Now consider displacement $\vec{r}$ of a particle at time t, given that it started at $\vec{r}_0$ with velocity $\vec{u}_0$ @ $t=0$:

$$\vec{r}-\vec{r}_0 = \int_0^t dt'\, \vec{u}(t') =$$

$$= \int_0^t dt' \left[\vec{u}_0 e^{-\beta t'} + e^{-\beta t'} \int_0^{t'} d\xi\, e^{\beta\xi} \vec{A}(\xi) \right] \text{, or}$$

$$\vec{r}-\vec{r}_0 - \beta^{-1}\vec{u}_0(1-e^{-\beta t}) = \int_0^t dt'\, e^{-\beta t'} \int_0^{t'} d\xi\, e^{\beta\xi} \vec{A}(\xi) \boxed{\equiv}$$

Further, we can integrate by parts:

$$\boxed{\equiv} - \beta^{-1} e^{-\beta t'} \int_0^{t'} d\xi\, e^{\beta\xi} \vec{A}(\xi) \Big|_0^t +$$

$$+ \beta^{-1} \int_0^t dt'\, \cancel{e^{-\beta t'}}\, \cancel{e^{\beta t'}}\, \vec{A}(t') =$$

$$= -\beta^{-1} e^{-\beta t} \int_0^t d\xi\, e^{\beta\xi} \vec{A}(\xi) + \beta^{-1} \int_0^t d\xi\, \vec{A}(\xi) \equiv$$

$$\equiv \int_0^t d\xi\, \psi(\xi) \vec{A}(\xi) \text{, where}$$

$$\psi(\xi) = \beta^{-1}\left[1 - e^{\beta(\xi - t)}\right].$$

Since $\displaystyle\int_0^t d\xi\, \psi^2(\xi) = \frac{1}{\beta^2} \int_0^t d\xi \left[1 - e^{\beta(\xi-t)}\right]^2 =$

$$= \frac{2\beta t - 3 + 4e^{-\beta t} - e^{-2\beta t}}{2\beta^3},$$

we immediately have

$$W(\vec{r},t;\vec{r}_0,\vec{u}_0) = \left[\frac{m\beta^2}{2\pi k_B T[2\beta t - 3 + 4e^{-\beta t} - e^{-2\beta t}]}\right]^{3/2} \times$$

$$\times\, e^{-\frac{m\beta^2[\vec{r}-\vec{r}_0 - \vec{u}_0(1-e^{-\beta t})\beta^{-1}]^2}{2k_BT(2\beta t - 3 + 4e^{-\beta t} - e^{-2\beta t})}}.$$

If $t \gg \beta^{-1}$,

$$W(\vec{r},t;\vec{r}_0,\vec{u}_0) \simeq \left[\frac{m\beta}{4\pi k_B T t}\right]^{3/2} e^{-\frac{|\vec{r}-\vec{r}_0 - \frac{\vec{u}_0}{\beta}|^2}{4\underbrace{\left(\frac{k_BT}{m\beta}\right)}_{\equiv D} t}}$$

Since $\langle|\vec{r}-\vec{r}_0|^2\rangle$ is $O(t)$, we can neglect the $\frac{\vec{u}_0}{\beta}$ constant in the exponent, s.t.

$$W(\vec{r},t;\vec{r}_0,\vec{u}_0) \simeq \frac{1}{(4\pi D t)^{3/2}} e^{-\frac{|\vec{r}-\vec{r}_0|^2}{4Dt}}, \quad t \gg \beta^{-1} \qquad (+)$$

Finally, (+) gives:

$$\langle(x-x_0)^2\rangle = \langle(y-y_0)^2\rangle = \langle(z-z_0)^2\rangle =$$

$$= \frac{1}{3}\langle|\vec{r}-\vec{r}_0|^2\rangle = 2Dt = \frac{k_BT}{3\pi a\eta}t = 2\frac{k_BT}{m\beta}t.$$

Einstein's result,

fluctuation-dissipation relation:

$$D\beta = \frac{k_BT}{m}.$$

Perrin tested that $\frac{\langle (x-x_0)^2 \rangle}{t}$ is a constant for many combinations of T, η & a.

Clearly, (+) shows that for $t \gg \beta^{-1}$ Brownian motion is diffusive.

More generally,

$$\langle |\vec{r}-\vec{r}_0|^2 \rangle = \frac{|\vec{u}_0|^2}{\beta^2}(1-e^{-\beta t})^2 + \frac{3k_BT}{m\beta^2} \times$$
$$\times (2\beta t - 3 + 4e^{-\beta t} - e^{-2\beta t}).$$

Average over all values of $\vec{u}_0$:
in equilibrium, $\langle \frac{m|\vec{u}_0|^2}{2} \rangle = \frac{3k_BT}{2}$ by equipartition theorem $\Rightarrow \langle |\vec{u}_0|^2 \rangle = \frac{3k_BT}{m}$.

Then $$\langle\langle |\vec{r}-\vec{r}_0|^2 \rangle\rangle = \frac{3k_BT}{m\beta^2}\left[1-2e^{-\beta t} + \cancel{e^{-2\beta t}} + \right.$$
$$\left. + 2\beta t - 3 + 4e^{-\beta t} - \cancel{e^{-2\beta t}}\right] =$$

$$= 6\frac{k_BT}{m\beta^2}[\beta t - 1 + e^{-\beta t}].$$

$t \to \infty$: $$\langle\langle |\vec{r}-\vec{r}_0|^2 \rangle\rangle = 6 \underbrace{\frac{k_BT}{m\beta}}_{D} t = 6Dt$$ as before

$t \to 0$: $$\langle\langle |\vec{r}-\vec{r}_0|^2 \rangle\rangle = 6\frac{k_BT}{m\beta^2}[\beta t \cancel{-1} + \cancel{1} - \beta t + \tfrac{1}{2}\beta^2 t^2] =$$
$$= 3\frac{k_BT}{m}t^2 = \langle |\vec{u}_0|^2 \rangle t^2$$, inertial motion

The Fokker-Planck Equation (FP)

[FP eq'n in ~~[illegible]~~ velocity space : Brownian motion of a free particle]

Consider

$$(*) \quad W(\vec{u}, t+\Delta t) = \int d(\Delta\vec{u})\, W(\vec{u}-\Delta\vec{u}, t)\, \Psi(\vec{u}-\Delta\vec{u}; \Delta\vec{u})$$

Transition prob. density:

$\Psi(\vec{u}; \Delta\vec{u})$ $\quad \vec{u} \to \vec{u}+\Delta\vec{u}$ in time Δt

Now, $\dfrac{d\vec{u}}{dt} = -\beta\vec{u} + \vec{A}(t)$ gives

$$\underbrace{\Delta\vec{u}}_{\vec{u}(t+\Delta t)-\vec{u}(t)} \simeq -\beta\vec{u}\Delta t + \underbrace{\int_t^{t+\Delta t} dt'\, \vec{A}(t')}_{\vec{B}(\Delta t)}$$

So, $\Delta\vec{u} + \beta\vec{u}\Delta t$ is distributed as $\vec{B}(\Delta t)$:

$$(**) \quad \frac{1}{(4\pi q\Delta t)^{3/2}}\, e^{-\frac{|\Delta\vec{u}+\beta\vec{u}\Delta t|^2}{4q\Delta t}} . \qquad \left[q = \frac{\beta k_B T}{m} \right]$$

But this is exactly $\Psi(\vec{u}; \Delta\vec{u})$, since $\vec{B}(\Delta t)$ is the change in velocity over Δt. (**) is convenient since it explicitly depends on $\Delta\vec{u}$ & Δt.

Expand everything in (*):

$$W(\vec{u}, t) + \frac{\partial W}{\partial t}\Delta t + O(\Delta t^2) \; \boxed{=}$$

$$\boxed{=} \int_{-\infty}^{\infty} d(\Delta u_1)\, d(\Delta u_2)\, d(\Delta u_3) \times \left[w(\vec{u},t) - \sum_i \frac{\partial w}{\partial u_i} \Delta u_i + \right.$$

$$\left. + \frac{1}{2} \sum_i \frac{\partial^2 w}{\partial u_i^2} \Delta u_i^2 + \sum_{i<j} \frac{\partial^2 w}{\partial u_i \partial u_j} \Delta u_i \Delta u_j + \ldots \right] \times$$

$$\times \left[\psi(\vec{u}; \Delta\vec{u}) - \sum_i \frac{\partial \psi}{\partial u_i} \Delta u_i + \frac{1}{2} \sum_i \frac{\partial^2 \psi}{\partial u_i^2} \Delta u_i^2 + \right.$$

$$\left. + \sum_{i<j} \frac{\partial^2 \psi}{\partial u_i \partial u_j} \Delta u_i \Delta u_j + \ldots \right].$$

Define $\langle \Delta u_i \rangle = \int_{-\infty}^{\infty} d(\Delta\vec{u})\, \Delta u_i \psi(\vec{u}; \Delta\vec{u})$, etc.

Then

$$\frac{\partial w}{\partial t} \Delta t + \theta(\Delta t^2) = \underline{- \sum_i \frac{\partial w}{\partial u_i} \langle \Delta u_i \rangle} + \frac{1}{2} \sum_i \frac{\partial^2 w}{\partial u_i^2} \langle \Delta u_i^2 \rangle +$$

$$+ \sum_{i<j} \frac{\partial^2 w}{\partial u_i \partial u_j} \langle \Delta u_i \Delta u_j \rangle \underline{- \sum_i w \frac{\partial}{\partial u_i} \langle \Delta u_i \rangle} +$$

$$+ \sum_i \frac{\partial}{\partial u_i} \langle \Delta u_i^2 \rangle \frac{\partial w}{\partial u_i} + \sum_{i \neq j} \frac{\partial}{\partial u_j} \langle \Delta u_i \Delta u_j \rangle \frac{\partial w}{\partial u_i} +$$

$$+ \frac{1}{2} \sum_i \frac{\partial^2}{\partial u_i^2} \langle \Delta u_i^2 \rangle w + \sum_{i<j} \frac{\partial^2}{\partial u_i \partial u_j} \langle \Delta u_i \Delta u_j \rangle w +$$

$$+ \theta(\Delta u^3).$$

So, $$\frac{\partial w}{\partial t} \Delta t + \theta(\Delta t^2) = - \sum_i \frac{\partial}{\partial u_i} (w \langle \Delta u_i \rangle) +$$

$$+ \frac{1}{2} \sum_i \frac{\partial^2}{\partial u_i^2} (w \langle \Delta u_i^2 \rangle) + \sum_{i<j} \frac{\partial^2}{\partial u_i \partial u_j} (w \langle \Delta u_i \Delta u_j \rangle) + \theta(\Delta u^3).$$

↑ FP eq'n

Now, with (**) we have:

$$\begin{cases} \langle \Delta u_i \rangle = -\beta u_i \Delta t \,, \\ \langle \Delta u_i \Delta u_j \rangle = \langle \Delta u_i \rangle \langle \Delta u_j \rangle = \mathcal{O}(\Delta t^2) \qquad (i \neq j) \\ \langle \Delta u_i^2 \rangle = 2q \Delta t + \mathcal{O}(\Delta t^2) \end{cases}$$

Then in the $\Delta t \to 0$ limit:

$$\frac{\partial W}{\partial t} = \beta \sum_i \frac{\partial}{\partial u_i}(W u_i) + q \sum_i \frac{\partial^2}{\partial u_i^2} W$$

One can show that this eq'n is satisfied by

$$W(\vec{u}, t; \vec{u}_0) = \frac{1}{\left(2\pi q (1 - e^{-2\beta t})/\beta\right)^{3/2}} \, e^{-\frac{\beta |\vec{u} - \vec{u}_0 e^{-\beta t}|^2}{2q(1 - e^{-2\beta t})}} ,$$

which was previously derived directly from Langevin's equations.

Likewise, we can generalize to:

$$\frac{d\vec{u}}{dt} = -\beta \vec{u} + \vec{A}(t) + \underbrace{\vec{K}(\vec{r}, t)}_{\text{acceleration due to external field: } \text{"}\frac{F_{ext}}{m}\text{"}}$$

Then as before

$$\begin{cases} \Delta \vec{u} = -(\beta \vec{u} - \vec{K}) \Delta t + \vec{B}(\Delta t) \,, \\ \Delta \vec{r} = \vec{u} \, \Delta t \,. \end{cases}$$

we have:

$$\overbrace{W(\vec{r},\vec{u},t+\Delta t)}^{\text{prob. density in phase space}} = \iint d(\vec{\Delta r})\,d(\vec{\Delta u}) \times$$

$$\times\, W(\vec{r}-\vec{\Delta r},\vec{u}-\vec{\Delta u},t)\,\underbrace{\Psi(\vec{r}-\vec{\Delta r},\vec{u}-\vec{\Delta u};\vec{\Delta r},\vec{\Delta u})}_{\text{transition prob. in phase space}}$$

$$\Psi(\vec{r},\vec{u};\vec{\Delta r},\vec{\Delta u}) = \overbrace{\psi(\vec{u};\vec{\Delta u})}^{\text{trans'n prob. in velocity space}}\,\delta(\Delta x-u_1\Delta t)\times$$

$$\times\,\delta(\Delta y-u_2\Delta t)\,\delta(\Delta z-u_3\Delta t).$$

Then $\int d(\vec{\Delta r})$ is trivial, and we obtain:

$$W(\vec{r},\vec{u},t+\Delta t) = \int d(\vec{\Delta u})\,W(\vec{r}-\vec{u}\Delta t,\vec{u}-\vec{\Delta u},t)\times$$

$$\times\,\psi(\vec{u}-\vec{\Delta u};\vec{\Delta u}).$$

Alternatively,

$$W(\vec{r}+\vec{u}\Delta t,\vec{u},t+\Delta t) = \int d(\vec{\Delta u})\,W(\vec{r},\vec{u}-\vec{\Delta u},t)\times$$

$$\times\,\psi(\vec{u}-\vec{\Delta u};\vec{\Delta u})$$

Expand in $\vec{\Delta u}$ & Δt:

$$\frac{\partial W}{\partial t}\Delta t+(\underbrace{\vec{u}\cdot\vec{\nabla}_{\vec{r}}}_{\sum_i u_i\frac{\partial}{\partial r_i}})W\Delta t+O(\Delta t^2) =$$

$$= -\sum_i\frac{\partial}{\partial u_i}(W\langle\Delta u_i\rangle)+\frac{1}{2}\sum_i\frac{\partial^2}{\partial u_i^2}(W\langle\Delta u_i^2\rangle)\quad\oplus$$

$$\oplus \sum_{i<j} \frac{\partial^2}{\partial u_i \partial u_j} \left(W \langle \Delta u_i \Delta u_j \rangle \right) + \mathcal{O}(\Delta u^3).$$

Here,

$$\Psi(\vec{u}; \Delta\vec{u}) = \frac{1}{(4\pi q \Delta t)^{3/2}} e^{-\frac{|\Delta\vec{u} + (\beta\vec{u} - \vec{K})\Delta t|^2}{4 q \Delta t}}.$$

This expression gives

$$\begin{cases} \langle \Delta u_i \rangle = -(\beta u_i - K_i)\,\Delta t, \\ \langle \Delta u_i^2 \rangle = 2 q \Delta t + \mathcal{O}(\Delta t^2), \\ \langle \Delta u_i \Delta u_j \rangle = \langle \Delta u_i \rangle \langle \Delta u_j \rangle = \mathcal{O}(\Delta t^2). \end{cases}$$

Accordingly,

$$\left[\frac{\partial W}{\partial t} + \sum_i u_i \frac{\partial W}{\partial r_i} \right] \Delta t + \mathcal{O}(\Delta t^2) =$$

$$= \left[\sum_i \frac{\partial}{\partial u_i} \left[(\beta u_i - K_i) W \right] + q \sum_i \frac{\partial^2 W}{\partial u_i^2} \right] \Delta t + \mathcal{O}(\Delta t^2)$$

$$\left[q = \overbrace{\frac{\beta k_B T}{m}}^{\beta^2 D} \right]$$

In the $\Delta t \to 0$ limit we obtain:

$$\frac{\partial W}{\partial t} + \vec{u} \cdot \vec{\nabla}_{\vec{r}} W + \vec{K} \cdot \vec{\nabla}_{\vec{u}} W = \beta \vec{\nabla}_{\vec{u}} (W \vec{u}) + q \nabla_{\vec{u}}^2 W.$$

FP eq'n in phase space; generalizes Liouville's theorem to include Brownian motion (through two terms on the RHS)