On the connections between single file dynamics and collective dynamics.

Single file dynamics: particles in a channel that cannot pass each other. Applications in biology and chemistry (flow through pores in a membrane, zeolites, traffic flows, etc).

Tagged particle transport dynamics closely related to collective transport, as first noticed by Alexander and Pincus (PRB 10, 2011 (1978)).

\[ \langle (x_i(t) - x_i(0))^2 \rangle \propto \frac{1}{n^2} \langle \left( \int_0^t f(x_i(t), \tau) \right)^2 \rangle \]
Warning: only correct in (average) rest frame of tagged particle. In moving frame
\[ \left\langle \Delta^2 \right\rangle = V_t^2 t^2 + \left\langle \Delta_0^2(t) \right\rangle \]
but fluctuations in \( \int J \, dt \) increase.

To leading order:
\[
\frac{\partial \delta n(x, t)}{\partial t} = -\frac{\partial}{\partial x} j(x, t)
\]
\[
\frac{\partial \hat{n}(x, t)}{\partial t} = -i\hbar \frac{\partial}{\partial x} \hat{j}(x, t)
\]
\[
\int_0^t dt' \hat{j}(x, t') = -\left( \hat{n}(x, t) - \hat{n}(x, 0) \right)
\]
\[
\int_0^t dt' \hat{j}(0, t') = N \left( X(t) - X(0) \right)
\]
\[
\left\langle (x_i(t) - x_i(0))^2 \right\rangle = \frac{1}{n^2 t^2} \left\{ \sum_{k \neq 0} \left\langle A_{k,0} \hat{n}(x, 0) \right\rangle \langle A_{k,0} \hat{n}(x, 0) \rangle + N^2 \left( X(t) - X(0) \right)^2 \right\}
\]
\[
= \sum_{k \neq 0} \frac{2 \langle \delta(x, t) \rangle \langle \delta(x, t) \rangle + \langle 1 - n, t \rangle \left( \frac{n^2 t^2}{N^2} \right)}{N t^2}
\]
\[ S(\mathbf{r}, t) = \langle \hat{n}(\mathbf{r}, t) \hat{n}(-\mathbf{r}, 0) \rangle \]

\[
\lim_{L \to \infty} \int \frac{d^3k}{2\pi} \frac{2S(k) - S(k, t) + S(-k, t)}{n^2k^2} \text{ in "rest frame"}
\]

\[ \langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle = \frac{1}{2\pi} \int \frac{d^3k}{2\pi} \frac{2S(k) - (S(k, t) + S(-k, t))}{n^2k^2} + V^2E^2 \text{ (fluctuating part of)}
\]

\[ \langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle \text{ vanishes to be added by hand if one wants expression in moving frame} \]
Simplest category: dynamics of independent particles that exchange identity on crossing (equivalent: what is MSD of 137^\text{th} particle in the row?)

In this case: \( S(k,t) = n \cdot S_{\text{single}}(t) \)

Suppose \( S(k,t) = \bar{S}(k) \cdot F(k \cdot v(t)) \)

\[ \langle (x_{137}(t) - x_{137}(0))^2 \rangle = -\left( \frac{\partial^2 \bar{S}(k,t)}{\partial k^2} \right)_{k=0} n^2 t^{2/\alpha} \]

but \( \langle (x_{137}(t) - x_{137}(0))^2 \rangle \sim n^2 t^{1/\alpha} \) [provided \( V=0 \)]

[Perca rule]

Examples:

1) Jepson gas. Equal mass point particles, which exchange velocities on colliding:

\[ S(k,t) = \int_\mathbb{R} e^{-ik \cdot \phi} \bar{S}(k) \cdot e^{-ik \cdot \phi} d\phi \]

\[ = \frac{N}{1} \sum_{j=1}^{\infty} e^{-ik \cdot \phi} \to n \int d\phi \phi (\text{rule of } \int_0^\infty \phi e^{-\phi n} d\phi) \]
\[ \Rightarrow \langle (x(t) - x(0))^2 \rangle = \frac{\langle V(t)^2 \rangle}{n} \]

2) Non-crossing Brownian particles (T.E. Harris)

Now \( S(n, t) = n e^{\frac{-Dh^2 t}{2}} \)

\[ \langle (x(t) - x(0))^2 \rangle = \frac{1}{\pi n} \int_0^\infty dh \frac{1 - e^{-Dh^2 t}}{h^2} \]

\[ \frac{\alpha}{n} \sqrt{D_0 t} \]

For Brownian particles will drift: add \( V(t)^2 \)

3) Lévy Flights: random flight with power law jump length distribution

\( S(n, t) = n e^{\frac{-D t^\alpha}{\alpha}} \)

\[ \langle (x(t) - x(0))^2 \rangle = \frac{1}{\pi n} \int_0^\infty dh \frac{1 - e^{-D h^\alpha t}}{h^2} \]

requires \( \alpha > 1 \) for convergence

\[ = \Gamma\left(\frac{\alpha - 1}{\alpha}\right) (D t^{\alpha - 1})^{1/\alpha} \]
\[
\lim_{N \to \infty} \frac{N^r}{n^r \cdot (\frac{\epsilon}{N})^n} = \frac{\epsilon^n}{n^r}
\]

\[
p(m) = \sum_n \frac{\epsilon^{2m+n}}{(m+n)! \cdot n!}
\]

\[
= \sum n \frac{\epsilon^{2m+n}}{(m+n)^{m+n} \cdot n}
\]

\[
\log \left( \frac{\epsilon^n}{n!} \right) = n \log \left( \frac{\epsilon^n}{n!} \right)
\]

\[
\frac{\partial}{\partial n} = \log \left( \frac{\epsilon^n}{n!} \right) - 1 = 0 \quad \text{for } n = 3
\]

\[
\frac{\partial^2}{\partial n^2} = -\frac{1}{n}
\]
Gaussian distribution of displacement in AP approximation, for long times.

Right of origin, very large number of identically distributed particles, all having same probability $\sqrt{T}$ of having crossed the origin.

Central limit theorem $\Rightarrow n_T(t)$ has Gaussian distribution with average $\sqrt{T}$ and variance $\frac{1}{\sqrt{T}}$.

Same for $n_T(t) = n_T^+ - n_T^-$ also Gaussian with average zero and variance $\sqrt{T}$. 

Second category: interacting systems

AP approximation remains valid, but variety of possibilities becomes richer.

A few examples:

SEP  Collective density satisfies diffusion equation ⇒ same result for MSD as for independent BM

ASEP  + other systems satisfying Fick.

Burger eq.

\[
\frac{\partial n}{\partial t} = - \frac{\partial}{\partial x} \left[ n u(n) \right] + D \frac{\partial^2 n}{\partial x^2} - \frac{\partial \mu}{\partial x}
\]

Expand \( u(n) = \bar{u} + (n-\bar{n}) \frac{\partial u}{\partial n} + \ldots \)

\[
\Rightarrow \frac{\partial n}{\partial t} = - \left( \bar{u} + \bar{n} \frac{\partial u}{\partial n} \right) \frac{\partial n}{\partial x} + \sum \left( \frac{\partial u}{\partial n} \right) \frac{\partial^2 n}{\partial x^2} + \frac{\partial}{\partial x} \left( \frac{\partial^2 n}{\partial x^2} \right) \frac{\partial \mu}{\partial x}
\]

Pattern velocity + \( D \frac{\partial^2 n}{\partial x^2} \frac{\partial \mu}{\partial x} \)

Average drift velocity equals \( \bar{u} \)

\[
\Rightarrow \frac{S(n,t)}{\sqrt{\bar{n} \left( \frac{\partial u}{\partial n} \right)}} = \frac{f(\mu t)}{t^{1/2}}
\]

in particle frame
For large $t e^{-\frac{t^2}{12}}$ dominates

$$\Rightarrow \int \frac{2 - S(k, n) - S(-k, n)}{\hbar^2} \sim t$$

(Notice: pattern velocity ≠ CM velocity)

Possible getting drift speed = pattern velocity?

Not with one species, but one may add mutually non-passing second-class particles and tune their jump rates. Should give $\text{MSD} \propto t^{2/3}$. 
Hamiltonian dynamics

1d hamilt. systems with short-ranged interactions

have \( S(k,t) = \sum_{\sigma=\pm} S^{\sigma}(k,t) + S^{H}(k,t) \)

\[ S^{\sigma}(k,t) = e^{-\sigma \alpha t \tau_{\sigma}} \tilde{F}_{\sigma}(k \pm \alpha t^{2/3}) \]

\[ S^{H}(k,t) = e^{-\alpha \frac{t}{t^{2/3}}} \] [like Levy flights]

\rightarrow 3 contributions to MSD:

\[ S^{\sigma} \Rightarrow c t \]

\[ S^{H} \Rightarrow \frac{t}{t^{3/5}} \]

\[ S \Rightarrow t \]
Finite size effects

1) Hamilton systems with fixed CM and PB
   a) Due to fixed CM the tr=0 term in summation over \( r \) vanishes. So one more \( \langle V_{\text{CM}} \rangle \uparrow \).
   b) Plus, having CM constrains displacement of a single particle to \( \frac{N-1}{N} \) from \( \bar{N} \)
   \( \Rightarrow \text{MSD saturates for long times} \)

Result Point

3) AP approximation ignores effect of systematic and stochastic deviation from fixed interparticle intervals.
   Can be calculated for \( k \to \infty \)

\[
\langle (\tilde{r}_i - \tilde{r}_i(0))^2 \rangle = \langle (y_i(1) - \langle y_i \rangle)^2 \rangle - \langle (y_i(1) - \langle y_i \rangle)(x_i - \langle x_i \rangle) \rangle
\]

\( \tilde{r}_i \) from equivalent configuration with same CM position
Diffuse systems with PBC

For long times CM performs diffuse motion with \( \text{Dcm} = \frac{D}{N} \)

Tagged particle:

\[
\langle (x_j(t) - x_j(0))^2 \rangle = \langle (x_j(t) - x_j(0)) - (x_j(0) - x_j(0)) \rangle^2 \\
= \langle (X(t) - X(0))^2 \rangle + 2 \langle (x_j - 2x_j) \rangle^2 
\]

So for large \( t \) differs from Hamiltonian result by additional \( \frac{2Dt}{N} \) only!

Attention for meeting on SFP in Erice from July 4-9, organized by Opher Florenceman; see single file dynamics conference . net
FIG. 2: Comparison of mean-squared deviation (MSD) (with error bars) for $N = 1024$.
Red: simulation value; blue: Alexander-Pincus approximation based on simulation values for $S(k,t)$
FIG. 3: Comparison of mean-squared deviation MSD (with error bars) for $N = 2048$. 

2048 particles, $n = 0.8$, $\varepsilon = 1.0$.
FIG. 7: Comparison of experimental and theoretical MSD for 4000 particles.
References on SFD:


T. E. Harris, J. Appl. Prob. 2, 323 (1965)


Conference on single file dynamics in Erice from July 4-9:

http://singlefiledynamicsconference.net/