The probability distribution of a diffusing particle

Let $G(x,t)$ be the probability distribution of a certain particle, created at the origin at time zero, which diffuses in n dimensions. According to Fick's second law of diffusion[1]:

$$\frac{\partial G(\mathbf{x},t)}{\partial t} = D\Delta G(\mathbf{x},t) + \delta(x,t)$$

Rearrange and perform a Fourier transform ($\mathbf{x} \mapsto \mathbf{k}$,t$\mapsto \omega$):

$$\begin{aligned}
\mathcal{L}G(\mathbf{x},t) = \left[\frac{\partial}{\partial t} - D\Delta\right] G(\mathbf{x},t) &= \delta(\mathbf{x},t) \\
\left(i\omega + D|\mathbf{k}|^2\right)\tilde{g}(\mathbf{k},\omega) &= 1 \\
\tilde{g}(\mathbf{k},\omega) &= \frac{1}{i\omega + D|\mathbf{k}|^2}
\end{aligned}$$

Now perform an inverse Fourier transform ($\omega \mapsto$t) using a contour integral on the upper half plane to enclose the singularity at $\omega = iD|\mathbf{k}|^2$. We apply the residue theorem to evaluate this integral:

$$\begin{aligned}
\tilde{g}(\mathbf{k},t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{it\omega}}{i\omega + D|\mathbf{k}|^2}\, d\omega \\
&= \frac{1}{2\pi}\oint_{UHP} \frac{e^{it\omega}}{i\omega + D|\mathbf{k}|^2}\, d\omega \\
&= \frac{2\pi i}{2\pi}\mathrm{Res}\left(\frac{\omega - iD|\mathbf{k}|^2}{i\omega + D|\mathbf{k}|^2} e^{it\omega}, iD|\mathbf{k}|^2\right) \\
&= \lim_{\omega \to iD|\mathbf{k}|^2} e^{it\omega} \\
&= e^{-Dt|\mathbf{k}|^2}
\end{aligned}$$

Now we can perform another set of inverse Fourier transforms, completing the square to make a Gaussian function and shifting horizontally to simplify:

[1]Notice that Fick's second law is intended to describe the change in concentration profile for an ensemble of molecules, but we have applied it to the probability distribution of a single particle.

$$
\begin{aligned}
G(\mathbf{x},t) &= \frac{1}{(2\pi)^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}e^{-Dt|\mathbf{k}|^2}\,dk_1\cdots dk_n \\
&= \frac{e^{-|\mathbf{x}|^2/4Dt}}{(2\pi)^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(\sum_{j=1}^{n} -Dtk_j^2 + ik_jx_j + \frac{x_j^2}{4Dt}\right)dk_1\cdots dk_n \\
&= \frac{e^{\frac{-|\mathbf{x}|^2}{4Dt}}}{(2\pi)^n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{j=1}^{n}\exp\left(-Dtk_j^2 + ik_jx_j + \frac{x_j^2}{4Dt}\right)dk_1\cdots dk_n \\
&= \frac{e^{\frac{-|\mathbf{x}|^2}{4Dt}}}{(2\pi)^n}\prod_{j=1}^{n}\int_{-\infty}^{\infty}\exp\left(-Dtk_j^2 + ik_jx_j + \frac{x_j^2}{4Dt}\right)dk_j \\
&= \frac{e^{\frac{-|\mathbf{x}|^2}{4Dt}}}{(2\pi)^n}\prod_{j=1}^{n}\int_{-\infty}^{\infty}\exp\left(\left(ik_j\sqrt{Dt} + \frac{x_j}{2\sqrt{Dt}}\right)^2\right)dk_j \\
&= \frac{e^{\frac{-|\mathbf{x}|^2}{4Dt}}}{(2\pi)^n}\prod_{j=1}^{n}\int_{-\infty}^{\infty} e^{-Dtk_j^2}\,dk_j = \frac{e^{\frac{-|\mathbf{x}|^2}{4Dt}}}{(2\pi)^n}\prod_{j=1}^{n}\sqrt{\frac{\pi}{Dt}} = \left(\frac{\pi}{Dt}\right)^{n/2}(2\pi)^n e^{\frac{-|\mathbf{x}|^2}{4Dt}} \\
&= \frac{1}{(4\pi Dt)^{n/2}}\exp\left(-|\mathbf{x}|^2/4Dt\right)
\end{aligned}
$$

$G(\mathbf{x},t)$, the Green's function for a diffusing particle whose location at time $t = 0$ is known with absolute accuracy, is a Gaussian function with mean zero. Its mean square displacement – which in this case is also equal to the variance in position – is:

$$
\begin{aligned}
\sigma^2 = \left\langle|\mathbf{x}|^2\right\rangle &= \frac{1}{(4\pi Dt)^{n/2}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}|\mathbf{x}|^2\exp\left(-|\mathbf{x}|^2/4Dt\right)dx_1\cdots dx_n \\
&= \frac{1}{(4\pi Dt)^{n/2}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(-\sum_{i=2}^{n}x_i^2/4Dt\right)\left[\int_{-\infty}^{\infty}|\mathbf{x}|^2 e^{\frac{-x_1^2}{4Dt}}\,dx_1\right]dx_2\cdots dx_n
\end{aligned}
$$

Focus on how to evaluate the innermost interval, using Gaussian integral identities:

$$
\begin{aligned}
\int_{-\infty}^{\infty}|\mathbf{x}|^2\exp\left(\frac{-x_1^2}{4Dt}\right)dx_1 &= \int_{-\infty}^{\infty}x_1^2\exp\left(\frac{-x_1^2}{4Dt}\right)dx_1 + \int_{-\infty}^{\infty}\left(\sum_{i=2}^{n}x_i^2\right)\exp\left(\frac{-x_1^2}{4Dt}\right)dx_1 \\
&= 2Dt\sqrt{4\pi Dt} + \left(\sum_{i=2}^{n}x_i^2\right)\sqrt{4\pi Dt} \\
&= \sqrt{4\pi Dt}\left[2Dt + \sum_{i=2}^{n}x_i^2\right]
\end{aligned}
$$

Plugging this result into the calculation for mean square distance, we get:

$$
\begin{aligned}
\left\langle|\mathbf{x}|^2\right\rangle &= \frac{1}{(4\pi Dt)^{(n-1)/2}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(-\sum_{i=2}^{n}x_i^2/4Dt\right)\left[2Dt + \sum_{i=2}^{n}x_i^2\right]dx_2\cdots dx_n \\
&= \frac{1}{(4\pi Dt)^{(n-2)/2}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(-\sum_{i=3}^{n}x_i^2/4Dt\right)\left[4Dt + \sum_{i=3}^{n}x_i^2\right]dx_3\cdots dx_n \\
&= 2nDt
\end{aligned}
$$