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On shrinking and expansion of radial wave packets

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Abstract

We study the effect of initial 'shrinking' of radial 'ring-shaped' wave packets with zero initial velocity distribution in two and more dimensions. Considering time evolution of probability densities described by explicit exact solutions of the free Schrödinger equation in d dimensions, we introduce and compare two different families of quantitative measures of 'expansion'. The measures of the first type are based on the mean values of arbitrary powers of radius, they characterize the 'total extension' of the packet. The measures of the second type quantify the 'internal' size of the packet (or an effective width of the 'ring'). We find that the effect of initial 'in-spreading', which is very small in two dimensions and absent in higher dimensions with respect to the mean value of radius, is much more pronounced, if one uses mean values of $\langle r^{\alpha}\rangle$ with $\alpha < 1$ and especially $\alpha < 0$ as the measure of packet extension. In this sense, the case of two dimensions is not distinguished, and shrinking packets exist in more than two dimensions, as well. On the other hand, we show that the effect of initial 'shrinking' or 'expansion' strongly depends on the chosen measure of spatial extension ('total' or 'internal') of the packet. Moreover, the conclusions concerning the initial evolution of the 'internal' packet extensions based on the 'volume' probability density $|\psi|^2$ may be sometimes opposite to the conclusions based on the 'radial probability density' $r^{d-1}|\psi|^2$.

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1. Introduction

Recently, renewed interest in propagation, reflection, scattering and diffraction of packets of matter waves in one and several dimensions has been observed [1–8]. In particular, it was

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shown in [6] that for 'ring-shaped' packets in d space dimensions, whose initial form depends only on radius as (we use dimensionless variables, assuming $m = \hbar = 1$)

$$\psi_d(r;0) = \mathcal{N}_d r^2 \exp(-r^2) \tag{1}$$

the mean value of the radius *decreases* with time in some interval $0 < t < t_*$ for $d = 2$, whereas for $d \geqslant 3$ it monotonically increases for all $t > 0$. This effect of initial *contraction* of the packet was interpreted as a manifestation of an effective 'quantum anticentrifugal potential' in two dimensions [9] (for other studies of different 'effective' or 'fictitious' quantum forces see [1, 3, 8, 10]). However, the effect of contraction considered in [6] seems to be extremely small, because the ratio of the minimal mean radius to its initial value equals 0.9978 for the initial packet (1) and 0.9953 for the best configuration among those considered in [6]. From a common point of view, such values are usually considered as practically undistinguishable from unity.

But the mean radius is only one of many reasonable quantitative measures of the packet extension. The aim of our paper is to show that the effect of initial 'shrinking' of the packet can be made much more pronounced if one uses other measures, in particular, the mean values of different (especially negative) powers of the radius, or some 'entropy-like' extensions. However, in terms of these generalized measures, the two-dimensional case loses its distinguished role (although it is distinguished in some other respects). Moreover, under certain conditions, three- and higher-dimensional packets may exhibit stronger initial shrinking than two-dimensional ones.

The plan of the paper is as follows. In section 2, we obtain explicit analytical expressions describing the evolution of 'scale-invariant' initial ring-shaped packets generalizing (1) for an arbitrary number of space dimensions d, giving also some graphical illustrations for the distribution of the probability density and phase velocity. Although the cases of $d = 2$ and $d = 3$ seem to be the most relevant, studying the general case provides some additional information which helps to understand the situation better. Besides, the cases of $d > 3$ could be interesting from the point of view of analysis of the behaviour of many-particle systems [6, 10]. In section 3 we analyse the mean values of arbitrary powers of the radius as measures of packet size. The 'entropy-like' measures of packet extension are considered in section 4. Section 5 contains a discussion of results and conclusions.

2. Spreading of scale-invariant ring-shaped packets

Integrating the well-known propagator of the free Schrödinger equation in d space dimensions

$$G(\mathbf{x}, \mathbf{x}', t) = (2\pi \mathrm{i} t)^{-d/2} \exp\left[\frac{\mathrm{i}}{2t}(\mathbf{x} - \mathbf{x}')^2\right] \tag{2}$$

over angular variables, one can easily find, using the known integral representations of the Bessel functions (see, e.g., formula 7.12.9 from [11]), that the evolution of initial wavefunctions depending only on the radius $r \equiv (\mathbf{x}^2)^{1/2}$ is given by effective radial propagators of the form (see also, e.g., [12])

$$\psi_d(r,t) = \frac{r}{t}\int_0^\infty \left(\frac{r'}{\mathrm{i}r}\right)^{d/2} J_{(d-2)/2}\left(\frac{rr'}{t}\right) \exp\left[\frac{\mathrm{i}}{2t}(r^2 + r'^2)\right] \psi_d(r',0)\,\mathrm{d}r' \tag{3}$$

where $J_\nu(z)$ is the Bessel function and d is the number of space dimensions.

We consider the following generalization of the initial packet (1):

$$\psi_d^{(k)}(r;0) = \mathcal{N}_{d,k} r^k \exp(-r^2) \qquad \mathcal{N}_{d,k}^2 = \frac{2^{k+d/2}\Gamma(d/2)}{\pi^{d/2}\Gamma(k+d/2)} \tag{4}$$

where $\Gamma(z)$ is Euler's gamma function. Then the integral (3) can be expressed in terms of the confluent hypergeometric function $\Phi(a; c; z)$ (see, e.g., equation 7.7.3(22) from [11]), so that

$$\psi_d^{(k)}(r; t) = \frac{\mathcal{N}_{d,k}\Gamma\left(\frac{k+d}{2}\right)(\mathrm{i}\tau)^{k/2}}{\Gamma(d/2)(1+\mathrm{i}\tau)^{\frac{k+d}{2}}} \exp\left(-\frac{r^2}{1+\mathrm{i}\tau}\right)\Phi\left(-\frac{k}{2}; \frac{d}{2}; \frac{\mathrm{i}r^2}{\tau(1+\mathrm{i}\tau)}\right) \quad (5)$$

where $\tau \equiv 2t$. If $k/2 = n$ is an integer, then the right-hand side of (5) can be expressed in terms of the associated Laguerre polynomials due to formula 10.12(14) from [11]:

$$\psi_d^{(2n)}(r; \tau) = \frac{\mathcal{N}_{d,2n} n!(\mathrm{i}\tau)^n}{(1+\mathrm{i}\tau)^{n+d/2}} \exp\left(-\frac{r^2}{1+\mathrm{i}\tau}\right) L_n^{(d/2-1)}\left(\frac{\mathrm{i}r^2}{\tau(1+\mathrm{i}\tau)}\right). \quad (6)$$

It is not difficult to generalize the solutions (5) or (6) to the case where the argument of the exponential in (4) is equal to $-(1+\mathrm{i}\kappa)r^2$. Such functions can be considered as generalizations of *correlated coherent states* of [13] or their special case—'contractive states' of [14], because the covariances $\langle \hat{\mathbf{x}}\hat{\mathbf{p}} + \hat{\mathbf{p}}\hat{\mathbf{x}}\rangle$ are different from zero in these states. However, if $\kappa \neq 0$, then the initial mean value of the radial momentum is also different from zero, so the effect of shrinking of the initial packet becomes trivial. For this reason we confine ourselves to the case of $\kappa = 0$.

2.1. Probability distribution

It is easy to see from equations (5) or (6) that for large τ (and fixed r) the packet 'forgets' its initial ring shape and spreads as the usual Gaussian packet:

$$\left|\psi_d^{(k)}(r; \tau)\right|^2 \sim \tau^{-d} \exp(-2r^2/\tau^2) \qquad \tau \gg 1.$$

However, since the initial 'ring-shaped' packet spreads both outside and inside, its shape may be quite different from the Gaussian and from the initial one at the initial stage of evolution (when $\tau < 1$) due to the interference effects. For example, using formula (6) with $n = 1$ one obtains the solutions of the Schrödinger equation corresponding to the initial function (1):

$$\psi_d^{(2)}(r; \tau) = \mathcal{N}_{d,2}(1+\mathrm{i}\tau)^{-2-d/2}(r^2 - \tau^2 d/2 + \mathrm{i}\tau d/2) \exp\left(-\frac{r^2}{1+\mathrm{i}\tau}\right). \quad (7)$$

It has the probability density

$$\rho_d(r; \tau) \equiv \left|\psi_d^{(2)}\right|^2 = \mathcal{N}_{d,2}^2 \frac{r^4 - r^2\tau^2 d + \tau^2(1+\tau^2)d^2/4}{(1+\tau^2)^{2+d/2}} \exp\left(-\frac{2r^2}{1+\tau^2}\right). \quad (8)$$

This function has one minimum and one maximum in the interval $0 < r < \infty$ (and one maximum at $r = 0$ for $\tau > 0$). For $\tau \gg 1$ their positions are given by the approximate expressions $r_{\min} \approx \tau\sqrt{d/2}$ and $r_{\max} \approx \tau\sqrt{1+d/2}$ (for $d = 2$ this is an *exact* formula), and the following approximate ratios hold:

$$\frac{\rho_{\max}}{\rho(r=0)} \approx (ed/2)^{-2}\,\mathrm{e}^{-d} \qquad \frac{\rho_{\min}}{\rho_{\max}} \approx (ed\tau/2)^{-2}.$$

Consequently, some remnants of the initial ring survive for $\tau \gg 1$, but this outer ring is very faint: its height is about 2% of the height of the central peak for $d = 2$ and less than 0.5% for $d = 3$.

The initial stages of evolution of the 'volume probability density' $\rho_d(r; \tau)$ and the 'radial probability density'

$$\chi_d(r; \tau) = \omega_d r^{d-1}|\psi_d(r; \tau)|^2 \qquad \omega_d \equiv \frac{2\pi^{d/2}}{\Gamma(d/2)} \quad (9)$$

for different values of k and d are demonstrated in figures 1–6.

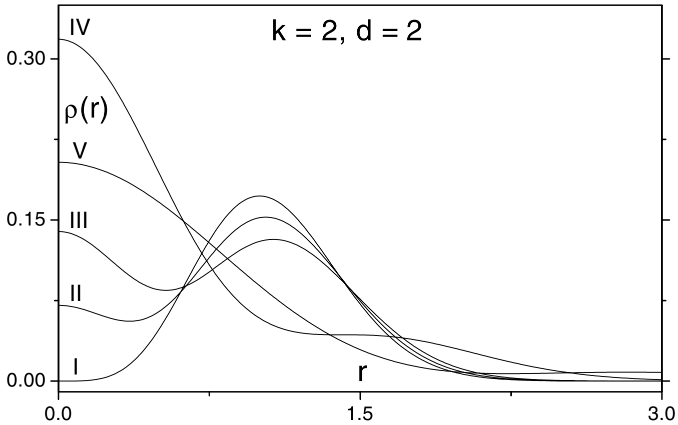

Figure 1. The volume probability density $\rho(r) = |\psi(r)|^2$ for $k = 2$ and $d = 2$ at different moments of time. I: $\tau = 0$, II: $\tau = 0.25$, III: $\tau = 1/\sqrt{7} \approx 0.38$, IV: $\tau = 1$, V: $\tau = 2$.

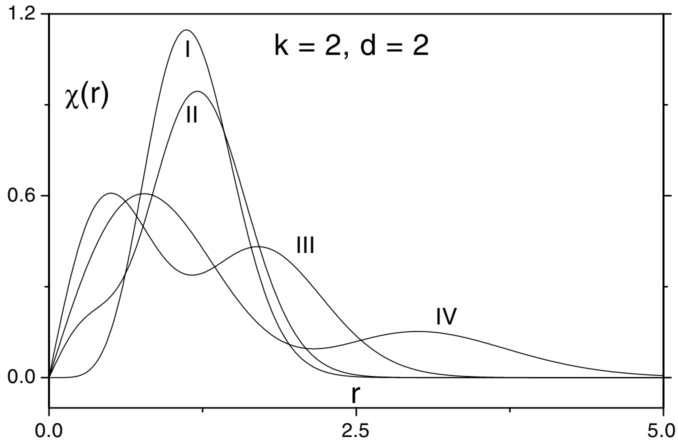

Figure 2. The radial probability density $\chi(r)$ (9) for $k = 2$ and $d = 2$ at different moments of time. I: $\tau = 0$, II: $\tau = 1/\sqrt{7} \approx 0.38$, III: $\tau = 1$, IV: $\tau = 2$.

Looking at the plots, we discover, first of all, that the visual impression depends on the kind of probability density considered. The radial probability distributions at $\tau > 0$ seem to always be wider than the initial ones, although it is not obvious whether their spreading is always monotonic or not (compare the curves III and IV in figure 2 and the curves II and III in figure 4).

The situation becomes even more complicated, if one looks at the evolution of the volume probability densities. For example, in the case of $k = d = 2$ (figure 1) the distributions of $\rho(r)$ at the moments $\tau = 1/\sqrt{7}$ (curve III) and $\tau = 2$ (curve V) seem to be obviously wider than at $\tau = 0$. However, it is not easy to answer whether the packet at the moment $\tau = 1$ (curve IV) is wider or narrower than the initial one, especially if one closes ones eyes to the 'tail' of the packet at $r > 1$. The same can be said about the volume distributions at the moments $\tau = 0.25$ (curve II), $\tau = 2$ (curve IV) and $\tau = \sqrt{2/3}$ (curve III) in the case of $k = 2$ and $d = 3$ (figure 3). And which curve is relatively narrower or wider with respect to the

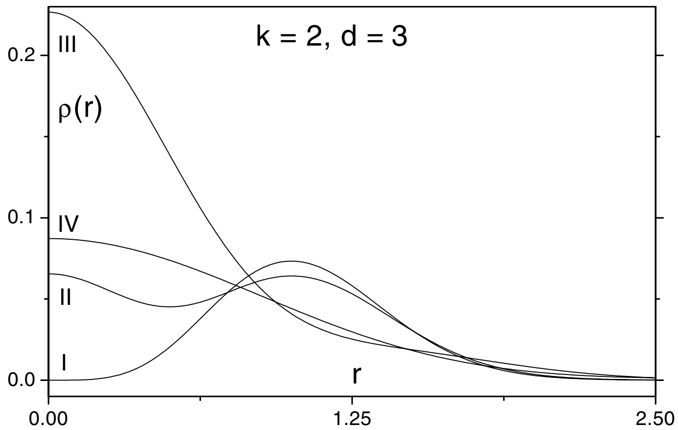

Figure 3. The volume probability density $\rho(r) = |\psi(r)|^2$ for $k = 2$ and $d = 3$ at different moments of time. I: $\tau = 0$, II: $\tau = 0.25$, III: $\tau = \sqrt{2/3} \approx 0.82$, IV: $\tau = 2$.

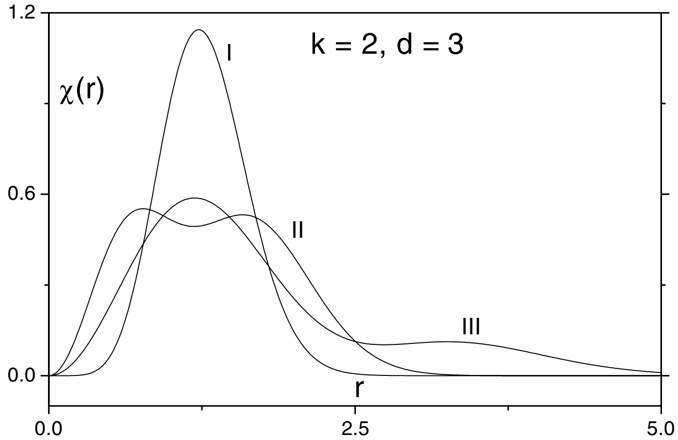

Figure 4. The radial probability density $\chi(r)$ (9) for $k = 2$ and $d = 3$ at different moments of time. I: $\tau = 0$, II: $\tau = \sqrt{2/3} \approx 0.82$, III: $\tau = 2$.

initial distribution: curve III in figure 1 (which corresponds to the smallest size of the packet according to results of [6]: see the next section) or curve III in figure 3? (According to the measure of extension adopted in [6], curve III describes the distribution whose size is greater than that corresponding to curve II in the same figure 3, although visually the distribution III is apparently narrower than the distribution II.) Analogously, in the case of $k = 20$ and $d = 2$ (figure 5) the distribution given by curve II seems to be obviously wider than the initial one, but what can be said about the distribution given by curve III ?

2.2. Velocity distribution

Additional useful information concerning the dynamics of the shrinking/expansion process is contained in the velocity distribution in the packet. Remembering that the probability density

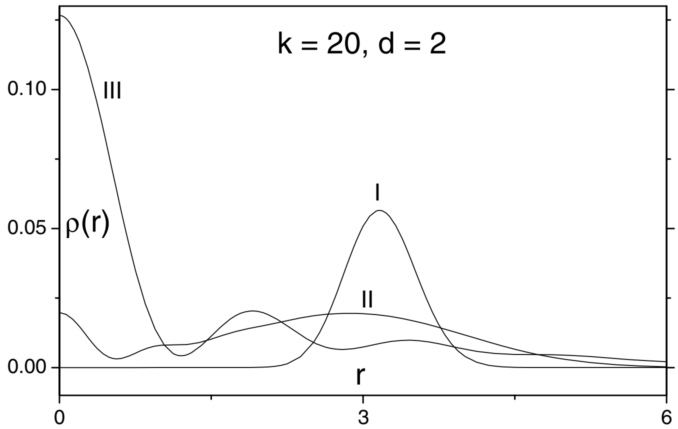

Figure 5. The volume probability density $\rho(r) = |\psi(r)|^2$ for $k = 20$ and $d = 2$ at different moments of time. I: $\tau = 0$, II: $\tau = 1.4$, III: $\tau = \sqrt{10} \approx 3.16$.

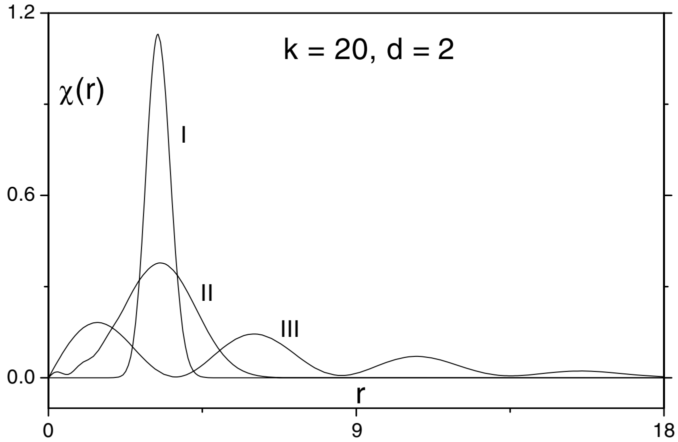

Figure 6. The radial probability density $\chi(r)$ (9) for $k = 20$ and $d = 2$ at different moments of time. I: $\tau = 0$, II: $\tau = 1.4$, III: $\tau = 10$.

flux is defined as $\mathbf{J} = \mathrm{Im}(\psi^* \nabla \psi)$ (we assume $\hbar = m = 1$), the local (phase) velocity is given by

$$\mathbf{v} = \mathbf{J}/\rho = \mathrm{Im}(\nabla \psi / \psi). \tag{10}$$

For the radial packets vector $\mathbf{v}$ has only a radial component. For the state (7) we obtain

$$v(r, \tau) = \frac{2r\tau[r^4 - r^2\tau^2 d + d(1+\tau^2)(\tau^2 d - 2)/4]}{(1+\tau^2)[(r^2 - \tau^2 d/2)^2 + \tau^2 d^2/4]}. \tag{11}$$

(Although the velocity grows as r for $r \to \infty$, this has no physical consequences, because the probability flux is suppressed by the exponentially decaying probability density $\rho(r)$.) The regions of shrinking correspond to negative values of $v(r)$. Their bounds are given by two roots of the quadratic (with respect to r^2) expression in the numerator of (11):

$$r_{\pm}^2(\tau) = \frac{d}{2}\tau^2 \pm \sqrt{\frac{d}{2}\left[1 - \tau^2\left(\frac{d}{2} - 1\right)\right]}. \tag{12}$$

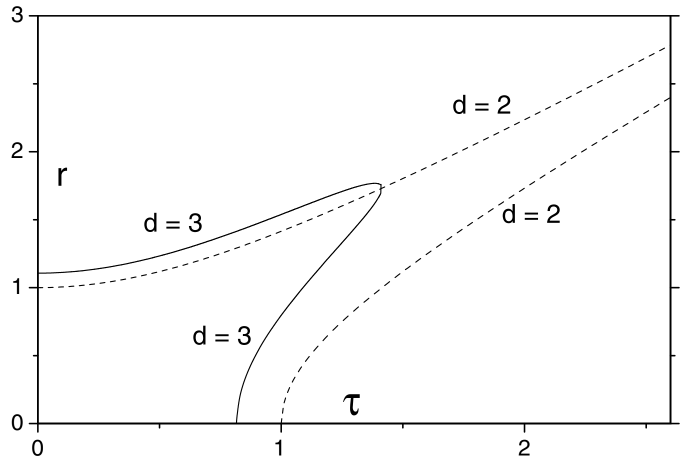

Figure 7. The regions of shrinking, corresponding to negative phase velocity (11), are located between two dashed curves for $d = 2$ and between two solid curves for $d = 3$ (for the initial packet with $k = 2$).

For $\tau < \sqrt{2/d}$ (this is exactly the moment when the probability density at the origin $|\psi(0,\tau)|^2$ attains its maximum) some local shrinking seems to exist for $0 < r < r_+(\tau)$. After that, the region near the origin begins to expand, and the shrinking region is limited by two values: $r_-(\tau) < r < r_+(\tau)$. Here we observe a qualitative difference between the cases of $d = 2$ and $d \geqslant 3$. In three and more dimensions the intermediate shrinking region exists only for $\tau < \sqrt{2/(d-2)}$, whereas in the case of two dimensions the shrinking region never disappears, although its size diminishes as soon as it moves outside; it is confined in the interval $\sqrt{\tau^2 - 1} < r < \sqrt{\tau^2 + 1}$. These 'regions of shrinking' for $d = 2$ and $d = 3$ are shown in figure 7.

However, to answer the question, whether the packet shrinks or expands as a whole, we need *quantitative measures* of packet extension.

3. Generalized mean radius as a measure of extension

One of the most frequently used quantities characterizing the 'size' of some distribution possessing the probability density $\rho(\mathbf{x})$ is the *mean square radius*

$$R^{(2)} \equiv \left(\int \mathbf{x}^2 |\psi(\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} \right)^{1/2}. \tag{13}$$

However, this quantity is totally insensitive to the form of freely expanding packet, because for any initial distribution without correlations between coordinates and momentum ($\langle \hat{\mathbf{x}}\hat{\mathbf{p}} + \hat{\mathbf{p}}\hat{\mathbf{x}} \rangle = 0$) the exact solution of the Heisenberg equations of motion for a free particle results in the monotonic time dependence

$$[R^{(2)}(t)]^2 = [R^{(2)}(0)]^2 + \langle \hat{\mathbf{p}}^2 \rangle t^2/m^2$$

(we calculate all mean values in the reference frame related to the 'centre of mass' of the packet, where $\langle \hat{\mathbf{x}} \rangle = \langle \hat{\mathbf{p}} \rangle = 0$).

Therefore, we have two possibilities. The first one is to assume that the mean square radius is the only 'true' measure of the packet extension, concluding immediately that 'shrinking' (free) packets do not exist and figures 1–6 are something like 'optical illusions'. The second possibility is to admit that there exist other measures of packet extension, which are not worse than (13), moreover, which could provide additional information on the properties of quantum systems. Making the second choice, we can try to find such measures which would be more sensitive to the details of packet evolution. The reason why the measure (13) 'does not feel' the form of the packet seems to be clear: the initial ring-shaped packet expands in both directions, outside and inside, but the factor $\mathbf{x}^2$ in the integrand of (13) (together with the factor r^{d-1} in the radial probability density) gives much more preference to the outer parts of the packet, so that its 'internal behaviour' becomes totally irrelevant. Thus the way to resolve the problem becomes also almost obvious: one should use such measures which would treat the 'external' and 'internal' parts of the packet on a 'more equal' footing.

The simplest possibility is to diminish the power of the factor $|\mathbf{x}|$ in (13) and to characterize the extension of the packet by the mean radius

$$\langle r \rangle_d = \int_0^\infty \mathrm{d}r\, r\, \chi_d(r). \tag{14}$$

Namely this measure was used in [6]. Calculating the integral (14) for the function (8) with the aid of the relation

$$\int_0^\infty r^n\, \mathrm{e}^{-2r^2/a}\, \mathrm{d}r = \frac{1}{2}\left(\frac{a}{2}\right)^{\frac{n+1}{2}} \Gamma\left(\frac{n+1}{2}\right) \tag{15}$$

and the known property of the Gamma function $\Gamma(z+1) = z\Gamma(z)$, we obtain the formula (given in [6] without derivation)

$$\langle r(\tau) \rangle_d = \langle r(0) \rangle_d \frac{1 + b\tau^2}{\sqrt{1+\tau^2}} \qquad b = \frac{d^2+3}{(d+3)(d+1)}. \tag{16}$$

In particular, for $d = 2$ and $d = 3$ one has [6]

$$\langle r(\tau) \rangle_2 / \langle r(0) \rangle_2 = \frac{1 + 7\tau^2/15}{\sqrt{1+\tau^2}} \qquad \langle r(\tau) \rangle_3 / \langle r(0) \rangle_3 = \frac{1 + \tau^2/2}{\sqrt{1+\tau^2}}. \tag{17}$$

The character of initial evolution of the mean radius is determined by the parameter

$$b - 1/2 = \frac{(d-3)(d-1)}{2(d+3)(d+1)}$$

(which is equal to the coefficient at the first nonzero term τ^2 in the Taylor expansion of $\langle r(\tau) \rangle / \langle r(0) \rangle$). This parameter is negative only for $d = 2$. On this ground, the authors of [6] concluded that the initial 'in-spreading' of radial packets is possible only in the case of two space dimensions. However, for $\tau \ll 1$ the actual difference between two functions in (17) is very small:

$$\frac{\langle r(\tau) \rangle_2}{\langle r(0) \rangle_2} = 1 - \frac{\tau^2}{30} + \frac{17}{120}\tau^4 + \cdots \qquad \frac{\langle r(\tau) \rangle_3}{\langle r(0) \rangle_3} = 1 + \frac{\tau^4}{8} + \cdots.$$

The function $\langle r(\tau) \rangle_2 / \langle r(0) \rangle_2$ attains a minimum for $\tau_* = 1/\sqrt{7}$ (this value explains the choice of parameters in figures 1 and 2), but the minimal value $\langle r(\tau_*) \rangle_2 / \langle r(0) \rangle_2 = \sqrt{224/225}$ is very close to unity and to the value $\langle r(\tau_*) \rangle_3 / \langle r(0) \rangle_3 = 1 + 1/392$. Therefore, it seems quite probable that even small variations in the definition of the measure of extension could change the situation.

On the other hand, as soon as one agrees that the measure (13) is not the only possible one, there are no grounds to believe that there are only two 'true' measures, (13) and (14). Moreover, the characterization of the dimension of the packet by its mean radius (14), i.e., by the average value of the first power of $|\mathbf{x}|$, being quite natural at first sight, has no visible advantages over the measures based on other powers of $|\mathbf{x}|$, say, $|\mathbf{x}|^{1/2}$, even from the point of view of simplicity of calculations. Indeed, in contrast to the mean square radius, which can be easily calculated by solving a simple closed set of (Ehrenfest) equations, there are no closed equations for the function $\langle r(\tau)\rangle$. In order to find it, one has to solve first the Schrödinger equation, find the time-dependent wavefunction and calculate the integral (14). For example, to obtain the result (17) one should calculate three integrals of the type (15) with $n = d + 2s$ and $s = 0, 1, 2$. However, the analytical form remains the same for arbitrary (not necessarily integral) values of the exponent n. Therefore, it seems reasonable to suppose that the measures (13) and (14) are nothing but special cases of a wide family of 'generalized mean radii', characterized by a real continuous parameter α:

$$R_d^{(\alpha)} = \left[\int_0^\infty \mathrm{d}r r^\alpha \chi_d(r)\right]^{1/\alpha}. \tag{18}$$

In the case of the probability density (8) (i.e., for $k = 2$) the calculations of the $R_d^{(\alpha)}$-extensions are reduced again to the integral (15), with the only difference that in the general case $n = d - 1 + \alpha + 2s$. Thus we obtain the following expression for the normalized function $\tilde{R}_d^{(\alpha)}(\tau) = R_d^{(\alpha)}(\tau) \big/ R_d^{(\alpha)}(0)$:

$$\tilde{R}_d^{(\alpha)}(\tau) = (1+\tau^2)^{1/2-1/\alpha}\left[1 + \frac{(\alpha - d)^2 + 2(\alpha + d)}{(\alpha + d)^2 + 2(\alpha + d)}\tau^2\right]^{1/\alpha}. \tag{19}$$

At $\tau \ll 1$ it equals

$$\tilde{R}_d^{(\alpha)}(\tau) = 1 + \frac{(\alpha + d)^2 + 2\alpha - 6d}{2(\alpha + d)(\alpha + d + 2)}\tau^2 + \cdots. \tag{20}$$

For $\alpha = 1$ formulae (19) and (20) give the same results as equations (16) and (17).

It is worth noting that the 'generalized extensions' of quantum packets based on the mean values of arbitrary powers of coordinates (radius) have been used for rather long time, beginning, perhaps, with Bargmann's work on generalized uncertainty relations [15] and its further generalizations [16–18] (actually, 'uncertainty relations' tell us about limitations on the extensions of quantum packets in complementary spaces, and the simplest inequalities of the Weyl–Heisenberg or Schrödinger–Robertson type, based on the mean squared values, constitute only a very small part of a large family of known relations, based on other definitions of 'extensions' [19]).

The coefficient at τ^2 in (20) is negative for $\alpha < \alpha_c$, where the critical exponent α_c equals

$$\alpha_c = \sqrt{1 + 8d} - d - 1. \tag{21}$$

For $d = 2, \alpha_c = \sqrt{17} - 3 \approx 1.12$. It is remarkable that for $d = 3, \alpha_c = 1$, therefore, the generalized effective radius of the initial packet (1) *diminishes* even in the three-dimensional case for any $\alpha < 1$. The minimal value of the function $\tilde{R}_d^{(\alpha)}(\tau)$ (19) with fixed parameters d and α equals

$$\tilde{R}_{d\,\min}^{(\alpha)} = \frac{\sqrt{8d}(1 - \alpha/2)^{1/2-1/\alpha}}{[(\alpha - d)^2 + 2(\alpha + d)]^{1/2-1/\alpha}[(\alpha + d)^2 + 2(\alpha + d)]^{1/\alpha}}. \tag{22}$$

It is attained for

$$\tau_*^2 = \frac{6d - 2\alpha - (\alpha + d)^2}{(\alpha - d)^2 + 2(\alpha + d)}. \tag{23}$$

The numerical values for some special cases are as follows:

α	0.9	0.75	0.5	0.25	0	−0.5	−1
$\tilde{R}^{(\alpha)}_{2\ \min}$	0.9929	0.9808	0.9499	0.9080	0.8576	0.7401	0.6042
$\tilde{R}^{(\alpha)}_{3\ \min}$	0.9989	0.9948	0.9816	0.9617	0.9368	0.8763	0.8046

The case of $\alpha = 0$ is understood in the sense of the limit $\alpha \to 0$ in equations (19) and (22):

$$\tilde{R}^{(0)}_d(\tau) = \sqrt{1+\tau^2}\exp\left[-\frac{4\tau^2}{(1+\tau^2)(d+2)}\right]$$

$$\tilde{R}^{(0)}_{d\ \min} = \sqrt{\frac{8}{2+d}}\exp\left[-\frac{6-d}{2(2+d)}\right] \qquad \tilde{R}^{(0)}_{2\ \min} = \sqrt{2/e}.$$

Diminishing the value of exponent α one can make the minima of $\tilde{R}^{(\alpha)}_d(\tau)$ quite pronounced, especially for α negative. In our opinion, there are no reasons to exclude negative values of α, provided $\alpha > -d$ to ensure the convergence of integrals. For instance, the value $R^{(-1)}_d$ could be called the 'Coulomb radius' of the packet, as soon as it characterizes the electrostatic potential energy in the given state of, e.g., a hydrogen atom. Note that namely the uncertainty relation including the average value of $\langle r^{-1}\rangle$ (and not of $\langle r^2\rangle$ or $\langle r\rangle$) is necessary in order to prove rigorously the existence of finite minimal energy of the hydrogen atom, as was shown by Lieb [20] (see also [18, 19]). Moreover, it is well known that the mean value of radius in the ground state of the hydrogen atom equals $\frac{3}{2}a_B$ (where a_B is Bohr's radius). At the same time, $R^{(-1)}$ equals exactly a_B in this case. The value $R^{(-2)}_d$ (for $d \geqslant 3$) characterizes an effective size of the packet with respect to the centrifugal potential, and uncertainty relations including this quantity have also been studied [15, 16, 18]. Note also that the critical exponent α_c (21) turns into zero for $d = 6$ and becomes negative for $d < 6$.

On the other hand, taking α close to $-d$ one can obtain the value $\tilde{R}^{(\alpha)}_{d\ \min}$ as close to zero as desired. Of course, this does not mean that the effect of shrinking is only a matter of convention. For example, in the case of symmetrical Gaussian packets ($k = 0$) one obtains $\tilde{R}^{(\alpha)}_{d,0}(\tau) = \sqrt{1+\tau^2}$ for any values of d and $\alpha > -d$, so that no measure can make truly expanding packets shrink. But a proper choice of the measure helps to visualize or emphasize the effect when it does exist. For $\alpha \to -d$ the time τ_* (23) (when the value $\tilde{R}^{(\alpha)}_{d\ \min}$ is achieved) tends to $\sqrt{2/d}$, and this is exactly the moment when the function $\left|\psi^{(2)}_d(0;\tau)\right|^2$ (the probability density (8) at the origin) attains its maximum. Obviously, the measures with α close to $-d$ are too sensitive to the behaviour of the wavefunction near the origin, and they practically do not take into account the form of the packet far from the origin (the opposite situation is observed for the mean square radius: it is sensitive to the behaviour of the 'tail' of the packet, but it practically does not feel what happens inside). Therefore, it seems reasonable to use negative values of α which are greater than, say, $1-d$ or perhaps, even -1.

3.1. Mean radius of packets with k arbitrary

One can make some conclusions concerning the initial evolution of the mean radius $\langle r(t)\rangle$ for an arbitrary (radial) packet, calculating the time derivatives of the right-hand side of equation (14) at the initial moment $t = 0$ with the aid of the Schrödinger equation

$$\partial\psi/\partial t = \frac{\mathrm{i}}{2}\Delta\psi = \frac{\mathrm{i}}{2}r^{1-d}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}\psi(r)\right). \qquad (24)$$

Evidently, the first derivative $\mathrm{d}\langle r\rangle/\mathrm{d}t$ equals zero at $t = 0$ for the packet (4). Using equation (24) twice, we obtain after some algebra the following formula:

$$\tilde{R}^{(1)}_{d,k}(\tau) = 1 + \frac{(d-3)(d-1)\tau^2}{2(2k+d-3)(2k+d-1)} + \mathcal{O}(\tau^4). \tag{25}$$

The coefficient at τ^2 is negative for $d = 2$ and $k > 1/2$, and its absolute value decreases with increasing k. Therefore, one could suppose that the packets of the form (4) with $1/2 < k < 2$ exhibit stronger initial shrinking than the packet (1). However, numerical calculations show a very small difference in the fifth digit only. For example, for $k = 1.5$ we have obtained the minimal value of $\tilde{R}^{(1)}_{2,1.5}(\tau)$ to be equal to 0.997 74, whereas the minimal value of $\tilde{R}^{(1)}_{2,2}(\tau)$ equals 0.997 78, but we are not sure that this small difference is not a result of numerical errors.

The coefficient at τ^2 in (25) is also negative for $d > 3$, if one of the two terms in the denominator is negative while the other is positive, for example, for $d = 6$ and $k = -2$ (although $\psi(r)$ diverges at $r = 0$ in this case, there is no divergence in the radial probability density $\chi(r)$). However, this case should be excluded, because formula (25) has sense only for $2k + d - 3 > 0$, otherwise some integrals arising in the course of its derivation become divergent. Actually, in the case of $d = 6$ and $k = -2$ the mean radius can be calculated analytically, because the confluent hypergeometric function is reduced to an elementary function [21]:

$$\Phi(1; 3; z) = 2z^{-2}(\mathrm{e}^z - 1 - z).$$

We find

$$\tilde{R}^{(1)}_{6,-2}(\tau) = (1+\tau^2)^{-1/2}\left[1 - 5\tau^2 + 6\tau^{3/2}\left(\tau + \sqrt{1+\tau^2}\right)^{1/2}\right].$$

Thus the expansion of $\tilde{R}^{(1)}_{6,-2}(\tau)$ begins not with the negative term proportional to τ^2, but with the positive term proportional to $\tau^{3/2}$, and the second derivative with respect to time simply does not exist at $\tau = 0$.

4. 'Entropy-like' measures of packet extensions

An obvious disadvantage of the generalized mean radii is that these measures possess some selectivity with respect to different parts of the packets. Namely, the values of $R^{(\alpha)}_d$ with negative exponent α are more sensitive to the details of the probability density near the origin, whereas the mean radii with $\alpha > 0$ are more sensitive to the behaviour of the probability density 'tail' for large values of r. Different measures of spatial (temporal) extensions of wave packets (signals), which do not give preference to large or small values of coordinates, were introduced by several authors [22–24] (for review see [19]). For example, a family of 'intrinsic volumes' of a quantum system described by the normalized probability distribution $\rho(\mathbf{x}) = |\psi(\mathbf{x})|^2$ (where $\mathbf{x}$ is the d-dimensional position vector) can be defined, following [22], as

$$\mathcal{V}^{(\beta)} = \left(\int [\rho(\mathbf{x})]^\beta\,\mathrm{d}\mathbf{x}\right)^{1/(1-\beta)}. \tag{26}$$

Such quantities were also considered, e.g., in deriving some inequalities characterizing bound states of quantum systems [18, 20]. In the case of a uniform distribution $\rho(x) = V^{-1}$ in some space region (not necessarily single-connected) of the volume V, the definition (26) results in $\mathcal{V}^{(\beta)} \equiv V$ for any β. Of course, the transition from the effective volume to the effective length is not unique, because it depends on the shape of the distribution. However, it seems reasonable simply to extract the root of the dth power from (26). So we define the 'total β-extension' of the symmetrical probability distribution $\rho(r)$ in d dimensions as

$$\mathcal{E}_d^{(\beta)} = \left(\int_0^\infty \omega_d r^{d-1}[\rho(r)]^\beta \, \mathrm{d}r\right)^{1/d(1-\beta)} \tag{27}$$

where the area of the sphere of unit radius in the d-dimensional space ω_d was defined in equation (9). Roughly speaking, in the case of the 'ring-shaped' packets the 'β-measures' characterize the effective width of the ring, whereas the 'α-measures' characterize in some way the effective radius of this ring (for $\alpha > 0$).

Taking the limit $\beta \to 1$ in (26), one arrives at the 'entropic internal volume'

$$\mathcal{V}^{(1)} \equiv \exp(S_{\mathbf{x}}) \qquad S_{\mathbf{x}} = -\int \rho(\mathbf{x}) \ln[\rho(\mathbf{x})] \, \mathrm{d}\mathbf{x}$$

introduced in [23] (see also [25]; there is a vast literature on the 'entropic uncertainty relations' formulated in terms of the 'entropies' such as $S_{\mathbf{x}}$: see, e.g., [26, 27] and reviews [19, 28]). However, we prefer to consider the special case of (27) with $\beta = 2$, due to the simplicity of the calculations:

$$\mathcal{E}_d^{(2)} = \left(\int_0^\infty \omega_d r^{d-1}[\rho(r)]^2 \, \mathrm{d}r\right)^{-1/d}. \tag{28}$$

For the distribution (8) we find

$$\tilde{\mathcal{E}}_d^{(2)} = \left[\frac{(1+\tau^2)^{(d/2+2)}}{1 + b\tau^2 + a\tau^4}\right]^{1/d} \tag{29}$$

where

$$\tilde{\mathcal{E}}_d^{(\beta)}(\tau) \equiv \mathcal{E}_d^{(\beta)}(\tau) \big/ \mathcal{E}_d^{(\beta)}(0) \tag{30}$$

and

$$a = \frac{81d^2 - 54d + 24}{d^2 + 10d + 24} \qquad b = \frac{18d^2 - 44d + 48}{d^2 + 10d + 24}.$$

The Taylor expansion of (29) for small τ yields

$$\tilde{\mathcal{E}}_d^{(2)} = 1 + \frac{d^2 - 22d + 152}{2(d+6)(d+4)}\tau^2 + \cdots.$$

One can check that the coefficient at τ^2 is always positive. Consequently, the function $\tilde{\mathcal{E}}^{(2)}(\tau)$ increases initially for any number of space dimensions. However, it has local minima for $d \leqslant 12$: see figure 8, which shows that the case of $d = 4$ is the best from the point of view of the $\mathcal{E}^{(2)}$-measure.

Another simple expression for the extension arises in the case of $\beta = \infty$, because one can verify that [22]

$$\mathcal{E}_d^{(\infty)} \equiv (\max[\rho(\mathbf{x})])^{-1/d}. \tag{31}$$

The usefulness of this form of extension was shown in the context of other problems (the degree of coherence of partially coherent optical beams and generalizations of uncertainty relations) in [29, 30]. Following [30] we shall call $\mathcal{E}^{(\infty)}$ 'superextension'. For the distribution $\rho(r)$ given by equation (8) the dependence $\tilde{\mathcal{E}}_d^{(\infty)}(\tau)$ can be found analytically. Indeed, one can easily verify that for $\tau > 0$ the function $\rho(r)$ has one maximum at $r = 0$ and another at $r > 1$ (it does not exist for all values of τ). The position of the right maximum can be found by solving a quadratic equation. Therefore, to find $\tilde{\mathcal{E}}_d^{(\infty)}(\tau)$, one should compare two functions:

$$f_0(\tau) = (\tau d e/2)^{-2/d}(1+\tau^2)^{(2+d)/2d} \tag{32}$$

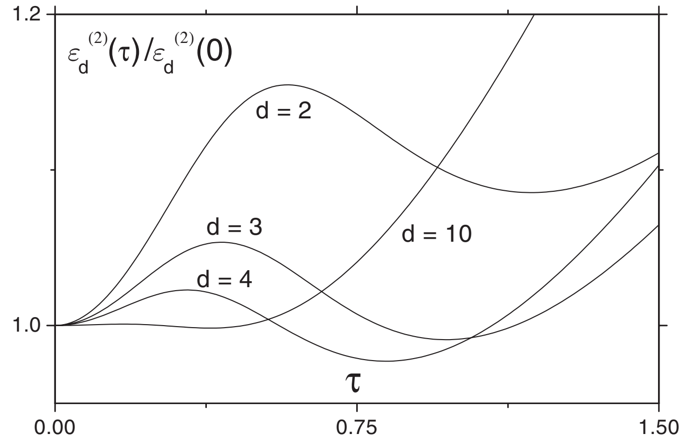

Figure 8. The time dependence of the 'volume' extension $\mathcal{E}_d^{(2)}$ for $k = 2$ and different space dimensions: $d = 2, 3, 4, 10$.

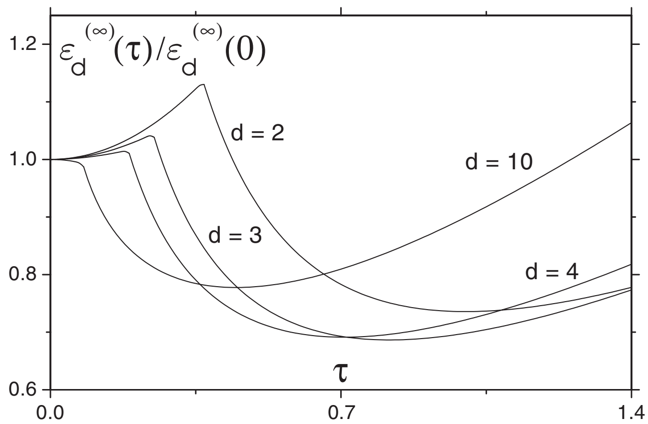

Figure 9. The time dependence of the 'volume' extension $\mathcal{E}_d^{(\infty)}$ for $k = 2$ and different space dimensions: $d = 2, 3, 4, 10$.

and

$$f_1(\tau) = \frac{2^{1/d}\sqrt{1+\tau^2}}{(1+R)^{1/d}} \exp\left[\frac{\tau^2}{1+\tau^2} - \frac{1-R}{d}\right] \qquad R = \left[1 - \frac{\tau^2 d^2}{(1+\tau^2)^2}\right]^{1/2} \tag{33}$$

choosing that one which gives the lower value. For small values of τ, one should use the function (33) (see figures 1 and 3), whereas for larger values of time the function $\tilde{\mathcal{E}}_d^{(\infty)}(\tau)$ is given by formula (32) (see figure 9). Expanding the function $f_1(\tau)$ in power series of τ we obtain

$$\tilde{\mathcal{E}}_d^{(\infty)}(\tau) \approx 1 + \frac{6-d}{4}\tau^2 + \cdots \qquad \tau \ll 1.$$

Consequently, the ring-shaped packets (1) initially increase their superextension $\mathcal{E}_d^{(\infty)}$ in the low-dimensional spaces with $d < 6$, whereas they shrink from the beginning (with respect to this measure of extension) if $d > 6$ (note that the dimension $d = 6$ is distinguished also from the point of view of the critical exponent α_c (21), which becomes negative if $d > 6$). However, even for $d \leqslant 6$ the initial expansion is changed by shrinking after some short interval of time (for large d the switch from f_1 to f_0 happens at $\tau_c \approx 2/(ed)$, and this relation gives a good approximation even for $d = 2$). The minimum of the function $f_0(\tau)$ is achieved at $\tau^2 = 2/d$; thus the minimal value of $\tilde{\mathcal{E}}_d^{(\infty)}$ equals

$$\tilde{\mathcal{E}}_{\min}^{(\infty)}(d) = (de^2/2)^{-1/d}(1 + 2/d)^{(2+d)/2d}. \tag{34}$$

It is less than 1 for any $d \geqslant 2$. In particular, $\tilde{\mathcal{E}}_{\min}^{(\infty)}(2) = 2/e$. Moreover, the table below shows that three-dimensional packets exhibit more strong shrinking than two-dimensional ones, according to the $\mathcal{E}^{(\infty)}$-measure:

d	2	3	4	6	10	20	100	1000
$\tilde{\mathcal{E}}_{\min}^{(\infty)}$	0.7358	0.6866	0.6915	0.7226	0.7776	0.8499	0.9522	0.9926

For $\tau \gg 1$ the $\tilde{\mathcal{E}}^{(\infty)}$-extension grows as $\tilde{\mathcal{E}}_d^{(\infty)}(\tau) \approx \tau(ed/2)^{-2/d}$.

For symmetrical radial packets one can also define the 'radial extensions' as

$$\mathcal{F}_d^{(\beta)} = \left(\int_0^\infty [\chi(r)]^\beta \,\mathrm{d}r\right)^{1/(1-\beta)} = \left(\int_0^\infty r^{\beta(d-1)}[\omega_d\rho(r)]^\beta \,\mathrm{d}r\right)^{1/(1-\beta)} \tag{35}$$

where $\chi(r)$ is the radial probability density introduced in (9). In particular,

$$\mathcal{F}_d^{(2)} = \omega_d^{-2}\left[\int_0^\infty r^{2(d-1)}|\psi_d(r)|^4 \,\mathrm{d}r\right]^{-1} \tag{36}$$

$$\mathcal{F}_d^{(\infty)} = (\max[\chi_d(r)])^{-1} \equiv \omega_d^{-1}(\max[r^{d-1}\rho(r)])^{-1}. \tag{37}$$

In the case of $\beta = 2$ and probability density (8) we now obtain, instead of (29), the following expression for the normalized radial extension (defined in the same way as in equation (30)):

$$\tilde{\mathcal{F}}_d^{(2)} = \frac{C(1+\tau^2)^{5/2}}{A\tau^4 + B\tau^2 + C} \tag{38}$$

where

$$A = 16d^4 + 128d^3 - 8d^2 + 32d - 15$$
$$B = 2(16d^4 - 32d^3 + 56d^2 + 8d - 15)$$
$$C = 16d^4 + 64d^3 + 56d^2 - 16d - 15.$$

Since $B/C < 2$, the function $\tilde{\mathcal{F}}_d^{(2)}(\tau)$ increases with τ for any d if $\tau \ll 1$. Moreover, making plots (which are not given here, because they show nothing interesting) one can see that this function never becomes less than 1 for any values of τ and d, as well as the function $\tilde{\mathcal{F}}_d^{(\infty)}(\tau)$.

4.1. Packets with k arbitrary

The superextension $\mathcal{E}^{(\infty)}$ permits us to analyse the evolution of packets having initially the form (4) with arbitrary values of parameter k. As we have seen for $k = 2$, the behaviour of the function $\mathcal{E}^{(\infty)}(\tau)$ for not very small values of τ is determined by the time dependence of the volume probability density $|\psi(r,\tau)|^2$ at the origin. The initial probability density has maximum at $r = \sqrt{k/2}$; therefore, the initial extension equals

$$\mathcal{E}_{d,k}^{(\infty)}(0) = \sqrt{\frac{\pi}{2}}\left[\frac{\mathrm{e}^k\Gamma(k+d/2)}{k^k\Gamma(d/2)}\right]^{1/d}. \tag{39}$$

Using Stirling's formula, one can check that the initial extension slowly increases as a function of k for $k \gg d$: $\mathcal{E}_{d,k}^{(\infty)}(0) \sim k^{(d-1)/2d}$. Taking the value of $|\psi(0,\tau)|^2$ from equation (5), we obtain the function

$$\mathcal{G}_{d,k}(\tau) = (2e\tau/k)^{-k/d}(1+\tau^2)^{(k+d)/2d}\left[\frac{\Gamma(d/2)}{\Gamma([d+k]/2)}\right]^{2/d} \tag{40}$$

which gives an upper bound for the relative extension $\tilde{\mathcal{E}}_{d,k}^{(\infty)}(\tau)$. This bound is obviously bad for $\tau \to 0$, but as soon as we are interested in the *minimal* value of the $\mathcal{E}^{(\infty)}$-extension, replacing the function $\tilde{\mathcal{E}}^{(\infty)}(\tau)$ by $\mathcal{G}(\tau)$ results in good (probably exact) evaluation. The minimum of function (40) is achieved for $\tau = \sqrt{k/d}$ (this formula explains the choice of moments $\tau = 1, \sqrt{2/3}$ and $\sqrt{10}$ in figures 1, 3 and 5):

$$\mathcal{G}_{\min}(d,k) = \sqrt{\frac{d+k}{d}}\left[\frac{k(d+k)}{4e^2}\right]^{k/2d}\left[\frac{\Gamma(d/2)}{\Gamma([d+k]/2)}\right]^{2/d}. \tag{41}$$

If $k = 2$, then (41) coincides with (34). For $d \gg 1$ we can replace the Gamma functions by their Stirling representations and simplify (41) as

$$\mathcal{G}_{\min}(d,k) \approx \left(\frac{k}{d+k}\right)^{k/2d}\left(\frac{d+k}{d}\right)^{1/d-1/2}. \tag{42}$$

In particular, if $d \gg k$, then $\mathcal{G}_{\min}(d,k) \approx (ed/k)^{-k/2d}$. If $k \gg d$, then formula (42) gives

$$\mathcal{G}_{\min}(d,k) \approx \mathrm{e}^{-1/2}(k/d)^{1/d-1/2}. \tag{43}$$

Consequently, it is possible to achieve arbitrarily large shrinking choosing the packets with $k \gg d > 2$. In this sense, the case of two dimensions is the worst, because formula (41) for $d = 2$ reads

$$\mathcal{G}_{\min}(2,k) = \sqrt{1+k/2}\,[k/2(1+k/2)]^{k/4}\,\mathrm{e}^{-k/2}[\Gamma(1+k/2)]^{-1} \tag{44}$$

so that for $k \to \infty$ it goes to the constant limit $\sqrt{e/(2\pi)} \approx 0.66$ (which is a little bit smaller than the value of $\tilde{\mathcal{E}}_{\min}^{(\infty)}(2,2)$). On the other hand, the asymptotical form of (41) for $d = 3$ and $k \gg 1$ reads

$$\mathcal{G}_{\min}(3,k) = \sqrt{e/3}(4k)^{-1/6} \tag{45}$$

which differs from (43) only in the numerical coefficient. It is worth noting that as soon as the evolution of the probability density of the *Gaussian* packet ($k = 0$) is reduced to the *uniform* scale transformation $r \to r/\sqrt{1+\tau^2}$, *all* measures give the same result in this specific case: the normalized extension increases as $\sqrt{1+\tau^2}$.

5. Conclusion

We have demonstrated that initial 'ring-shaped' radial packets can exhibit significant 'shrinking' at the initial stages of their free evolution. The degree of shrinking essentially depends on the chosen measure of the packet extension and the kind of probability density ('volume' or 'radial') used for the evaluation, because different regions of the 'ring' can move initially in different directions, and some measures are more sensitive to the structure of the 'internal' regions, while the others are more sensitive to the probability distribution of the 'external' parts. The case of two space dimensions is not distinguished from the point of view of measures different from the mean value of the radius. We have found the examples of measures for which the distinguished dimensions are $d = 3, 4$ or 6. Moreover, choosing suitable combinations of the parameters k and d characterizing the initial packets and the parameters α and β of the measures of packet extension one can obtain the minimal value of the normalized time-dependent extension as small as desired. However, asymptotically, as $\tau \to \infty$, all packets 'forget' their initial forms and spread almost as usual symmetrical Gaussian packets (although some faint remnants of the initial ring remain forever). The problem of shrinking packets in one dimension was considered recently in [8].

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