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Comments and Addenda

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Anomalous self-diffusion for one-dimensional hard cores

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The time-displaced self-correlation function for a one-dimensional hard-core fluid with independent stochastic forces acting on each core is solved exactly and concisely. At long time, the distribution has a spread given by $\delta x(t) = [R(t)/n]^{1/2}$, where $R(t)$ is the absolute dispersion in position of a noninteracting particle and n the free-volume reduced density. The diffusional behavior without stochastic background, and non-Fickian diffusion of Levitt with Brownian background, are reproduced.

There are, understandably, very few classical many-body systems whose macroscopic time development can be followed exactly. A trivial example is that of free particles, but this is rendered nontrivial by the observation of a one-to-one correspondence with the dynamics of point hard cores in one-dimensional space,[1] and indeed with that of finite-diameter hard cores as well.[2] Interestingly enough, many of the transport properties of real, e.g. three-dimensional, systems are mimicked by the one-dimensional hard cores. However, more detailed correspondence with the space-time pair-correlation structure of a real system is achieved only by special choice of the initial hard-core velocity distribution,[3] which is clearly invariant under collision in one dimension and hence constant in time.

Levitt[4] has made the interesting observation that if a Brownian mechanism is introducted to allow for the relaxation of the hard-core velocity distribution to a Maxwell-Boltzmann distribution, an abnormal diffusion results. Thus, there is an intrinsic distinction between most physical realizations of one-dimensional hard-core statistical dynamics and anticipated fluid dynamics (see also Ref. 5). It is the purpose of this communication to present the matter in a somewhat more general context.

We consider a set of N point hard cores $x_1, \ldots, x_N$—with possibly stochastic background—on the line $-\frac{1}{2}L \leq x \leq \frac{1}{2}L$. Assume now a state of homogeneous current-free equilibrium with density $n = N/L$ [to be replaced by the free-volume reduced density $n/(1-na)$ for hard cores of finite diameter a] and velocity probability distribution $g(v)$. Then the time-displaced one-body self-distribution function for a particle initially at position-velocity $(0, v')$ to end up at a time t later at (x, v) is defined by

$$f_s(xvt\,|\,v')g(v') = \sum_i \langle \delta(x_i(0))\,\delta(x_i(t)-x) \times \delta(v_i(0)-v')\,\delta(v_i(t)-v)\rangle \quad (1)$$

now normalized to N. If the X_i are the particle positions without velocity interchange on collision, i.e., behaving as noninteracting particles, Eq. (1) may be rewritten[2] as

$$f_s(xvt\,|\,v')g(v') = \sum_{i,j} \Big\langle \delta(X_i(0))\,\delta(X_j(t)-x)\,\delta(V_i(0)-v') \times \delta(V_j(t)-v)\,\delta_{\text{Kron}}\Big(\sum_{k\neq i}\epsilon(X_i(0)-X_k(0)),\ \sum_{k\neq j}\epsilon(X_j(t)-X_k(t))\Big)\Big\rangle, \quad (2)$$

where $\delta_{\rm Kron}$ is the Kronecker δ function and ϵ the unit step function.

Straightforward algebraic manipulation in the thermodynamic limit $L\to\infty$, $n=$const can now be carried out in the fashion of Ref. 2, Appendix A. The result is that if $h(xvt\,|\,v')$ denotes the time-displaced one-body self-probability (normalized to unity) in the absence of direct or indirect two-body interactions, and the partially integrated time-displaced probabilities are defined by

$$h(xvt)\equiv\int h(xvt\,|\,v')g(v')\,dv', \qquad h(xt\,|\,v')\equiv\int h(xvt\,|\,v')\,dv,$$
$$h(xt)\equiv\int h(xvt)\,dv=\int h(xt\,|\,v')g(v')\,dv', \tag{3}$$

then

$$f_s(xvt\,|\,v')=nh(xvt\,|\,v')\int\frac{d\theta}{2\pi}\exp\{-n[ix\sin\theta+R(xt)(1-\cos\theta)]\}$$
$$+n^2\int\frac{d\theta}{2\pi}\int e^{-i\theta\epsilon(x-X)}h(Xt\,|\,v')\,dX\int e^{i\theta\epsilon(Y-x)}h(Yvt)\,dY\exp\{-n[ix\sin\theta+R(xt)(1-\cos\theta)]\}\,. \tag{4}$$

Here

$$R(xt)\equiv\int h(Xt)\,|\,X-x\,|\,dX \tag{5}$$

is the absolute dispersion of an excursion about x in time interval t for a noninteracting particle.

The θ integrations in (4) are easy enough to do. It is more useful to look directly at some limiting cases. For $x>0$ on the tail of the underlying distribution $h(xt)$, we have as well $R(xt)\to x$, and (4) reduces to

$$f_s(xvt\,|\,v')\to ne^{-nx}h(xvt\,|\,v'), \tag{6}$$

essentially the probability of a gap in the particle distribution between the origin and x.

On the other hand, in the body of the distribution, we can perform a time-asymptotic evaluation in the sense of the small expansion parameter

$$\lambda\equiv\frac{1}{n[R(xt)^2-x^2]^{1/2}}\,. \tag{7}$$

[Note that for even $h(xt)$, $R(xt)-|x|$ decreases monotonically from $R(0t)$ to 0.] To leading order in λ, the replacement $e^{i\theta}\to[R(xt)+x/R(xt)-x]^{1/2}\times e^{i\theta}$ in (4), followed by second-order expansion about $\theta=0$ yields at once

$$f_s(xvt\,|\,v')\to n\{2\pi n[R(xt)^2-x^2]^{1/2}\}^{-1/2}$$
$$\times\exp(-n\{R(xt)-[R(xt)^2-x^2]^{1/2}\})$$
$$\times[h(xvt\,|\,v')+ng(v)], \tag{8}$$

or except for a portion of vanishing integral at long time,

$$f_s(xvt\,|\,v')\to[n/2\pi R(t)]^{1/2}[h(xvt\,|\,v')+ng(v)]\,e^{-nx^2/2R(t)},$$

where

$$R(t)\equiv R(0t)=\int|X|\,h(Xt)\,dX\,. \tag{9}$$

In particular, the breadth of the distribution is given by

$$[\delta x(t)]^2=\langle x^2(t)\rangle\to n^{-1}R(t)\,. \tag{10}$$

If the particles suffer only collisional interaction, then for an initial velocity distribution $g(v)$, we clearly have $h(Xt)=t^{-1}g(X/t)$, so that

$$R(t)=t\int|V|\,g(V)\,dV\,. \tag{11}$$

Thus $\delta x\propto t^{1/2}$ evinces the canonical diffusive behavior. This is the situation originally analyzed,[1,2] which indicated that the model was not entirely alien to real three-dimensional physics.

However, it is now seen that in the presence of any mechanism—aside from interparticle collision—which independently interrupts the rectilinear propagation of the particles, the ensuing reduction of $R(t)$ will destroy the $t^{1/2}$ dependence of δx. For example, for a Brownian background—without specifying the precise realization of the one-dimensional geometry which makes this relevant—$R(t)$ starts at small time at the value (11), but after a transition time depending upon the parameters involved achieves its asymptotic form

$$R(t)=\gamma t^{1/2}, \tag{12}$$

so that $\delta x\propto t^{1/4}$. There are two complementary consequences. First, the diffusion constant vanishes:

$$D=\lim\frac{1}{2}\frac{d\langle x^2(t)\rangle}{dt}\bigg|_{t\to\infty}=0\,.$$

But the velocity autocorrelation

$$\langle v(0)v(t)\rangle=\frac{1}{2}\frac{d^2\langle x^2(t)\rangle}{dt^2}$$

becomes

$$\langle v(0)v(t)\rangle \to -(\gamma/8n)t^{-3/2}, \qquad (13)$$

with a very-long-range negative tail in time. Both qualitative consequences are seen from (10) to be evoked by the coupling of an intrinsic velocity distribution relaxation mechanism with collisional transfer, and are not special to the Brownian nature of the background.

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