Is the Spreading of Quantum Mechanical Wave Packets Indeed Inevitable?

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Abstract

It is demonstrated that – contrary to the common belief – it is possible to construct solutions of the non-relativistic Schrödinger equation of a free particle, that do not exhibit dispersion. However, it seems that no normalizable wave packets can be built up by their use, so the spreading of the wave packets is indeed inevitable.

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1. Introduction

It is usually considered that the limiting transition from the quantum mechanical description to the classical mechanical one is not as straightforward as is the transition from the mechanics of the special theory of relativity to the classical mechanics. In fact, Ehrenfest theorem stating that the center of a wave packet moves according to Newton’s laws could be sufficient to follow a smooth transition from quantum mechanics to the classical one as \( \hbar \to 0 \), but the picture is spoiled by the observation that quantum mechanical wave packets are spreading in the time until they fill the whole space. This is the case because it is usually considered that the solutions of the Schrödinger equations of a free (unbounded) particle always exhibit dispersion: the phase speed of a de Broglie wave differs from the velocity of the particle it describes.

It is to be mentioned that non-spreading solutions have been described in the literature, but not for free particles. Thus, such solutions are possible if there is also an external potential. The well-known example is a Gaussian wave packet in the potential well of a harmonic oscillator, but also non-spreading wave-packets have been considered in the field of a microwave source, etc. [2–4]. Non-spreading wave packets can be constructed also by adding a non-linear term to the Schrödinger equation [5].

A special word is appropriate about the one-dimensional case. Berry and Balazs [6] showed that there is a sort of “Airy-packets” that is a solution of the Schrödinger equation of a free particle and moves without spreading—however, it is accelerating in a manner as if there were a constant external potential. Later the uniqueness of this solution was also proved [7], which means that (except, of course, the standart infinite sinusoidal waves) these accelerating Airy packets are the only possible solutions for an one-dimensional Shrödinger equation for a free particle that move without change of shape. Admitting three dimensions, however, some additional mathematical freedom appears, too.

From the reasons mentioned above, it seems to be of interest to check whether the wave packets moving with a constant speed in the three-dimensional free space are indeed inevitably spreading out in the time. For that reason one has to consider the most general wave packets that are non-spreading by construction. It will be seen that by using cylindrical coordinates one can, indeed, construct solutions of the non-relativistic Schrödinger equation of a free particle that do not exhibit dispersion, but there appears an unsurmountable normalization problem that prevents them to be used to build up physically meaningful wave packets.
2. Cylindrical waves without dispersion

Let us consider a free particle moving with the velocity $v$ along the positive direction of the axis $z$ of a cylindrical system of coordinates $z, r, \phi$. We shall search the wave function in the form

$$\Psi = R(r)f(z - vt)$$

(1)

This means that for sake of simplicity we shall assume the wave function $\Psi$ to be independent of coordinate $\phi$, so $\partial \Psi / \partial \phi = 0$. (Admitting a $\phi$-dependence would not be significant from our point of view; it has also been shown that solutions with $\phi$-dependence can always be generated from the $\phi$-independent ones in a trivial manner [8].)

Obviously, any function of form (1) represents a “wave” moving with the phase-velocity $v$ in the positive direction of the axis $z$. This function $\Psi$ is required to be a solution of the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$$

(2)

As we are dealing with a free particle, the Hamiltonian is simply

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta$$

(3)

where $m$ is the mass of the particle. Using the expression of the Laplacian in the cylindrical coordinates selected, and taking into account that $\Psi$ is independent of the angle $\varphi$, we get

$$i\hbar R \frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m} \left[ R \frac{\partial^2 f}{\partial z^2} + f \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial R}{\partial r} \right) \right]$$

(4)

By performing a standard separation of variables, and taking into account that $f$ depends on $z$ and $t$ only through their combination $z - vt$, we get the coupled system of ordinary differential equations

$$f'' - i \frac{2nv}{\hbar} f' - qf = 0$$

$$\frac{1}{r} \frac{d}{dr} \left( r \frac{dR}{dr} \right) + qR = 0$$

(5)

where $q$ is an arbitrary constant. (Also see below.)

The general solution of the system (5) is, as easy to see,

$$f(u) = C_1 \exp \left[ \frac{1}{\hbar} \left( inv + \sqrt{q\hbar^2 - m^2v^2} \right) u \right]$$

$$+ C_2 \exp \left[ \frac{1}{\hbar} \left( inv - \sqrt{q\hbar^2 - m^2v^2} \right) u \right]$$

(6)
where we have introduced the notation

\[ u = z - vt \]  

(7)

and

\[ R(r) = C_3 J_0(\sqrt{q} r) + C_4 Y_0(\sqrt{q} r) \]  

(8)

where \( J_0 \) and \( Y_0 \) are the standard cylindrical (Bessel) functions.

The solutions obtained remain finite everywhere if one requires

\[ 0 \leq q \leq \frac{m^2 v^2}{\hbar^2} \]  

(9)

and sets

\[ C_4 = 0 \]  

(10)

In the special case of selecting \( q = 0 \) one has for \( R(r) \) the special solution

\[ R(r)|_{q=0} = C_3 + C_4 \ln(r) \]  

(11)

which again remains finite only if \( C_4 = 0 \). However, in this case we have simply \( R(r) = \text{Const} \) and we recover the special case of the plane wave which is constant in the directions orthogonal to \( z \). In that case

\[ f(u) = C_1 + C_2 \exp \left( \frac{2mv}{\hbar} u \right) \]  

(12)

thus – disregarding the constant part, i.e., by setting \( C_1 = 0 \) – we get a standard exponential plane wave for which the phase velocity is half of the group velocity \(^1\) which equals the conventional velocity of the particle.

Independently of the value of the parameters \( q \) and \( C_i \), all these solutions for the Schrödinger equation of the free particle are simply shifted by the same distance \( vt \) along the positive axis \( z \) after the period of time \( t \), as they depend only on the combination \( u = z - vt \) but not on \( z \) and \( t \) separately. That means that these functions do not exhibit dispersion and any their linear combinations conserve their forms, only are shifted in the space as time passes. Therefore the wave packets formed as linear combinations of these functions

\[ \Psi(z, r, t) = \int_{0}^{q_{\text{max}}} \left\{ A(q) \exp \left[ \frac{i}{\hbar} \left( mv + \sqrt{m^2 v^2 - q \hbar^2} \right) (z - vt) \right] + B(q) \exp \left[ \frac{i}{\hbar} \left( mv - \sqrt{m^2 v^2 - q \hbar^2} \right) (z - vt) \right] \right\} J_0(\sqrt{q} r) dq \]  

(13)

\(^1\)At the beginning we have selected the phase velocity to be equal \( v \), therefore Eq. (12) describes a de Broglie wave corresponding to the conventional velocity \( 2v \).
where \( q_{\text{max}} = (mv/\hbar)^2 \) and \( A(q), B(q) \) are arbitrary functions, do not spread out in the space, as consist of components having the same phase velocity \( v \). That is the fundamental difference with respect to the “usual” wave packets formed of the plane waves, the different components of which always have different phase velocities, and therefore are inevitably spreading out.

However, these wave packets are clearly not normalizable. Even the first inspection shows that the components corresponding to a given \( q \) do not decay to zero as variable \( z \) tends to \( \pm \infty \). It is clear that one simply cannot select the functions \( A(q) \) and \( B(q) \) as to provide a thorough cancellation of the terms at infinite intervals. In full accord with this, by utilizing the closure-relation of Bessel functions,

\[
\int_0^\infty x J_\alpha(ux) J_\alpha(vx) \, dx = \frac{1}{u} \delta(u-v), \quad \alpha > -\frac{1}{2};
\]

one obtains for the normalization integral of the wave function (13), calculated for \( t=0 \) (or any fixed value of \( t \)), the expression

\[
\langle \Psi | \Psi \rangle \big|_{t=0} = 2\pi \int_{-\infty}^{\infty} dz \int_0^{q_{\text{max}}} \left\{ |A(q)|^2 + |B(q)|^2 + 2 \text{Re} \left[ A(q) B^*(q) e^{i \left( \frac{2zi}{\hbar} \sqrt{m^2v^2 - q^2\hbar^2} \right)} \right] \right\} \frac{dq}{q}
\]

This is an integral over an infinite interval with a non-negative integrand: the oscillating third terms of the integrand cannot overcompensate the positive first two – at most, if \( |A(q)| = |B(q)| \), it can just compensate them in individual points. Therefore the normalization integral diverges.

### 3. Conclusions

It is demonstrated that using cylindrical coordinates one can form wave packets out of different functions all of which have the same phase velocity and all of them are solutions of the non-relativistic Schrödinger equations of a free particle. Such wave packets do not spread out—but are not normalizable. Therefore the spreading of the physically relevant normalizable wave packets is indeed inevitable.

\[ \text{[2]} \quad \text{That can be seen by subtracting and adding } 2|A(q)||B(q)|. \text{ Then the first two terms of the integrand give } (|A(q)| - |B(q)|)^2 \text{ while the second becomes } |A(q)||B(q)|2\text{Re} \left\{ 1 + e^{i \left( [\psi_A(q) - \psi_B(q)] + \frac{m^2v^2 - q^2\hbar^2}{\hbar^2} \right)} \right\}, \text{ neither of which can be negative. [Here } \psi_A(q) \text{ and } \psi_B(q) \text{ are the phases of } A(q) \text{ and } B(q), \text{ respectively.] } \]

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