Evolution of Wave-Packet Spread under Sequential Scattering of Particles of Unequal Mass

L. S. Schulman*

Physics Department, Clarkson University, Potsdam, New York 13699-5820, USA

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Under assumptions on initial wave-packet spreads and particle interactions, different mass particles scattering off one another will have the product $\sigma_i^2 m_i$ converge to a common value, where σ_i is the spread and m_i is the mass of the ith particle. When this relation is satisfied, kinematic entanglement vanishes.

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Theoretical developments suggest that a good way to describe naturally occurring quantum states is as spatially localized Gaussian wave packets, or as density matrices built from them [1–4]. The principal concern of these works (and others) is to justify the effective diagonalization of the density matrix in a coordinate space basis and to calculate a time scale for this process. In particular, thinking of the density matrix as a weighted sum of pure-state projections, wave packets do *not* spread indefinitely, but in any particular environment arrive at a statistically defined size. As far as I know, there have not been experiments to test the sizes that emerge. The existence of a stabilized spread size will be the working assumption of this article. "Spread," for our purposes, means $(\Delta x)^2 \equiv \langle (x - \langle x \rangle)^2 \rangle$, although the demonstrations of spread limitation often address density matrix diagonalization. Δx is well defined and in general nonzero, even for density matrices that are diagonal in coordinate space.

In this Letter, I report a surprising feature of wave-packet evolution that takes place when unequal-mass particles scatter. In particular, absent other influences, a collection of mixed-mass particles with Gaussian wave packets will evolve so that wave-packet spreads, σ^2, are related to corresponding particle masses, m, by $m\sigma^2 \sim$ const. Moreover, if the wave packet was not quite Gaussian, our calculation suggests that it will tend to lose non-Gaussian components in collisions (another kind of evidence for the thesis of [1–4]). Finally, it turns out that when $m\sigma^2 \sim$ const, and the wave function is Gaussian, there is *no* kinematic entanglement. By this I refer to the fact that after a scattering the coordinates of the colliding particles are intertwined, and even if the collision has but a single outcome, momentum conservation alone suggests—but apparently does not require—entanglement. These conclusions are based on dynamical assumptions that will be elaborated below.

In [5] features of this sort were noted, but under limited circumstances. What I have now found is that (i) the result can be extended to three dimensions (3D), (ii) for multiple collisions mutually interacting particles evolve so that all simultaneously satisfy the relation, (iii) the possibility of multiple outcomes (quantum induced) does not limit the result, and (iv) there are indications that non-Gaussian factors tend to shrink.

I begin with a demonstration of the result in [5]. A density matrix, ρ, can be represented as a weighted sum over projections (pure states). $\rho(t)$ evolves by evolving each pure state and recombining (a trivial consequence of $[\psi \to U\psi] \Leftrightarrow [\rho \to U\rho U^\dagger]$). Scattering calculations in this Letter will be done for pure states, subsequent to which they can be recombined. Moreover, properties shared by all the pure states are properties of the density matrix. The following is an example (with pure states summed over k'):

$$\rho_{\text{In Envir}} \sim \exp\{-(x^2 + y^2)/4\sigma^2 + ik(x - y) - \beta(x - y)^2\} = \sqrt{\frac{1}{4\pi\beta}} \int dk' \times \exp\left\{-\frac{(k' - k)^2}{4\beta} - \frac{x^2 + y^2}{4\sigma^2} + ik'(x - y)\right\}. \quad (1)$$

The quantity $\rho_{\text{In Envir}}$ was shown [2] to be the typical form of a density matrix after interaction with its environment. The salient environment-induced feature is the off-diagonal cutoff, governed by β. In Eq. (1), I have taken all pure-state spreads (σ) to be the same.

Begin then with an initial one-dimensional (1D) two-particle momentum-space wave function of the form $\Psi_I(p_1, p_2) = \exp[-\sigma_1^2(p_1 - k_1)^2 + ip_1a_1 - \sigma_2^2(p_2 - k_2)^2 + ip_2a_2]$, where the indices refer to the particles, k and a are the central momenta and positions, normalization is ignored, and $\hbar = 1$. In fact, all but quadratic terms in the p_i are ignorable for our argument. For the (position) spreads, σ^2, I adopt the notation ω so that the negative of the quadratic part (in the momenta) of the logarithm of the initial wave function is $Q_I(p_1, p_2) \equiv \omega_1 p_1^2 + \omega_2 p_2^2$. Although other dependencies of Ψ are important, the spread can be read from the coefficients of the quadratic part alone. We assume that scattering occurs on a time scale short compared to natural wave-packet spreading as well as environmental truncation (which in general requires many scatterings). These and other assumptions will be elaborated below. Only the real part of ω will be considered. With hard core repulsion, in 1D there is only

one outcome, and the propagator is best expressed in collective coordinates. These are $P \equiv p_1 + p_2$ (conjugate to $r_1x_1 + r_2x_2$) and $p = r_2p_1 - r_1p_2$ (conjugate to $x_1 - x_2$), where $r_i \equiv m_i/(m_1 + m_2)$. Thus, $Q_I = \omega_1(r_1P + p)^2 + \omega_2(r_2P - p)^2$. Aside from phase factors, whose possible impact on packet shape will be discussed below, the propagator is $G \sim \delta(P_f - P_i)\delta(p_f + p_i)$ (see [5]). The final shape factor is found by reversing p in Q_I and reexpressing in the original variables:

$$\begin{aligned} Q_F(p_1, p_2) = {} & p_1^2[\omega_1(r_1 - r_2)^2 + 4r_2^2\omega_2] \\ & + p_2^2[\omega_2(r_2 - r_1)^2 + 4r_1^2\omega_1] \\ & + 4(r_1 - r_2)p_1p_2[r_1\omega_1 - r_2\omega_2]. \end{aligned} \tag{2}$$

As noted [5], this implies that if $\sigma_i^2 = \text{const}/m_i$ ($\Leftrightarrow r_1\omega_1 = r_2\omega_2$) then the entangled portion, arising from the coefficient of p_1p_2, is zero and the wave function factors. Following the 1-2 encounter, the particles go off to others, say a collision of No. 1 and another particle [6]. If No. 1 is not entangled with No. 2, it is clear what wave function should be attributed to No. 1 for its next collision. Otherwise, we take the 1-2 density matrix, trace out p_2, and either use what is left for a density matrix calculation, or select exemplars from a projection expansion of the density matrix, with appropriate weights. Thus, we form $\hat{\rho}(p_1, p_1')$ from $\int dp_2 \exp[-Q_F(p_1, p_2) - Q_F(p_1', p_2) + \cdots]$. This turns out to have a single value for its new spread (Δx), which can be evaluated by transforming $\hat{\rho}$ to coordinate space and finding the coefficient of x^2 (in the exponent) on the diagonal. Details will be presented in the 3D case. The result is that after the 1-2 collision the particles have new spreads (independent of the original central momenta, etc.) given by the diagonal part of Q_F alone:

$$\begin{aligned} \xi_1' &= \xi_1\cos^2 2\theta + \xi_2\sin^2 2\theta, \\ \xi_2' &= \xi_1\sin^2 2\theta + \xi_2\cos^2 2\theta, \end{aligned} \tag{3}$$

where $\xi_i \equiv r_i\omega_i$ and $\cos^2\theta \equiv r_1$. Consider a gas of two species with many scatterings [6]. For equal mass scattering, Eq. (2) shows that there is no entanglement, only interchange of spread. With each successive *other-mass* scattering, the transformation (3) is applied. The result is convergence to $\xi_1 = \xi_2 = [\xi_1^{(0)} + \xi_2^{(0)}]/2$, where "0" indicates initial condition. ($\sum \xi$ is invariant; for $N \geq 2$, $\sum_{i=1}^N m_i\omega_i$ is invariant). The convergence is exponential, with $|\xi_2 - \xi_1|$ decreasing by $|\cos 4\theta|$ on successive iterations. For example, a 3-to-1 mass ratio sends that difference to less than 1% of its original value in seven collisions. Going from ξ back to the spreads, this shows $\sigma_i^2 m_i$ to be constant. Moreover, collision no longer induces kinematic entanglement [7].

Next, suppose the initial wave function is not perfectly Gaussian. Add terms $\sum_{i=1,2} g_i p_i^4$ to Q_I and redo the above: Write the p_i in terms of P and p, switch $p \to -p$ in the collision, and reexpress using (p_1, p_2). If the induced entangling does not affect the outgoing one-particle packet shape, as for the quadratic case, the coefficients g_i undergo the transformation

$$\begin{aligned} r_1^2 g_1' &= r_1^2 g_1\cos^4 2\theta + r_2^2 g_2\sin^4 2\theta, \\ r_2^2 g_2' &= r_1^2 g_1\sin^4 2\theta + r_2^2 g_2\cos^4 2\theta. \end{aligned} \tag{4}$$

Except for the equal or zero mass cases, all eigenvalues of this transformation are less than one in magnitude, indicating a flow of quartic terms to 0. Similar arguments hold for other nonquadratic terms. Nevertheless, these results do not have the force of the previous ones because discarding the entangled terms has not been fully justified. Heuristic arguments, lowest order in non-Gaussian terms and using the near independence of $\hat{\rho}(p, p')$ from $(p + p')$ when $\hat{\rho}(x, x')$ is near diagonal, justify the result, but I do not have a complete proof.

If the interparticle potential allows transmission as well as reflection, surmountable complications ensue, as will be discussed in the richer 3D case.

In 3D, the propagator is a δ function in the center-of-mass momentum times a potentially more elaborate object for the relative coordinate. Consider a wave packet in the relative coordinate. If the prescattering wave function is $\psi(\boldsymbol{r}, 0)$, then under the standard assumptions of scattering theory (see below) it ultimately becomes

$$\psi(\boldsymbol{r}, t) = \psi(\boldsymbol{r} - \boldsymbol{v}t, 0)e^{iEt} + \frac{1}{r} f_{\boldsymbol{k}}(\hat{\boldsymbol{r}})\psi(r\hat{\boldsymbol{k}} - \boldsymbol{v}t, 0)e^{iEt}, \tag{5}$$

where $\boldsymbol{k}$ is ψ's central momentum, $\boldsymbol{v} = \boldsymbol{k}/m$, $E = k^2/2m$, the scattering occurs near $\boldsymbol{r} = 0$, and $f_{\boldsymbol{k}}(\hat{\boldsymbol{r}})$ is the scattering amplitude in the direction $\hat{\boldsymbol{r}}$ ([8], Section 11.2). The density matrix constructed from this consists of transmitted plus scattered components, and assuming environmental decoherence [9] we can select wave functions from this collection so as to follow the particle's time evolution. The immediate message of Eq. (5) is that the *shape* of the wave function does not change: You can find the particle where it kinematically needs to be, given $\hat{\boldsymbol{r}}$, t, etc., but, except for resonances, the *form* of its wave function is still $\psi(\cdot, 0)$.

In momentum space, this leads to a simple description. The new wave function is the same as the old, but the relative momentum has rotated, as in classical mechanics. For our purposes—following the shape of the two-particle wave function—each "branch" of the wave function, i.e., the pure state moving in a single definite direction that is extracted from the environmentally truncated density matrix, can be obtained from the original wave function using an effective propagator, $G \sim \delta(P_f - P_i)\delta(p_f - Rp_i)$, where each momentum is a column three vector and $R \in \text{SO}(3)$ (dropping boldface). The richness in the phase of f does not enter the discussion of spreads.

The significant assumptions underlying the Low-Merzbacher [8] representation, Eq. (5), which become the assumptions of the present article, are that the distance between scatterings is large compared to the wave

function spread, that the spread is in turn larger than the scatterer, and that the energy is not near resonance. (See [10] for an example.)

With this characterization of the time evolution of a single component of the density matrix, we follow what happens to the spreads. For the initial wave function we again assume a Gaussian, but the spreads, ω_i, are now 3×3 positive-definite matrices. The quadratic part of the negative of the logarithm of the initial wave packet is therefore $Q_I(p_1, p_2) \equiv p_1^\top \omega_1 p_1 + p_2^\top \omega_2 p_2$, where $\top$ indicates transpose. To analyze the scattering, as above, Q_I is reexpressed in collective coordinates, and the relative momentum is sent to its image, in this case Rp. Following this, the p_i are restored and only quadratic terms retained. Using $R^{-1} = R^\top$ and $\omega^\top = \omega$, the result is

$$\begin{aligned} Q_F = {} & p_1^\top\{(r_1 + r_2R)\omega_1(r_1 + r_2R^{-1}) + r_2^2(1 - R)\omega_2(1 - R^{-1})\}p_1 \\ & + p_2^\top\{(r_2 + r_1R)\omega_2(r_2 + r_1R^{-1}) + r_1^2(1 - R)\omega_1(1 - R^{-1})\}p_2 \\ & + 2p_1^\top\{(r_1 + r_2R)r_1\omega_1(1 - R^{-1}) + (1 - R)r_2\omega_2(r_2 + r_1R^{-1})\}p_2. \end{aligned} \tag{6}$$

As for 1D, the entanglement term, $p_1^\top\{\ldots\}p_2$, vanishes when $r_1\omega_1 = r_2\omega_2 = \text{const}$, except that now the ω's must be multiples of the identity. Under this condition, the spread is unchanged by scattering.

We next calculate the effective spread of the scattered particles if the entanglement term does *not* vanish. For particle No. 1 trace out No. 2's coordinates, calculating $\hat{\rho}(p_1, p_1')$ from $\int dp_2 \exp[-Q_F(p_1, p_2) - Q_F(p_1', p_2) + \cdots]$, as before, except that now the p's are three vectors. Define A_1, A_2, and B as matrices by writing $Q_F(p_1, p_2) = p_1^\top A_1 p_1 + p_2^\top A_2 p_2 + 2p_1^\top B p_2$. Then the integral over p_2 yields (dropping the "1" on p_1 and suppressing irrelevant dependencies) $\hat{\rho}(p, p') = \exp(-p^\top A_1 p - p'^\top A_1 p') \times \exp[(p + p')^\top C(p + p')]$, with $C \equiv B^\top A_2^{-1} B/2$. To find the new spread, it is convenient to go to coordinate space. With $x = x_1$, $\hat{\rho}$ is

$$\begin{aligned} \hat{\rho}(x, x') &= \int dp\, dp'\, e^{ipx - ip'x'} \\ &\quad \times e^{-p^\top A_1 p - p'^\top A_1 p' + (p+p')^\top C(p+p')} \\ &= \exp(-\xi^\top M^{-1}\xi/4), \end{aligned} \tag{7}$$

with $M \equiv \begin{pmatrix} A_1 - C & -C \\ -C & A_1 - C \end{pmatrix}$ and $\xi \equiv \begin{pmatrix} x \\ -x' \end{pmatrix}$. M^{-1} can be written $\begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}$ with α and β symmetric, since A_1 and C are symmetric. A straightforward identity shows that $\xi^\top M^{-1}\xi = x^\top(\alpha - \beta)x + x'^\top(\alpha - \beta)x' + (x - x')^\top \times \beta(x - x')$. To find the new σ (Δx) we need only the diagonal elements in the x-space basis, yielding for the quadratic form for the x portion of the density matrix $(\alpha - \beta)/4$. Returning to momentum space, the new spread [the quadratic form for $p^\top(\ldots)p$] is $(\alpha - \beta)^{-1}$. It is easily shown that this quantity is equal to the original A_1. As a result, the new spread for No. 1, ω_1', is A_1, and $\omega_2' = A_2$. The packet spread iteration rule is therefore

$$\begin{aligned} \xi_1' &= (r_1 + r_2R)\xi_1(r_1 + r_2R^{-1}) \\ &\quad + r_1r_2(1 - R)\xi_2(1 - R^{-1}), \\ \xi_2' &= (r_2 + r_1R)\xi_2(r_2 + r_1R^{-1}) \\ &\quad + r_1r_2(1 - R)\xi_1(1 - R^{-1}), \end{aligned} \tag{8}$$

where again the ω's have been replaced by $\xi_i \equiv r_i\omega_i$. Note that Eq. (8) preserves the symmetry and positivity of the ω's. [Also, (8) reduces to (3) for $R \to -1$.]

I will not dwell on the mathematical properties of Eq. (8), but report only that, as for Eq. (3), it converges to limiting ω values when the transformation is iterated, using a variety of R's, as in a gas where the impact parameter takes many values [6,11,12]. Under the transformation, $\text{Tr}\sum \xi = \text{const}$, and the final ξ values are $\text{Tr}[r_1\omega_1^{(0)} + r_2\omega_2^{(0)}]/6$ times the 3×3 identity. [I have also shown that certain nonquadratic terms in $\log(\psi)$ flow to zero (as for 1D) and expect this to be true in general.] The consequence of repeated use of Eq. (8) is therefore that the spreads for a collection of varied-mass particles converge to isotropic values, inversely proportional to their masses.

The focus of this article has been on the shape of naturally occurring wave packets and, in particular, on the size of the position-space spread. Can this be measured in the laboratory? The issue of measuring the wave function goes back at least to the 1930s [13], and continues to engage researchers both in principle and in practice [15–28]. To test our results, emphasis would be on measurement of interference phenomena for massive particles [27–29]. One would seek less information than is often contemplated—spread alone is needed. Such a measurement can be performed with a two-slit interferometer by varying slit separation. If the separation is greater than the transverse spread, interference could not be observed, so the threshold for interference becomes a rough measure of spread [30]. One point though needs to be emphasized. While experiments have measured subtle properties, including coherence lengths, some of those properties are created in the state-preparation process, which can involve beam choppers, monochromators, collimators, and other devices. An experimental probe of the present work should take particles from the environment in which they scatter off one another (a "natural" environment) without changing the spread.

The calculation of this article is straightforward, but the circumstances under which the assumptions apply are less clear. In particular, a relevant and unknown quantity is how large the environmentally "stabilized" spreads are (without the scattering discussed here), a topic that has been explored in theoretical discussions and for which experimental work has been contemplated [25]. It is further implicit that the spread evolution studied here occurs rapidly compared to the environmental size stabilization

of spreads [31]. Whether or not this is true, as for our assumptions on the size of the stabilized spread, is unknown. What theory can contribute is to suggest situations in which the assumptions are more likely to be true. In selecting candidates for experiment, one should consider cross sections, resonances, and mass ratios. The assumptions may also hold more widely than at first appears. Noninteracting species in a walled container can separately come to "spread equilibrium" with the wall, so that the ratios of their spreads are inverse to that of their masses, despite a lack of direct interaction [32]. If the container is itself buffeted by outside influences, the three of them will come to a joint steady state (of spreads) with the scale set by the container.

As in [5,33], I find the nonentanglement property of the spread equilibrium intriguing. Entanglement can occur when more than one distinct final state is available in a scattering, but from the perspective of [34] the phenomenon described in the present article makes the finding of "special" states easier.

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*Electronic address: schulman@clarkson.edu

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