Wind-tree model in two dimensions with internal degrees of freedom: Exact solution

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The two-dimensional wind-tree model with particles with four allowed velocities, which can scatter off obstacles with internal degrees of freedom, is solved exactly. Depending on initial conditions the distribution functions and entropy of obstacles can display a nonmonotonic time dependence with over- and underpopulations followed by transient relaxation.

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The wind-tree model introduced by P. and T. Ehrenfest early in this century [1] is an important testing ground to check many ideas of nonequilibrium statistical mechanics. It consists of two sorts of particles: light, noninteracting particles are moving and are being scattered off a system of immobile obstacles. The density of the obstacles is low, and they are noninteracting. The light particles can have only a finite, small number of velocities. In the simplest version [2], only four velocities are allowed, $\mathbf{v}_i$, $i=1,\ldots,4$ with $|\mathbf{v}_i|=1$. Usually it is assumed that the whole system is spatially uniform.

We present here a generalization of this model in which the collisions of the light particles with the obstacles can induce the transitions between internal degrees of freedom of the obstacles. Let us assume for simplicity that the obstacles can be in two distinct states, left (L) or right (R). The system of such obstacles is now exposed to collisions with incoming particles. We identify the L and R directions with the x axis of particle velocity. Thus effectively the internal states of the obstacles are also one-dimensional. The interaction between the particles and obstacles is also anisotropic: the state R can be obtained from L through a collision with $\mathbf{v}=(1,0)$, and the state L is produced from R through a collision with $\mathbf{v}=(-1,0)$. The state of the system is given by one-particle distribution functions for particles $\varphi_i(t)$, $i=1,\ldots,4$, and for obstacles $\Psi_L(t)$ and $\Psi_R(t)$, which are normalized $[\sum_{i=1}^{4}\varphi_i(t)=1,\ \Psi_L(t)+\Psi_R(t)=1]$ and which have the usual probabilistic interpretation. The collision rules for the model are depicted in Fig. 1, and the kinetic equations read

$$\frac{d}{dt}\Psi_L(t)=g(\varphi_3\Psi_R-\varphi_1\Psi_L)\ ,$$
$$\frac{d}{dt}\Psi_R(t)=g(\varphi_1\Psi_L-\varphi_3\Psi_R)\ , \tag{1}$$

$$\frac{d}{dt}\varphi_1(t)=k(\varphi_2+\varphi_4-2\varphi_1)\ ,$$
$$\frac{d}{dt}\varphi_2(t)=k(\varphi_1+\varphi_3-2\varphi_2)\ ,$$
$$\frac{d}{dt}\varphi_3(t)=k(\varphi_2+\varphi_4-2\varphi_3)\ , \tag{2}$$
$$\frac{d}{dt}\varphi_4(t)=k(\varphi_1+\varphi_3-2\varphi_4)\ .$$

We observe that, according to Eqs. (2), the state of the particles is not influenced by the obstacles, and the state of the obstacles depends on φ_1 and φ_3 only (velocities parallel and antiparallel to the x axis). The coupling constants g and k are simple functions of velocities and are related to appropriate cross sections. We choose them as constants here, with $g>0$ and $k>0$.

In the following, we shall demonstrate that Eqs. (1) and (2) can be analytically solved for any finite ratio of coupling constants g/k and for any set of initial conditions $\varphi_i(0)$ and $\Psi_{R,L}(0)$. We first solve Eqs. (2), then substitute

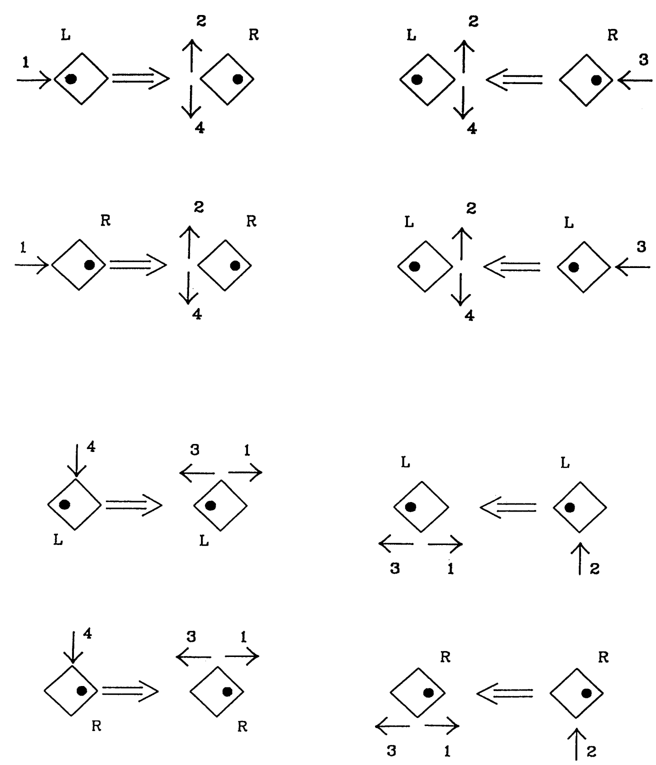

FIG. 1. Complete set of collision rules for the model. Incoming particles are scattered with a probability $\frac{1}{2}$ in each perpendicular direction. The internal degrees of freedom of the obstacles are one dimensional, chosen in the x direction. Only collisions with particles with velocities $\mathbf{v}=(1,0)$ or $(-1,0)$ (particles 1 or 3) can modify the state of the obstacles, as seen from the two first diagrams. This leads directly to Eqs. (1) and (2).

$\varphi_i(t)$, $i=1,3$, into (1), which can be then completely integrated in terms of known functions.

The solution of (2) is then given in terms of three constants $C_1=\varphi_1(0)-\varphi_3(0)$, $C_2=\varphi_2(0)-\varphi_4(0)$, and $C_3=\varphi_1(0)+\varphi_3(0)-\frac{1}{2}$:

$$\begin{aligned}\varphi_1(t)&=\tfrac{1}{2}(\tfrac{1}{2}+C_1e^{-2kt}+C_3e^{-4kt}) ,\\ \varphi_2(t)&=\tfrac{1}{2}(\tfrac{1}{2}+C_2e^{-2kt}-C_3e^{-4kt}) ,\\ \varphi_3(t)&=\tfrac{1}{2}(\tfrac{1}{2}-C_1e^{-2kt}+C_3e^{-4kt}) ,\\ \varphi_4(t)&=\tfrac{1}{2}(\tfrac{1}{2}-C_2e^{-2kt}-C_3e^{-4kt}) .\end{aligned} \tag{3}$$

In the following, we choose $C_3>0$, and, with (3), transform (1) into

$$\frac{d}{dt}\Psi_L(t)+g(\tfrac{1}{2}+C_3e^{-4kt})\Psi_L(t)=\frac{g}{2}\left[\frac{1}{2}-C_1e^{-2kt}+C_3e^{-4kt}\right] . \tag{4}$$

It is now convenient to introduce a reduced coupling constant $\Theta=g/8k$ and a new variable $y(t)=\exp(2C_3\Theta e^{-gt/2\Theta})$, in terms of which the general solution of (4) is

$$\Psi_L(y)=\exp(y)y^{\Theta}\int \exp(-y)\left[-\frac{1}{2y^{\Theta}}+\frac{C_1\sqrt{\Theta}}{\sqrt{2C_3}}\frac{1}{y^{\Theta+1/2}}-\frac{\Theta}{2}\frac{1}{y^{\Theta+1}}\right]dy . \tag{5}$$

The additive integration constant in (5) is, as usual, determined through $\Psi_L(t=0)$. The integrals in (5) can be expressed for arbitrary $\Theta>0$ in terms of Whittaker functions $W_{\mu,\nu}(y)$ [3] as follows:

$$\Psi_L(y)=e^{y/2}\left[-\frac{1}{2}y^{\Theta/2}W_{-\Theta/2,(1-\Theta)/2}(y)+\frac{C_1\sqrt{\Theta}}{\sqrt{2C_3}}y^{(\Theta-1/2)/2}W_{-(\Theta+1/2)/2,(1/2-\Theta)/2}(y)-\frac{\Theta}{2}y^{(\Theta-1)/2}W_{-(\Theta+1)/2,-\Theta/2}(y)\right] . \tag{6}$$

Equations (3) and (6) represent the solution of the problem. The time dependence of Ψ_L can be obtained from (6) even without the cumbersome analysis of Whittaker functions, as those can be expressed through more common functions for any integer or half-integer value of Θ ($\Theta>0$), as shown in the Appendix. In the following, we shall display the results only for such a set of Θ values. As will be shown, the distribution functions $\Psi(t)_{L,R}$ and the entropy of the obstacles $S(t)=-\Psi_L(t)\ln\Psi_L(t)-\Psi_R(t)\ln\Psi_R(t)$ can have a variety of different time behaviors, which may be either monotonic or nonmonotonic, as a function of the initial conditions for $\varphi_i(t)$ and $\Psi_i(t)$ and the coupling constant Θ. Our choice of constants implies that φ's, Ψ's and S are dimensionless, and t is expressed in units of g^{-1}. In all subsequent cases, we have chosen, without loss of generality, $\varphi_2(0)=\varphi_4(0)=0$ ($C_2=0$), i.e., we have assumed that at $t=0$, the particles are moving only in the x direction. We note that the value of C_2 does not enter the expression for $\Psi_L(t)$, Eq. (5).

In Fig. 2(a), the time dependence of $\Psi_k(t)$, $k=L,R$, for fixed Θ, g, and $\Psi_k(0)$, is illustrated as a function of the initial conditions on φ. For $\varphi_1(0)=0$, $\Psi_k(t)$ is nonmonotonic with initial overshoot at small times. For small values of $\varphi_1(0)$, $\Psi_k(t)$ becomes monotonic, and for larger [$\varphi_1(0)>0.5$] value of $\varphi_1(0)$, the nonmonotonicity sets in again, with very strong undershoots. The nonmonotonic behavior of $\Psi_k(t)$ is very clearly reflected in $S(t)$ in Fig. 2(b), which shows regions where $dS(t)/dt<0$. For a very anisotropic case $\varphi_1(0)=1$ (all particles are coming in $-x$ direction), the initial slope of $S(t)$ is negative, followed by a local minimum. In Fig. 3(a), we study in detail the very anisotropic case $\varphi_1(0)=1$, this time as a function of $\Psi_k(0)$, for $g=\Theta=1$. Here again, only for the most asymmetric case $\Psi_L(0)=0$, the behavior is monotonic; otherwise $\Psi_k(t)$ presents strong local extrema for short times. In Fig. 3(b), the behavior of entropy is illustrated. A local maximum is followed by a minimum before the equilibrium value is reached asymptotically. In Fig. 4(a), we have displayed the dependence of $\Psi_k(t)$ on the coupling constant Θ for fixed initial values of both Ψ and φ. With Θ increasing from $\frac{1}{2}$ to 5, the response of the obstacles is increasing: $\Psi_k(t)$ shows more and more pronounced overshoots, which occur for all Θ at approximately equal times. The entropy, Fig. 4(b), shows the behavior similar to Figs. 2 and 3. We stress here that the peculiar form of entropy with time regions with $dS(t)/dt<0$, concerns the subsystem of obstacles. The total entropy $S_t(t)=-(\Psi_L\ln\Psi_L+\Psi_R\ln\Psi_R+\sum_{i=1}^{4}\varphi_i\ln\varphi_i)$ is everywhere nondecreasing ($dS_t/dt>0$), and consequently the Boltzmann H theorem is not violated [4].

The nonmonotonic time behavior of the statistical properties is a feature of certain special classes of kinetic-theory models. It has been discussed at length in [5] in conjection with exactly soluble Boltzmann equations, and it appears, for example, in the solutions of the Tjon-Wu model [6]. We have obtained this effect from a very simple, but exactly soluble, spatially uniform model.

Several extensions of the model are under study. If we add some interactions to otherwise free particles, the model is still soluble but with considerably richer structure. The inclusion of space variables in φ and Ψ would be of great interest, but appears to be rather difficult.

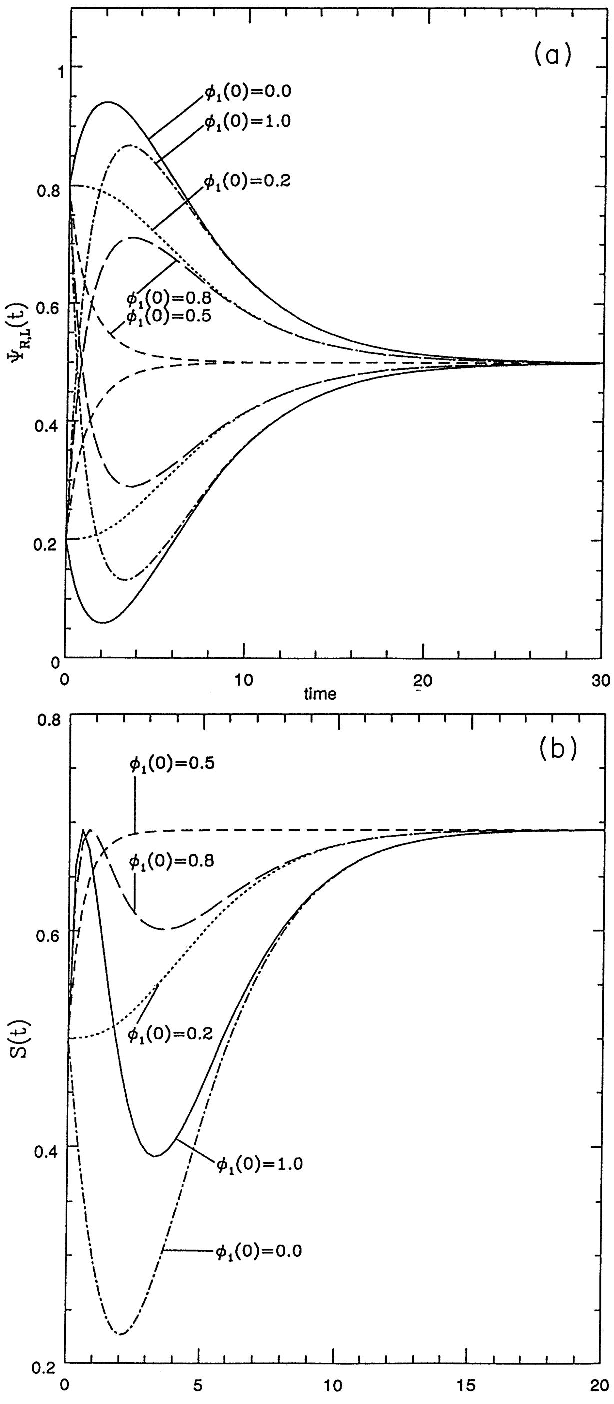

FIG. 2. (a) Obstacle distribution functions $\Psi_L(t)$ and $\Psi_R(t)$ for $g=1$, $\Theta=1$, $\Psi_L(0)=0.8$, $\Psi_R(0)=0.2$, $\varphi_1(0)+\varphi_3(0)=1$, for different $\varphi_1(0)$. (b) Entropy of the obstacles $S(t)$ for the same set of parameters as in Fig. 2(a). Time t is expressed in units of g^{-1}.

APPENDIX

The integrals $I(\Theta)$ occurring in Eq. (5) can be expressed through more common functions for any integer or half-integer positive Θ, the number of terms increasing rapidly with increasing Θ. We give here, with obvious notation, two examples for low values of Θ:

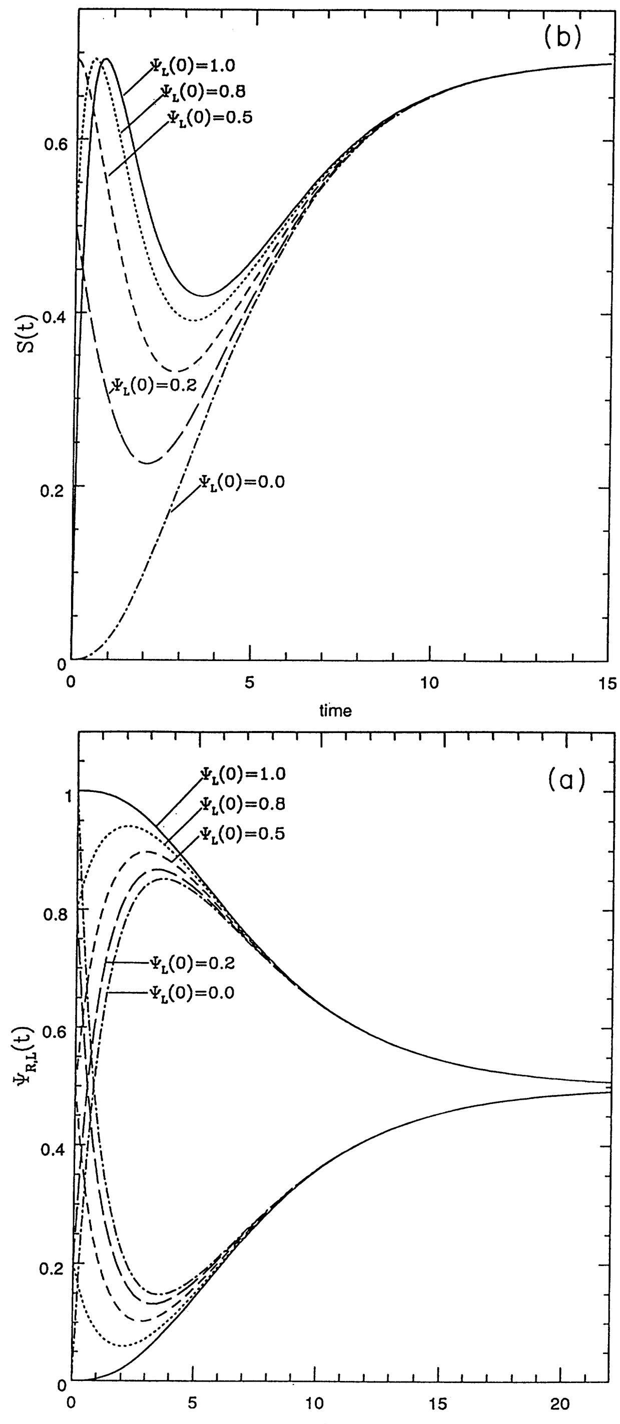

FIG. 3. (a) Obstacle distribution functions $\Psi_L(t)$ and $\Psi_R(t)$ for $g=\Theta=1$, $\varphi_1(0)=1$ as a function of $\Psi_L(0)$ and $\Psi_R(0)$. (b) Entropy of the obstacles $S(t)$ for the same set of parameters as in Fig. 3(a). Time t is expressed in units of g^{-1}.

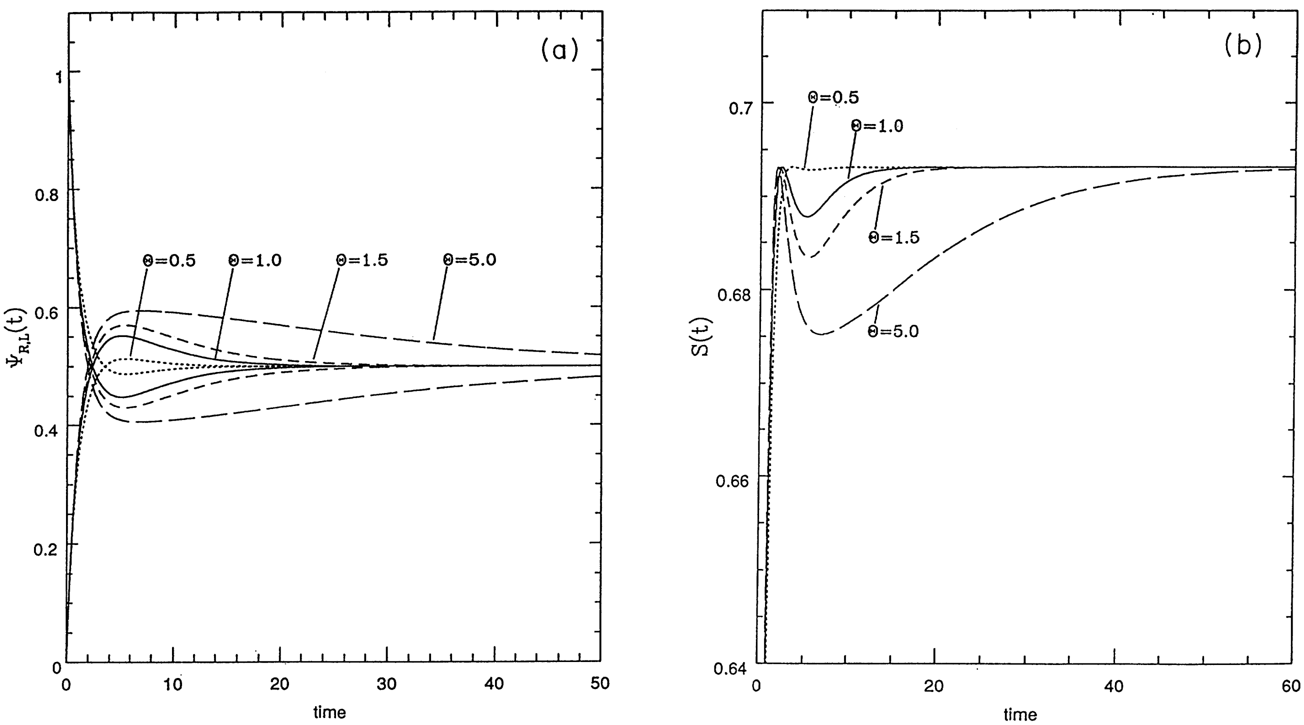

FIG. 4. (a) Obstacle distribution functions $\Psi_L(t)$ and $\Psi_R(t)$ for $g=1$, $\Psi_L(0)=1$, $\varphi_1(0)=0.6$, $\varphi_3(0)=0.4$, as a function of Θ. (b) Entropy of the obstacles $S(t)$ for the same set of parameters as in (a). Time t is expressed in units of g^{-1}.

$$I(\tfrac{3}{2})=\int e^{-y}\left[\frac{a_1}{y^{5/2}}+\frac{a_2}{y^2}+\frac{a_3}{y^{3/2}}\right]dy$$

$$=2a_1\left[-\frac{1}{3e^y y^{3/2}}+\frac{2}{3e^y y^{1/2}}+\frac{2}{3}\sqrt{\pi}\,\mathrm{erf}(\sqrt{y}\,)\right]-2a_2\left[-\frac{1}{2e^y y}+\frac{1}{2}\mathrm{Ei}(-y)\right]-2a_3\left[\frac{1}{e^y y^{1/2}}+\sqrt{\pi}\,\mathrm{erf}(\sqrt{y}\,)\right], \quad \text{(A1)}$$

$$I(3)=\int e^{-y}\left[\frac{a_1}{y^4}+\frac{a_2}{y^{7/2}}+\frac{a_3}{y^3}\right]dy$$

$$=2a_1\left[\frac{1}{6e^y y}\left[-\frac{1}{y^2}+\frac{1}{2y}-\frac{1}{2}\right]-\frac{1}{12}\mathrm{Ei}(-y)\right]$$

$$+2a_2\left[\frac{1}{5e^y\sqrt{y}}\left[-\frac{1}{y^2}+\frac{2}{3y}-\frac{3}{4}\right]-\frac{4\sqrt{\pi}}{15}\mathrm{erf}(\sqrt{y}\,)\right]+2a_3\left[\frac{1}{4e^y y}\left[-\frac{1}{y}+1\right]+\frac{1}{4}\mathrm{Ei}(-y)\right], \quad \text{(A2)}$$

where erf(x) and Ei(x) are error function and exponential integral, respectively. For higher values of Θ, the formulas become very long and will not be quoted here.

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