum_{m_T=-\infty}^{\infty} \cdots \sum_{m_1=-\infty}^{\infty} \prod_{i=0}^{T} \int_0^{2\pi} \frac{dx_i}{2\pi} S_T^2 \exp\left(\sum_{j=1}^{T} \left[-\tfrac{1}{2}\sigma m_j^2 + i m_j (x_j - x_{j-1} - v_0 - S_{j-1})\right]\right), \tag{17}$$

$$S_j = \epsilon \sum_{p=0}^{j} \sin x_p.$$

In the case $m_j = 0$ the calculations are trivial and we find

$$D_{\rm QL} = \epsilon^2/4. \tag{18}$$

This case corresponds to the random-phase approximation often made in quasilinear theory. To evaluate D for $m_j \neq 0$, we make use of the identity

$$\exp(\pm iz \sin x) = \sum_{n=-\infty}^{\infty} J_n(z) \exp(\pm inx). \tag{19}$$

Here $J_n(z)$ are Bessel functions and $z > 0$.

If we make use of Eq. (19), it is easy to see that the series in Eq. (17) involves products of Bessel functions. In the region of large ϵ the Bessel functions decay as $1/\sqrt{\epsilon}$ so that we can keep just a few low-order terms in Eq. (17). The expression obtained for D is

$$D = \tfrac{1}{2}\epsilon^2\left[\tfrac{1}{2} - J_2(\epsilon)e^{-\sigma} - J_1^2(\epsilon)e^{-\sigma} + J_3^2(\epsilon)e^{-3\sigma}\right], \tag{20}$$

which is obtained from Eq. (17) from those terms in which two or three of the $m_j \neq 0$, and all others are zero. The J_2 term arises from terms with $m_l = \pm 1$, $m_{l-1} = -m_l$, $l = 2, 3, \ldots, T$. The J_1^2 term is similar, with $m_{l-2} = -m_l$, $l = 3, 4, \ldots, T$, and the J_3^2 term comes from $m_l = \pm 1$, $m_{l-1} = -2m_l$, $m_{l-2} = m_l$, $l = 3, 4, \ldots, T$. We have neglected products involving three or more Bessel functions. Our numerical computations suggest that convergence of the series approximated by Eq. (20) in the region $\epsilon \gg 1$ is much faster than that due simply to the exponential factors $\exp(-\tfrac{1}{2}\sigma m_j^2)$. The possible relation between this fast convergence and exponential orbit divergence for Eqs. (4) and (5) which takes place in the region $\epsilon \gg 1$ (the so called stochastic instability[1,2]) has not yet been examined. The leading asymptotic terms in Eq. (20) are

$$\frac{D}{D_{\rm QL}} \approx 1 - 2e^{-\sigma}\left(\frac{2}{\pi\epsilon}\right)^{1/2} \cos\left(\epsilon - \frac{5\pi}{4}\right). \tag{21}$$

Thus D approaches $D_{\rm QL}$ in the limit $\epsilon \gg 1$; the usual quasilinear limit corresponds to $\epsilon \to \infty$. We recall here that the spectrum of ω is assumed to be continuous in quasilinear theory. Within our model a continuous spectrum can be achieved by considering the limit $\omega_0 \to 0$. Then in order that the power density per unit frequency bandwidth remain constant we need to rescale $E_0 \sim \omega_0^{1/2} \to 0$ and $\epsilon \sim \omega_0^{-3/2} \to \infty$ [see Eq (5)].

The contribution to D from terms with $m_j \neq 0$ can be comparable to or even bigger than $D_{\rm QL}$ for some values of ϵ (see also Fig. 1). This could have practical implications especially for the problems of radiofrequency heating.[6] We will address this question in future publications.

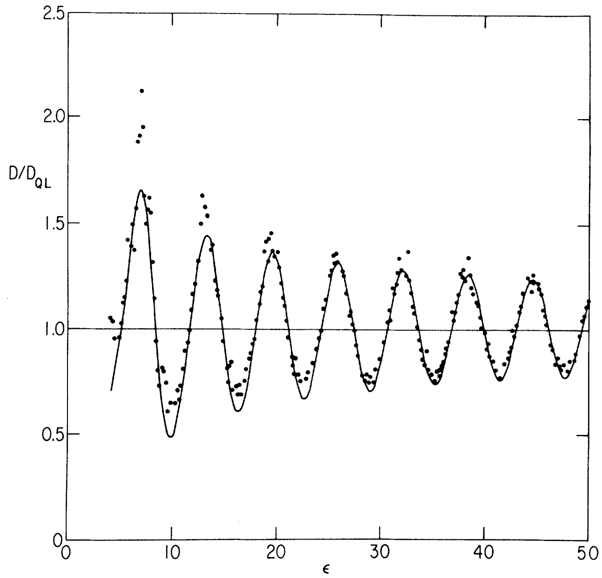

FIG. 1. The ratio of the numerically obtained diffusion to the quasilinear value as a function of ϵ. Here $\sigma = 10^{-5}$. Also plotted is the analytic expression given by Eq. (20).

We have made extensive numerical study of Eqs. (4) and (5), introducing a small random step in x with a normal distribution of mean σ. Some of the results of these computations are shown in Fig. 1 for the case $\sigma = 10^{-5}$. To obtain sufficient accuracy in the evaluation of D we used the number of particles $N_p = 3000$, the fluctuations in D behaving as $1/(N_p)^{1/2}$, and advancing the equations to $T = 50$. We also verified that introducing a random step in v rather than in x leads to essentially the same results for small σ and large ϵ. The oscillations in D/D_{QL} were apparently first noted by Chirikov,[1] but were independently found by Hizanidis[8] and pointed out to the present authors. We also note from this figure that D approaches D_{QL} in the limit of large ϵ. Also plotted on Fig. 1 is the function given by Eq. (20). It is clear that there is good agreement for large ϵ, but for ϵ of the order of unity we need to retain more terms in the evaluation of Eq. (17). We think that the method outlined may prove useful in other problems where apparently chaotic behavior arises from deterministic equations.

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