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# Reconciling Kinetic and Quantum Theory

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**Abstract**
We show that in a dilute gas the wave function's spreading is limited by scattering off other particles. This shows that quantum mechanics can be consistent with the kinetic theory of gases.

**Keywords** Kinetic theory · Spread of wave packet

## 1 Introduction

In the kinetic theory of gases one has a picture of little balls bouncing around, a concept of mean free path and related ideas. In more sophisticated theories the balls may become gaussian wave packets and the mean free path not simply given by *mean free path* $\equiv \ell = 1/n\sigma$, with $n$ the number density of particles and $\sigma$ the scattering cross section [1]. By contrast in quantum mechanics you have a wave function involving (say) $10^{23}$ coordinates [2], preferably plane waves (assuming the particles do not interact strongly). And even if you are ready to talk about single particle wave functions, and even if these are gaussians, they inevitably spread. Admittedly the kinetic theory picture is at best semiclassical, but there should also be a way to describe it by quantum mechanics, including the spreading. There is a concept of mean free path in quantum theory [3], but it is a kind of dissipation, leading to viscosity [4] and other effects.

In this article we do not fully solve the problem, but report ideas that lead to a resolution of sorts. In an appendix to a previous paper [5] we assumed the wave function was gaussian and that measurement caused a resumption of localization. In that heuristic treatment the size of a wave packet was on the order of $\sqrt{\ell\lambda_{\text{th}}}$ where the thermal wavelength is $\lambda_{\text{th}} = \hbar/\sqrt{mk_B T}$, $k_B$ is Boltzmann's constant and $T$ is the

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temperature. The main assumption was that scattering off another particle would localize a wave function, that is, reset the clock that allowed it to spread. This seemed reasonable in the context of that article in that the body of the article was devoted to a rigorous proof that scattering acted to squeeze the off-diagonal matrix elements and make them quite short, on the order of $\lambda_{\text{th}}$. In the present treatment there is also a dependence on the range of the potential that does the scattering, although in some sense that range was already present in $\ell$.

There is a common idea that we here lay to rest. Particles in a gas do not spread indefinitely. Our previous result suggested that a scattering would localize a particle, that spreading of the wave packet ceases. We here confirm that assumption.

As suggested earlier we consider only gases that interact weakly.

## 2 The Wave Packet is Localized

A single gaussian in 3 dimensions at time-0 can have the form

$$\psi(\boldsymbol{r},0)=\frac{1}{(2\pi\Delta^2)^{3/4}}\exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_0)^2}{4\Delta^2}+\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{r}-\boldsymbol{r}_0)\right). \tag{1}$$

It is localized at $\boldsymbol{r}_0$ and travels with momentum $\boldsymbol{p}$. At a later time, $t$, if it is freely propagating (with $H=\frac{p^2}{2m}$) it becomes

$$\psi(\boldsymbol{r},t)=\left(\frac{\Delta^4+\left(\frac{\hbar t}{2m}\right)^2}{2\pi\Delta^2}\right)^{-3/4}\exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_0-\frac{\boldsymbol{p}t}{m})^2}{4\left(\Delta^2+i\frac{\hbar t}{2m}\right)}+\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{r}-\boldsymbol{r}_0)-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}\right). \tag{2}$$

Now consider two such particles and condition on their colliding. Both have spread parameters $\Delta$ and mass $m$. They are approximately on a line (so $\boldsymbol{p}_1+\boldsymbol{p}_2\approx 0$) and meet approximately at position zero. One begins centered at $-\boldsymbol{r}_0$ and the other at $+\boldsymbol{r}_0$. Thus the initial wave function is

$$\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,0)=\frac{1}{(2\pi\Delta^2)^{3/2}}\exp\left(-\frac{(\boldsymbol{r}_1+\boldsymbol{r}_0)^2}{4\Delta^2}+\frac{i}{\hbar}\boldsymbol{p}_1(\boldsymbol{r}_1+\boldsymbol{r}_0)-\frac{(\boldsymbol{r}_2-\boldsymbol{r}_0)^2}{4\Delta^2}+\frac{i}{\hbar}\boldsymbol{p}_2(\boldsymbol{r}_2-\boldsymbol{r}_0)\right). \tag{3}$$

At time-$t$ the wave function becomes

$$\begin{aligned}\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=&\left(\frac{\Delta^4+(\frac{\hbar t}{2m})^2}{2\pi\Delta^2}\right)^{-3/2}\exp\left(-\frac{(\boldsymbol{r}_1+\boldsymbol{r}_0-\frac{\boldsymbol{p}_1t}{m})^2}{4\left(\Delta^2+i\frac{\hbar t}{2m}\right)}+\frac{i}{\hbar}\boldsymbol{p}_1(\boldsymbol{r}_1+\boldsymbol{r}_0)-\frac{i}{\hbar}\frac{\boldsymbol{p}_1^2t}{2m}\right)\\&\times\exp\left(-\frac{(\boldsymbol{r}_2-\boldsymbol{r}_0-\frac{\boldsymbol{p}_2t}{m})^2}{4\left(\Delta^2+i\frac{\hbar t}{2m}\right)}+\frac{i}{\hbar}\boldsymbol{p}_2(\boldsymbol{r}_2-\boldsymbol{r}_0)-\frac{i}{\hbar}\frac{\boldsymbol{p}_2^2t}{2m}\right).\end{aligned} \tag{4}$$

It is convenient to go to center of mass coordinates

$$\begin{aligned} \boldsymbol{R} &= \tfrac{1}{2}\left(\boldsymbol{r}_1 + \boldsymbol{r}_2\right) \qquad & \boldsymbol{r}_1 &= \boldsymbol{R} + \tfrac{1}{2}\boldsymbol{r} \\ \boldsymbol{r} &= \boldsymbol{r}_1 - \boldsymbol{r}_2 \qquad & \boldsymbol{r}_2 &= \boldsymbol{R} - \tfrac{1}{2}\boldsymbol{r}\,. \end{aligned} \tag{5}$$

Similarly

$$\begin{aligned} \boldsymbol{P} &= \boldsymbol{p}_1 + \boldsymbol{p}_2 \qquad & \boldsymbol{p}_1 &= \tfrac{1}{2}\boldsymbol{P} + \boldsymbol{p} \\ \boldsymbol{p} &= \tfrac{1}{2}\left(\boldsymbol{p}_1 - \boldsymbol{p}_2\right) \qquad & \boldsymbol{p}_2 &= \tfrac{1}{2}\boldsymbol{P} - \boldsymbol{p}\,. \end{aligned} \tag{6}$$

In these coordinates the argument of the exponential is (the normalization is unchanged)

$$-\frac{(\boldsymbol{R} + \frac{\boldsymbol{P}t}{2m})^2}{2\left(\Delta^2 + i\frac{\hbar t}{2m}\right)} - \frac{(\boldsymbol{r} + 2\boldsymbol{r}_0 + \frac{\boldsymbol{p}t}{m/2})^2}{2\left(4\Delta^2 + i\frac{\hbar t}{m/2}\right)} - \frac{i}{\hbar}\left(\boldsymbol{R}\boldsymbol{P} + (\boldsymbol{r} - 2\boldsymbol{r}_0)\boldsymbol{p}\right) - \frac{i}{\hbar}\left(\frac{\boldsymbol{P}^2}{4m} + \frac{\boldsymbol{p}^2}{m}\right)t\,. \tag{7}$$

To find the wave function after the scattering we use the Born approximation, in particular, since we are conditioning on a scattering having occurred, the wave function is $\int dt \frac{i}{\hbar} V(\boldsymbol{r})\Psi(\boldsymbol{R}, \boldsymbol{r}, t)$. Because of the conditioning we must divide by the appropriate probability in evaluating expectation values. (One can also look at this as a normalization of $\Psi$ to get correct expectation values.) Since the actual interaction is brief this can be approximated by $\delta t \frac{i}{\hbar} V(\boldsymbol{r})\Psi(\boldsymbol{R}, \boldsymbol{r}, t)$ for some small $\delta t$.

For convenience in calculating we take the potential to be a gaussian, of the form $V(\boldsymbol{r}) = V_0 \exp\left(-\frac{\boldsymbol{r}^2}{4a^2}\right)$ with $\boldsymbol{r}$ the relative coordinate. This is an assumption, to be discussed in Sect. 3. The quantity that we shall evaluate is the expectation of $(\Delta\boldsymbol{r}_1)^2$. Because the absolute value (squared) of the wave function will be used, there is no need to carry the phase terms. Moreover since we have conditioned on the particles' actually scattering we must divide by the quantity integrated, without the $(\Delta\boldsymbol{r}_1)^2$. Thus *after* the scattering, $\Psi$ (so $\Psi$ now has the potential as a factor) can be taken to be (omitting factors that cancel when divided by the conditioning)

$$|\Psi|^2 = \exp\left(-\frac{\boldsymbol{r}^2}{2a^2} - \frac{(\boldsymbol{R} + \frac{\boldsymbol{P}t}{2m})^2}{\left|\Delta^2 + i\frac{\hbar t}{2m}\right|} - \frac{(\boldsymbol{r} + 2\boldsymbol{r}_0 + \frac{\boldsymbol{p}t}{m/2})^2}{\left|4\Delta^2 + i\frac{\hbar t}{m/2}\right|}\right). \tag{8}$$

The quantity to be calculated is $(\Delta\boldsymbol{r}_1)^2 = \langle \Delta(\boldsymbol{R} + \boldsymbol{r}/2)^2 \rangle$ but because the integrand is even, cross terms vanish, and we can do separate evaluations, to obtain $(\Delta\boldsymbol{R})^2 + \frac{1}{4}(\Delta\boldsymbol{r})^2$. Finally, we must calculate

$$\langle A \rangle = \frac{\int d\boldsymbol{R}\, d\boldsymbol{r} A |\Psi|^2}{\int d\boldsymbol{R}\, d\boldsymbol{r} |\Psi|^2}\,, \tag{9}$$

for $A = \boldsymbol{r}, \boldsymbol{R}, \boldsymbol{r}^2$ and $\boldsymbol{R}^2$. For convenience we write $\theta \equiv \frac{\hbar t}{m}$ and

$$F \equiv |\Psi|^2 = \exp\left(-\frac{\boldsymbol{r}^2}{2a^2} - \frac{4\Delta^2}{4\Delta^4+\theta^2}\left(\boldsymbol{R}+\frac{\boldsymbol{P}t}{2m}\right)^2 - \frac{\Delta^2}{4\Delta^4+\theta^2}\left(\boldsymbol{r}+2\boldsymbol{r}_0+\frac{2\boldsymbol{p}t}{m}\right)^2\right)$$
$$= \exp\Bigg(-\frac{4\Delta^2}{4\Delta^4+\theta^2}\left(\boldsymbol{R}+\frac{\boldsymbol{P}t}{2m}\right)^2 - \frac{4\Delta^4+\theta^2+2\Delta^2a^2}{2a^2(4\Delta^4+\theta^2)}$$
$$\left(\boldsymbol{r}+\frac{2\Delta^2a^2}{4\Delta^4+\theta^2+2\Delta^2a^2}(2\boldsymbol{r}_0+2\boldsymbol{p}t/m)\right)^2$$
$$+\ \text{term that cancels because of normalization}\Bigg), \tag{10}$$

From Eq. (10) we evaluate (using Eq. (9))

$$\langle \boldsymbol{R}\rangle = -\frac{Pt}{2m}, \tag{11}$$

$$\langle \boldsymbol{r}\rangle = -\frac{2\Delta^2a^2}{4\Delta^4+\theta^2+2\Delta^2a^2}\left(2\boldsymbol{r}_0+\frac{2\boldsymbol{p}t}{m}\right), \tag{12}$$

so that

$$\langle(\Delta\boldsymbol{R})^2\rangle = \langle\boldsymbol{R}^2\rangle - \langle\boldsymbol{R}\rangle^2 = 3\,\frac{4\Delta^4+\theta^2}{8\Delta^2}, \tag{13}$$

and

$$\langle(\Delta\boldsymbol{r})^2\rangle = \langle\boldsymbol{r}^2\rangle - \langle\boldsymbol{r}\rangle^2 = 3\,\frac{a^2(4\Delta^4+\theta^2)}{4\Delta^4+\theta^2+2\Delta^2a^2}, \tag{14}$$

and

$$\langle(\Delta\boldsymbol{r}_1)^2\rangle = \frac{3}{4}\left[\frac{4\Delta^4+\theta^2}{2\Delta^2}+\frac{a^2(4\Delta^4+\theta^2)}{4\Delta^4+\theta^2+2\Delta^2a^2}\right]. \tag{15}$$

By symmetry

$$\langle(\Delta\boldsymbol{r}_2)^2\rangle = \langle(\Delta\boldsymbol{r}_1)^2\rangle. \tag{16}$$

Our final step is to impose a consistency condition. This will give us a value of $\Delta$ (the spread) that returns to itself after collision. Since the spread has turned out to be finite, and dependent on the initial $\Delta$ this is possible. Thus we require

$$\text{initial spread} = 3\Delta^2 = \text{final spread} = \frac{3}{8}\left(\frac{4\Delta^4+\theta^2}{\Delta^2}\right)\left(\frac{4\Delta^4+\theta^2+4\Delta^2a^2}{4\Delta^4+\theta^2+2\Delta^2a^2}\right). \tag{17}$$

Defining $x \equiv \Delta^2$ and using Eq. (17) implies that $x$ satisfies

$$16x^4 - 4a^2\theta^2 x - \theta^4 = 0\,, \tag{18}$$

with (recall) $\theta \equiv \frac{\hbar t}{m}$ (note that to a good approximation it is also true that $\theta = \lambda_{\rm th}\ell$). The solution can be approximated by $\frac{\theta}{2} + \frac{a^2}{4}$.

For dry air at STP, the mean free path is about 68 nm and the number per cubic meter is about $0.025 \times 10^{27}$, so that $\Delta$, the width of a wave packet, is about 3.78 Å, while the separation (one over the cube root of the number density) is about 10 times that.

## 3 Conclusion

Although there are many assumptions in our demonstration, the overall conclusions should be independent of those assumptions. The surprise (to us) was that a scattering caused localization. Such an assumption was plausible but until now not proved.

The assumption of a gaussian wave packet is a reasonable approximation to the "little balls" of kinetic theory. The assumption of a gaussian potential seems to us just a way to give the potential a finite range. It also made things easy to calculate.[1]

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[1] For example, if $V$ is a constant of height $V_0$ and of range $a$ we would have $\exp(-\boldsymbol{r}^2\Delta^2/(\Delta^4+\theta^2))V(\boldsymbol{r}) \le a^2 V_0$, and the relevant integral would again be finite.

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