What is the limit $\hbar \to 0$ of quantum theory ?

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Abstract

An analysis is made of the relation between quantum theory and classical mechanics, in the context of the limit $\hbar \to 0$. Several ways in which this limit may be performed are considered. It is shown that Schrödinger's equation for a single particle moving in an external potential V does not, except for special cases, lead, in this limit, to Newtons equation of motion for the particle. This shows that classical mechanics cannot be regarded as the limiting case of quantum mechanics for $\hbar \to 0$.

1 Introduction

In Dirac's famous book [6] on quantum theory one finds the statement: "*...classical mechanics may be regarded as the limiting case of quantum mechanics when $\hbar$ tends to zero*". A bright student, having read this statement might ask his teacher the following question: "In quantum mechanics a single particle in an external potential is described by Schrödinger's equation

$$\left[\frac{\hbar}{\imath}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\sum_{k=1}^{3}\left(\frac{\partial}{\partial x_k}\right)^2 + V(x,t)\right]\psi(x,t) = 0. \tag{1}$$

If Dirac is right then Newton's equation,

$$\frac{\mathrm{d}}{\mathrm{d}t} m r_k(t) = p_k(t), \qquad \frac{\mathrm{d}}{\mathrm{d}t} p_k(t) = -\frac{\partial V(x,t)}{\partial x_k}\Big|_{x=r(t)}. \tag{2}$$

should follow from Schrödinger's equation in the limit $\hbar \to 0$. Can you tell us, how this calculation is actually performed ? " Nobody has ever performed a general exact calculation showing that (1) implies (2) in the limit $\hbar \to 0$. An experienced teacher will nevertheless find an answer to this question. We will not discuss the variety of his possible responses but think that these will probably not include one of the following two statements: (i) Dirac is wrong, (ii) the answer is not known. A typical response is the statement that this limit cannot be understood in such a simple way. A closer look in Dirac's book shows, however, that, at least as Dirac's original intentions are concerned, this statement should in fact be interpreted in this simple way.

The attitude of the scientific community with regard to this point - which is extremely important for the interpretation of quantum theory (QT) as well as for more general questions such as the problem of reductionism - is somewhat schizophrenic. On the one hand, Dirac's dictum - which has been approved by other great physicists - is considered to be true. On the other hand it cannot be verified. Since the beginnings of QT a never ending series of works deal with this question, but the deterministic limit of QT, in the sense of the above *general* statement, has never been attained. Frequently, isolated 'classical properties' which indicate asymptotic 'nearness' of deterministic physics, or structural similarities (such as those between Poisson brackets and commutators) are considered as a substitute for the limit. The point is that in most of these papers (see e.g. [22],[28],[1] to mention only a few) the question "what is the limit $\hbar \to 0$ of quantum theory ?" is *not* studied. It is taken for granted that the final answer to this question has already been given (by Dirac and others) and the remaining problem is just how to confirm, or illustrate it by concrete calculations. But none of these attempts is satisfying.

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In the present paper the question formulated in the title will be studied without knowing the answer. A detailed step-by-step style of exposition has been chosen in order to understand this singular limit. In fact, the paper has been written with the idea in mind to provide an in-depth answer to a student's question concerning the mathematical details of the transition from (1) to (2). The questions how to perform a limit and how to characterize the relations between different (related) physical theories are closely connected to the basic question how to characterize physical theories themselves. We take a pragmatic position with respect to this question and characterize a physical theory simply by the set of its *predictions*. It turns out that this leads automatically to a reasonable definition of limit relations between different physical theories. We start by discussing, in section 2, two well-understood concrete limiting relations between two pairs of classical physical theories. These classical limiting relations, referred to as 'standard limit' and 'deterministic limit', define possible meanings of the term "the limit $\hbar \to 0$" in QT. In section 3 we use the variables introduced by Madelung to obtain the 'standard limit' of QT, previously found by Rosen [21], Schiller [23] and others. In section 4 we derive the deterministic limit of the 'standard limit' of QT. We find that Ehrenfest's relations, which have not been taken into account in previous treatments [21, 3, 15, 20, 9], provide the missing link between the 'standard limit' (field) theory and the trajectory equations of Newtonian mechanics (NM). In section 5 we investigate the 'deterministic limit' of QT and conclude that this limit does not exist. In section 6 we try to reconstruct the states of NM from QT by *combining* the 'deterministic limit' and the 'standard limit'. In this way we are indeed able to identify a class of (three) potentials and states which allow for a transition from QT to NM in the limit $\hbar \to 0$; these include among others the coherent states of the harmonic oscillator [24]. In section 7 we try to extend this process to arbitrary potentials. The obtained results are discussed and interpreted in section 8 and the final conclusion is drawn in section 9.

2 Two examples for limit relations in classical physics

As our first example we consider the relation between relativistic mechanics and NM. As is well-known, in relativistic mechanics a new fundamental constant, the speed of light c, appears, which is absent (infinitely large) in NM. Otherwise, the mathematical structures of both theories are similar. The basic equations of relativistic mechanics differ from (2) only by factors γ, which depend on v/c and disappear (reduce to 1) if c becomes large,

$$\gamma = \sqrt{1 - \frac{v^2}{c^2}}, \qquad \lim_{c \to \infty} \gamma = 1. \tag{3}$$

The relation between relativistic mechanics and NM may be summarized as follows:

- Both theories have the same mathematical structure: ordinary differential equations for trajectories. A new fundamental constant c appears in relativistic mechanics.
- The limit $1/c \to 0$ transforms the basic equations of relativistic mechanics in the basic equations of NM; the same is true for the solutions of relativistic mechanics and NM respectively.

We see that relativistic mechanics and NM provide a perfect realization of a limit relation (NM is the limit theory of relativistic mechanics) or a covering relation (relativistic mechanics is the covering theory of NM), respectively. The significant feature is the appearance of a new fundamental constant which allows for a transition between two different theories of the same mathematical type. We will refer to the type of limit relation encountered in this first example as 'standard limit' relation.

Our second example concerns the relation between NM and a probabilistic version of NM, which can be constructed according to the following well-known recipe. We consider a phase space probability density $\rho(x, p, t)$ and assume that the total differential of ρ vanishes,

$$\mathrm{d}\rho(x, p, t) = \frac{\partial \rho}{\partial x_k} \mathrm{d}x_k + \frac{\partial \rho}{\partial p_k} \mathrm{d}p_k + \frac{\partial \rho}{\partial t} \mathrm{d}t = 0. \tag{4}$$

This means that ρ is assumed to be constant along arbitrary infinitesimal changes of x_k, p_k, t. Next we postulate that the movement in phase space follows classical mechanics, i.e. we set $\mathrm{d}x_k = (p_k/m)\mathrm{d}t$ and $\mathrm{d}p_k = -(\partial V/\partial x_k)\mathrm{d}t$. This leads to the partial differential equation (Liouville equation)

$$\frac{\partial \rho}{\partial t} + \frac{p_k}{m} \frac{\partial \rho}{\partial x_k} - \frac{\partial V}{\partial x_k} \frac{\partial \rho}{\partial p_k} = 0, \tag{5}$$

which has to be solved by choosing initial values $\rho(x, p, 0)$ for the new dynamical variable $\rho(x, p, t)$. The relation between the probabilistic version (of NM) and NM may be summarized as follows:

- The probabilistic version and NM have a different mathematical structure; the probabilistic version is ruled by a partial differential equation, NM by an ordinary differential equation. No new constant appears in the probabilistic version.

- The probabilistic version and NM belong to fundamentally different epistemological categories. NM is a deterministic theory. The probabilistic version is a probabilistic (indeterministic) theory; predictions about individual events cannot be made because the initial values for individual particles are unknown.

The absence of a new fundamental constant prevents a simple transition between the two theories as found in our first example. Nevertheless, a kind of limit relation can be established by means of appropriate (singular) *initial values.* A probability density which is sharply peaked at $t = 0$ retains its shape at later times. Inserting the Ansatz

$$\rho(x, p, t) = \delta^{(3)}(x - r(t))\delta^{(3)}(p - p(t)), \tag{6}$$

into Eq. (5), it is easily shown that admissible particle trajectories $r_k(t)$, $p_k(t)$ are just given by the solutions of Newton's equations (2). Thus, NM can be considered as a limit theory of the probabilistic version in the sense that the manifold of solutions of a properly (with regard to singular initial values) generalized version of the probabilistic version leads to NM. This limit relation is 'weaker' than the one encountered in our first example, because there is no mapping of individual solutions. By allowing for singular solutions we have essentially constructed the *union* of the deterministic theory NM and the original probabilistic version of NM; it is then no surprise that the generalized probabilistic version theory contains NM as a special case. Considered from a formal point of view, however, the (generalized) probabilistic version is a perfect covering theory since its manifold of solutions is larger than that of NM. We shall refer to the kind of limit relation found in this second example as a 'deterministic' limit relation.

3 The 'standard limit' of quantum theory

Let us now compare QT and NM [Eqs. (1) and (2)] in the light of the above examples. Both theories differ obviously with respect to their mathematical structure; this indicates the possibility to obtain NM from QT by means of a 'deterministic' limiting process. However, in addition, a new fundamental constant (the number $\hbar$) appears in QT; this indicates the possibility to obtain NM from QT by means of a 'standard' limiting process. This shows that the limiting process which leads from QT to NM is either nonexistent or more complex than any one of the above examples.

Let us try, as a first step, to perform the 'standard limit' of QT - as defined by the first example in section 2. Performing the limit $\hbar \to 0$ in Eq. (1) produces a nonsensical result. This indicates that the real and imaginary parts of ψ are not appropriate variables with regard to this limiting process; probably because they become singular in the limit $\hbar \to 0$. Thus, a different set of dynamical variables should be chosen, which behaves regular in this limit. There is convincing evidence, from various physical contexts, that appropriate variables, denoted by ρ and S, are defined by the transformation

$$\psi = \sqrt{\rho}\, \mathrm{e}^{\imath \frac{S}{\hbar}}. \tag{7}$$

This transformation has been introduced by Madelung [19]. Note that using these variables in a meaningful limiting process requires that the modulus of ψ remains regular while its phase diverges like $\hbar^{-1}$ for small $\hbar$. This singular behavior, which has been noted very early [27], is the behavior of the majority of 'well-behaved' quantum states. Other, more singular, states may, however, behave in a different manner and will then require a different factorization in terms of $\hbar$. This may also lead to different equations in the limit $\hbar \to 0$; an example will be given in section 6.

In terms of the new variables Schrödinger's equation takes the form of two coupled nonlinear differential equations. The first is a continuity equation which does not contain $\hbar$,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} \frac{\rho}{m} \frac{\partial S}{\partial x_k} = 0. \tag{8}$$

The second equation contains $\hbar$ as a proportionality factor in front of a single term,

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \sum_k \left(\frac{\partial S}{\partial x_k} \right)^2 + V - \frac{\hbar^2}{2m} \frac{\triangle \sqrt{\rho}}{\sqrt{\rho}} = 0. \tag{9}$$

Eq. (9) is referred to as quantum Hamilton-Jacobi equation (QHJ). The $\hbar$-dependent 'quantum term' in (9) describes the influence of ρ on S (It is frequently denoted as "quantum potential", which is an extremely misleading nomenclature because a potential is, as a rule, an externally controlled quantity). Its physical meaning, as interpreted by the present author, has been discussed in more detail elsewhere [12].

In the limit $\hbar \to 0$ the quantum term disappears. Thus the 'standard limit' of QT is given by two partial differential equations, the continuity equation (8), which depends on ρ and S, and the Hamilton-Jacobi (HJ) equation,

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \sum_k \left(\frac{\partial S}{\partial x_k} \right)^2 + V = 0, \tag{10}$$

which depends only on S. The two equations (8) and (10) which will be referred to as probabilistic Hamilton-Jacobi theory (PHJ) constitute the classical limit of Schrödinger's equation or 'single-particle' QT, respectively. Clearly, this limit does not agree with the trajectory equations (2) of NM.

Much confusion has been created by the fact, that the Hamilton-Jacobi formulation of classical mechanics allows the determination of particle trajectories with the help of the HJ equation. From the fact that this equation can be obtained from QT in the limit $\hbar \to 0$ it is often concluded, neglecting the continuity equation, that classical mechanics is the $\hbar \to 0$ limit of QT. However, the limit $\hbar \to 0$ of QT does not provide us with the theory of canonical transformations, which is required to actually calculate particle trajectories. Note also that for exactly those quantum-mechanical states which are most similar to classical states (e.g. coherent states, see section 6) the classical limit of QHJ *differs* from HJ. There *is* in fact a connection between the PHJ and NM but this requires a second limiting process, as will be explained in section 4.

Both the PHJ and its (standard) covering theory QT are probabilistic theories, which provide statistical predictions (probabilities and expectation values) if initial values for S and ρ are specified. Although we have now partial differential equations, the relation between QT and PHJ resembles in essential aspects the relation between relativistic mechanics and NM.

4 The 'deterministic limit' of the 'standard limit' of quantum theory

The deterministic limit of the classical-limit PHJ of QT is of considerable interest for the present problem, despite the fact that the PHJ does no longer contain $\hbar$. Existence of a deterministic limit implies that $\rho(x,t)$ takes the form of a delta-function peaked at trajectory coordinates $r_k(t)$ [which, hopefully, should then be solutions of the classical equations (2)]. Thus, adopting a standard formula, we may write $\rho(x,t)$ as an analytic function

$$\rho_\epsilon(x,t) = \left(\frac{1}{\pi\epsilon} \right)^{\frac{3}{2}} \exp\left\{ -\frac{1}{\epsilon} \sum_{k=1}^{3} \left[x_k - r_k(t) \right]^2 \right\}, \tag{11}$$

which represents $\delta^{(3)}(x - r(t))$ under the integral sign in the limit $\epsilon \to 0$,

$$\lim_{\epsilon \to 0} \rho_\epsilon(x,t) = \delta^{(3)}(x - r(t)). \tag{12}$$

In order to check whether or not this deterministic representation of $\rho(x,t)$ is compatible with the basic equations of PHJ, we insert the Ansatz (11) into the continuity equation (8) and calculate the derivatives. After some rearrangement (8) takes the form [20]

$$\rho_\epsilon(x,t) \left\{ [x_k - r_k(t)] \left(p_k(t) - \frac{\partial S(x,t)}{\partial x_k} \right) + \frac{\epsilon}{2} \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_k} S \right\} = 0, \tag{13}$$

where $p_k(t) = m\dot{v}_k(t)$. At this point we recall that in the PHJ a momentum field $p_k(x,t)$, defined by

$$p_k(x,t) = \frac{\partial S(x,t)}{\partial x_k}, \tag{14}$$

exists. The trajectory momentum $p_k(t)$ should be clearly distinguished from this field momentum $p_k(x,t)$.

In the limit $\epsilon \to 0$, ρ_ϵ becomes a distribution and both sides of Eq. (13) have to be integrated over three-dimensional space in order to obtain a mathematically well-defined expression. The first term in the bracket vanishes as a consequence of the term $x_k - r_k(t)$ (at this point we start to disagree with

Ref [20]). The second term vanishes too for $\epsilon \to 0$ provided the second derivative of S is regular at $\epsilon = 0$. But this can safely be assumed since the equation for S does not contain ρ. We conclude that the singular (deterministic) Ansatz (11) is a valid solution of PHJ for arbitrary S.

The present theory is incomplete since differential equations for the particle trajectories $r_k(t)$ have still to be found. Generally, two conditions must be fulfilled in order to define particle coordinates in a probabilistic theory, namely (i) the limit of 'sharp' (deterministic) probability distributions must be a valid solution, and (ii) an evolution law for the time-dependent expectation values must exist. We have just shown that the first (more critical) condition is fulfilled; Ehrenfest-like relations corresponding to the second condition exist in almost all statistical theories. For the PHJ these take exactly the same form as in QT, namely [16, 13]

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{x_k} = \frac{\overline{p_k}}{m} \tag{15}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p_k} = -\overline{\frac{\partial V(x,t)}{\partial x_k}}, \tag{16}$$

where average values such as $\overline{x_k}$ are defined according to the standard expression

$$\overline{x_k}(t) = \int \mathrm{d}^3x\, \rho(x,t)\, x_k. \tag{17}$$

From (15) and the continuity equation (8) we obtain the following useful relation

$$\overline{p_k}(t) = \int \mathrm{d}^3x\, \rho(x,t)\, \frac{\partial S(x,t)}{\partial x_k}. \tag{18}$$

Since we have shown that the deterministic limit for ρ is a valid solution of PHJ, we may now use Eq. (12) and obtain in the limit $\epsilon \to 0$ the following identification of trajectory quantities,

$$\overline{x_k}(t) = r_k(t), \qquad \overline{p_k}(t) = m\dot{r}_k(t) = p_k(t), \tag{19}$$

from the definitions of the expectation values. The differential relations connecting these quantities, follow from Ehrenfest's theorem and agree with the basic equations (2) of NM. A completely different type of physical law has 'emerged' from the field theoretic relations of the PHJ theory. Thus, classical mechanics is, indeed, contained in PHJ as deterministic limit, in analogy to the second example of section 2.

Eq. (18) takes in this limit the form

$$p_k(t) = \frac{\partial S(x,t)}{\partial x_k}\Big|_{x=r(t)} = \frac{\partial S(r(t),t)}{\partial r_k(t)}, \tag{20}$$

which provides an interesting *link* between a particle-variable and a field-variable. We expect for consistency that this link admits a derivation of the equation for $\dot{p}$ [see (2)] from the (field-theoretic) HJ-equation. This is indeed the case. We calculate the derivative of the HJ equation (10) with respect to x_i, change the order of derivations with respect to x_i and t, and project the resulting relation on the trajectory points $x_k = r_k(t)$. This leads to the equation

$$\frac{\partial}{\partial t}\Big|_{2.} \frac{\partial S(r(t),t)}{\partial r_i(t)} + \frac{1}{m}\frac{\partial S(r(t),t)}{\partial r_k(t)}\frac{\partial^2 S(r(t),t)}{\partial r_i(t)\partial r_k(t)} + \frac{\partial V(r(t),t)}{\partial r_i(t)} = 0, \tag{21}$$

where the notation indicates that the time derivative operates on the second argument of S only. Using now Eq. (20) and the definition of particle momentum we see that the first two terms of (21) agree exactly with the (total) time-derivative of $p_i(t)$ and (21) becomes the second Newton equation. This establishes the connection between the PHJ equations and trajectory differential equations mentioned in section 3 and completes our treatment of the deterministic limit of the PHJ theory. This derivation of NM seems to be new; it is based on several interesting papers [21, 3, 15, 20, 9] reporting important steps in the right direction.

5 The 'deterministic limit' of quantum theory

In QT, the coupling term in QHJ [see (9)] prevents a deterministic limit of the kind found for the PHJ. To see this, we start from the assumption that a quantum mechanical system exists which admits a solution of the form (11) for arbitrary t. Inserting (11) into (8),(9) leads to two equations. The first is the continuity equation which takes the same form (13) as before. The second is the QHJ, which takes the form

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\sum_k \left(\frac{\partial S}{\partial x_k}\right)^2 + V + \frac{1}{2m}\left(\frac{\hbar}{\epsilon}\right)^2 \left\{3\epsilon - \sum_{k=1}^{3}\left[x_k - r_k(t)\right]^2\right\} = 0. \tag{22}$$

Eq. (22) shows that the coupling term diverges (for finite $\hbar$) in the limit $\epsilon \to 0$. Consequently, there is no reason to expect, that the second derivative of S with respect to x_k [see Eq. (13)] is regular at $\epsilon \to 0$ and that a delta-function-like $\rho(x,t)$, as given by Eq. (11), can be a solution of (8), (9). Thus, the deterministic limit of QT (if it exists) cannot be obtained in the same way as in the PHJ.

We next consider several concrete solutions of QT which lead to probability densities 'similar' to (11). As a first example we consider an ensemble of free particles which are distributed at $t = 0$ according to a probability density (11) centered at $r_k(0) = 0$ [set $r_k(t) = 0$ in (11)]. The initial value for $S(x,t)$ is given by $S(x,0) = p_{0,k}x_k$, i.e. $S(x,t)$ fulfills at $t = 0$ the 'deterministic' relation (20). These initial values describe for small ϵ a localized, classical particle in the sense that there is no uncertainty with respect to position or momentum. A calculation found in many textbooks leads to the following solution of Schrödinger's equation for ρ :

$$\rho(x,t) = \left(\frac{1}{\pi A(t)}\right)^{\frac{3}{2}} \exp\left\{-\frac{1}{A(t)}\sum_{k=1}^{3}\left[x_k - r_k(t)\right]^2\right\}, \tag{23}$$

where $mr_k(t) = p_{0,k}t$ and $A(t) = A_f(t) = \epsilon[1 + (\hbar/\epsilon)^2(t/m)^2]$. We see from Eq. (23) that the peak of ρ moves in agreement with NM, but the width of the wave packet increases with increasing time as well as with *decreasing* ϵ. A complete localization can only be achieved at $t = 0$. At later times the quantum uncertainty, due to the finite $\hbar$, dominates the behavior of the ensemble completely, despite our choice of 'deterministic' initial conditions.

As a second example, we consider an ensemble of particles moving in a harmonic oscillator potential $V(x) = (m\omega^2/2)x_k x_k$ using exactly the same initial conditions as in the above example of force-free motion. The result for ρ takes the same form (23) as for the force free ensemble, but with $mr_k(t) = (p_{0,k}/\omega)\sin\omega t$ and

$$A(t) = A_h(t) = \epsilon\left[\cos^2\omega t + \frac{1}{m^2\omega^2}\left(\frac{\hbar}{\epsilon}\right)^2 \sin^2\omega t\right]. \tag{24}$$

The width $A_h(t)$ increases again with decreasing ϵ and prevents again a deterministic limit. We mention, without going into details [25], that a third example showing the same behavior may be found, namely an ensemble of particles moving under the influence of a constant force.

The three examples considered in this section correspond to three potentials proportional to x_k^n, where $n = 0, 1, 2$. For these potentials the expectation values of the corresponding forces fulfill the relation $\overline{F_k(x)} = F_k(\overline{x})$. Therefore, equations of motions for $\overline{x_k}$ and $\overline{p_k}$ exist as a consequence of Ehrenfest's theorem. Despite of these classical features, even these 'optimal' states do not permit a deterministic limit of QT. We conclude, in agreement with common wisdom, that this limit does not exist.

6 The 'combined limit' of quantum theory

Let us summarize what has been achieved so far. In section 3 the limit $\hbar \to 0$ has been performed for arbitrary states (including wave packets with fixed width ϵ). The result of this first 'standard limiting process' was a classical statistical theory referred to as PHJ. In section 4 the limit $\epsilon \to 0$ of PHJ has been performed. The result of this second 'deterministic limit' was NM. Therefore NM is a subset of the classical limit PHJ of QT but NM is not the classical limit of QT, since we cannot neglect almost all of the (statistical) states of PHJ. Thus, the two limiting processes performed in this order have not led us from QT to NM in the sense that NM can be said to be the classical limit $\hbar \to 0$ of QT. In section 5 it has been shown that inverting the order of the two limiting processes (first $\epsilon \to 0$ then $\hbar \to 0$) does not solve the problem either since the limit $\epsilon \to 0$ (with $\hbar$ fixed) does not exist. The two limiting processes clearly do not commute. Thus, it is impossible to obtain NM as the classical limit of QT, no matter which order of the two (separate) limiting processes is chosen.

Fortunately, we have still the option to *combine* both limits; i.e. we could assume that the width of the wave packets is a monotone function of $\hbar$. This means that the localization of wave packets (the 'deterministic limit') and the change of the basic equations of QT (the 'standard limit') takes place *simultaneously* in the limit $\hbar \to 0$. Such states seem artificial from the point of view of experimental verification since the numerical value of $\hbar$ is not under our control. Nevertheless, a construction of NM from QT along these lines would certainly provide a kind of justification for Dirac's claim that QT reduces to NM in the limit $\hbar \to 0$. Note also, that the subject of our study is essentially of a formal nature. We are asking whether or not all predictions of NM can be obtained by means of some limiting process $\hbar \to 0$, from the basic equations of QT. There are no in-principle constraints how to perform his limit.

A brief look at the above examples for $A(t)$ shows that a *linear* relation between $\hbar$ and ϵ seems most promising. Thus, we set ,

$$\epsilon = k\hbar, \tag{25}$$

were k is an arbitrary constant. In order to use a notation similar to section 4 [see (11)], ϵ will be used instead of $\hbar$ as small parameter; it may be identified with $\hbar$ in most of the following relations. Let us perform the identification (25) for the two examples considered in section 5, with potentials $V(x) = V_f(x) = 0$ and $V(x) = V_h(x) = (m\omega^2/2)x_k x_k$, respectively. Using the same initial conditions as in section 5, the solutions for ρ and S of (8), (9) take essentially the same form in both cases, namely

$$\rho(x,t) = \left(\frac{1}{\pi\epsilon(t)}\right)^{\frac{3}{2}} \exp\left\{-\frac{1}{\epsilon(t)}\sum_{k=1}^{3}\left[x_k - r_k(t)\right]^2\right\}, \tag{26}$$

$$S(x,t) = \frac{m}{4}\frac{\dot{\epsilon}(t)}{\epsilon(t)}\sum_{i=1}^{3}\left[x_i - r_i(t)\right]^2 - \frac{1}{2}p_k(t)r_k(t) + p_k(t)x_k - \sum_{i=1}^{3}\frac{\epsilon}{2k}\tan^{-1}\frac{r_i(t)}{kp_i(t)}. \tag{27}$$

The solutions ρ_f, S_f and ρ_h, S_h for particle ensembles in force-free regions and linear-force fields may be obtained from Eqs. (26), (27) by using different widths $\epsilon(t) = \epsilon_f(t)$ and $\epsilon(t) = \epsilon_h(t)$, as given by

$$\epsilon_f(t) = \epsilon\left(1 + \frac{t^2}{k^2m^2}\right), \qquad \epsilon_h(t) = \epsilon\left[\cos^2\omega t + \frac{1}{k^2m^2\omega^2}\sin^2\omega t\right], \tag{28}$$

and different trajectory components $r_k(t) = r_k^{(f)}(t)$ and $r_k(t) = r_k^{(h)}$ (as well as momentum components $p_k(t) = m\dot{r}_k(t)$), as given by

$$r_k^{(f)}(t) = \frac{p_{0,k}}{m}t, \qquad r_k^{(h)} = \frac{p_{0,k}}{m\omega t}\sin\omega t. \tag{29}$$

As Eq. (28) shows, both widths are time-dependent; for the free-particle ensemble the width increases quadratically, for the bounded motion of the harmonic oscillator it varies periodically. However, both widths vanish in the limit $\epsilon \to 0$ for arbitrary (finite) times t. This means that the deterministic probability density we were looking for is, in fact, created in this limit. The solutions for S are well-behaved at $\epsilon = 0$. The limiting process in the continuity equation (8) can be performed in a similar way as in section 4 (an additional term due to the time-dependence of $\epsilon(t)$ is regular at $\epsilon = 0$). The remaining steps, the derivation of Newton's equations and their field-theoretic derivation from the QHJ can be performed in the same way as in section 4. Note also that the QHJ is regular at $\epsilon = 0$ and *differs* in this limit from the HJ equation [cf. the discussion following Eq. (7)]. In view of a recent discussion [18], [11] it should be noted that this field-theoretic limit is not equivalent to its projection on the trajectory.

The above solutions, with ϵ and $\hbar$ considered as *independent* parameters (as in section 5), have been reported many times in the literature. It has also been pointed out that the special value $\epsilon = \hbar/m\omega$, in the harmonic oscillator example, produces the coherent states found by Schrödinger [24]. On the other hand, the relevance of the weaker statement $\epsilon = k\hbar$ for the classical limit problem has apparently not been recognized. It is not necessary to restrict oneself to the coherent states of the harmonic oscillator (the special case $k = 1/m\omega$) in order to obtain deterministic motion; the latter may be obtained for a much larger class of force-free states, harmonic oscillator states, and constant-force states (this last example has not been discussed explicitly) as shown above. Summarizing this section, we found three potentials $V(x) \sim x^n$, $n = 0, 1, 2$ which allow for a derivation of NM from QT in the limit $\hbar \to 0$. For these potentials equations of motion for $\bar{x_k}$, $\bar{p_k}$ exist, as mentioned already. Home and Sengupta [10] have shown that for these potentials the form of the quantum-mechanical solution may be obtained with the help of the classical Liouville theorem.

7 Can the 'combined limit' be performed for all potentials ?

We know now that three potentials exist which, for properly chosen initial wave-packets, lead to deterministic equations of motion in the limit $\hbar \to 0$. We shall refer to such potentials for brevity as 'deterministic potentials'. A (complete) reconstruction of NM from QT requires that *all* (or almost all) potentials are deterministic. In this section we ask if this can be true.

As a first point we note that the probability density $\rho(x,t)$ of all deterministic wave packets takes, by definition, a very specific functional form, namely one that reduces, like Eq. (26), in the limit $\hbar \to 0$ to a delta function. This fixes essentially one of our two dynamic variables; we have two differential equations for a single unknown variable $S(x,t)$. It seems unlikely that this overdetermined system of equations admits solutions for $S(x,t)$ for *arbitrary* potentials V.

The second point to note is, that the existence of a deterministic limit does not only fix the functional form of ρ but also its argument. Let us assume, that a deterministic solution for ρ and S, with $\rho(x,t)$ taking the form (26) with unspecified $\epsilon(t)$, exists. The probability density $\rho(x,t)$ depends necessarily on $\vec{x} - \vec{r}(t)$, where the position vector $\vec{r}(t)$ is a solution of Newton's equation for the same potential $V(x)$ that occurs in the Schrödinger equation. The crucial point is that this dependence is not created by the limiting process $\hbar \to 0$ but is already present for finite $\hbar$, in the exact quantum-mechanical solution. For given initial conditions it has been created, so to say, by the quantum-theoretical formalism. This implies that $\vec{r}(t)$ describes for finite $\hbar$ not the time-dependence of a particle trajectory but of a position expectation value. Since $\vec{r}(t)$ is (again for finite $\hbar$) the solution of Newton's equations, such equations for expectation values must already be present in the quantum-theoretical formalism. Of course, in the deterministic limit $\hbar \to 0$ the difference between particle trajectories and expectation values vanishes, but the important point is that Newton's equations must hold already for finite $\hbar$. We conclude that the existence of the equations of motion of NM for position expectation values is a necessary condition for the existence of deterministic potentials.

This line of reasoning leads to a mathematical condition for deterministic potentials. Let us assume that we have a deterministic potential $V^{(det)}(x)$ in our quantum-theoretical ($\hbar$ finite) problem. We calculate the expectation value $\overline{x_k}(t)$ as defined by (17) using the deterministic probability density (26). We obtain $\overline{x_k}(t) = r_k(t)$, i.e. the expectation value follows the time-dependence of the trajectory [the peak of $\rho(x,t)$]. The latter must fulfill Newton's equation with the force derived from $V^{(det)}(x)$, otherwise the deterministic limit could not exist. Using these facts in Ehrenfest's theorems (15) and (16) we obtain immediately the following integral equation for deterministic potentials

$$F_k^{(det)}(r) = \int \mathrm{d}^3x \, \delta_\epsilon^{(3)}(x-r) F_k^{(det)}(x), \tag{30}$$

where $F_k^{(det)}(x) = -\partial V^{(det)}(x)/\partial x_k$. The quantity $\rho(x,t)$ has been renamed $\delta_\epsilon^{(3)}(x - r(t))$ in order to show the convolution-type structure of the equation. Note that (30) is only for $\epsilon > 0$ a constraint for $V^{det}(x)$. It is easy to see that a particular solution is given by $V^{(det)}(x) = a + b_k x_k + c_{i,k} x_i x_k$, where the coefficients may depend on time. This is essentially a linear combination of the three deterministic potentials x^n, $n = 0, 1, 2$ found already in the last section. According to a theorem by Titchmarsh [26] (a simple proof may be obtained with the help of the theory of generalized functions [17], see section 10) other solutions of (30) do not exist. This theorem shows that the 'combined limit' cannot be performed for all potentials. Although the present treatment does not cover all conceivable physical situations, the results obtained so far imply already definitively that the limit $\hbar \to 0$ of QT does not agree with NM.

8 Discussion

In our first limiting procedure, which is appropriate for 'well-behaved' quantum states, we found that QT agrees in the limit $\hbar \to 0$ with a classical statistical theory referred to as PHJ. The latter contains as a limiting case the deterministic states ruled by NM. Let us stress once again that the fact that these deterministic states are 'contained' in QT does not mean that NM is the limit of QT. This limit is PHJ which contains a much larger number of (probabilistic) states not belonging to NM. In a second attempt the limit $\hbar \to 0$ was simultaneously performed in the wave-packet width and in the basic equations. We found that almost all states do *not* admit a transition from QT to NM in the limit $\hbar \to 0$.

Our final result is then that NM is not the limit $\hbar \to 0$ of QT. This result has been obtained in the framework of standard QT using the Schrödinger picture to describe the quantum dynamics. One may ask whether this conclusion is specific for these choices, or remains true for other dynamical pictures, such as e.g. the Heisenberg picture, and other formulations of QT, such as e.g. Feynman's path-integral formulation. Recall that the present approach is (as discussed in 1) solely based on predictions i.e. the *numerical output* of the quantum theoretical formalism. These numbers do not depend on a particular picture of quantum dynamics. They are also independent from the choice of a particular formulation of QT since all formulations of QT must lead to the same predictions.

Let us illustrate the last point by a discussion of the path-integral formulation of QT [8]. The central quantity of this approach, the propagator, is an infinite sum of terms of the form $\sim \exp \imath \frac{S}{\hbar}$, where S is the classical action and each term in the sum is to be evaluated at a different path between the initial and final space-time points x_0 and x_1. In the classical limit $\hbar \to 0$ the dominating contribution to the sum comes from the classical path between x_0 and x_1, which extremizes S. The fact that this path obeys the differential equations (2) of NM is sometimes interpreted in the sense of a transition from QT to NM, which the path-integral formulation reveals in a particular rigourous and straighforward way. Such an interpretation is not justified. The form of the propagator says nothing about the fact whether or not a particle is really present at the initial space-time point x_0; it tells us just what will happen *given that* a particle occupies the point x_0 with certainty. The second variable of QT, the probability density ρ, must also be taken into account; it enters the initial state and makes the final state uncertain despite the 'deterministic' form of the propagator. A general classification scheme for probabilistic theories, taking the different roles of initial values and evolution equations into account, has been reported recently [13]. It is a general feature of classical statistical theories that the time-evolution in the event space (configuration or phase space) is deterministic and the impossibility to make deterministic predictions (on single events) is solely due to uncertainty in the initial values. This classical feature is also visible in the phase-space theory (5) and (though in a less explicit way) in the configuration-space theory PHJ [see (8) and (10)]. It is this feature, and not the transition from QT to NM, which is most explicit in the path-integral formalism. The classical limit of Feynman's version of QT is equivalent to the classical limit of Schrödinger's version of QT (the PHJ) since both versions are equivalent.

Our final result, the fact that NM is not the limit $\hbar \to 0$ of QT, is in disagreement with Dirac's statement quoted at the beginning of our study. Dirac discusses the problem of the classical limit in section 31 of his book. He formulates the following general principle:

> For any dynamical system with a classical analogue, a state for which the classical description is valid as an approximation is presented in quantum mechanics as a wave packet,...so in order that the classical description be valid, the wave packet should remain a wave packet and should move according to the laws of classical dynamics. We shall verify that this is so.

The following calculation is intended to show that such a wave packet always exists. Unfortunately, a systematic investigation of different classes of potentials or initial values is not performed. Instead, Dirac imposes several conditions for the considered wave packets, formulated verbally or in the form of inequalities, which he assumes to be true for arbitrary potentials but which need not necessarily be true. He arrives at the canonical equations of motions for the peaks of supposedly arbitrary wave packets. In reality, these conditions impose strong restrictions on the form of initial values and potentials and can only be fulfilled in few very special cases. Quantum-mechanical solutions for the three 'deterministic potentials', where Ehrenfest's relations agree with NM, are often used to demonstrate 'classical behavior' of wave packets. It should be borne in mind that this behavior is not generic but represents the exception(s) from the rule.

After the discovery of QT the community was shocked by the breakdown of NM in the microscopic world and it seemed inconceivable that NM should not even survive as the classical limit of QT. Schrödinger, like Dirac, considered it as evident, and wrote at the end of his famous paper about coherent states [24]:

> We can definitely foresee that, in a similar way, wave groups can be constructed which move round highly quantized Kepler ellipses and are the representation by wave mechanics of the hydrogen electron.

The coherent states of the harmonic oscillator have been generalized to arbitrary potentials in various ways [29] but none of these generalizations admits a clear transition to the classical (deterministic) limit. Special attention was, of course, devoted to the Coulomb potential, but despite intense research, Schrödinger's idea could not be realized and this chapter has apparently already been closed [30].

The classical limit of QT is the PHJ, a classical statistical theory defined by Eqs. (8), (9). The limit $\hbar \to 0$ transforms a quantum probabilistic theory into a classical probabilistic theory. The behavior of the uncertainty relation illustrates this conclusion in a simple way. For $\hbar \to 0$ it takes the form

$$\Delta x \Delta p \geq 0, \tag{31}$$

which means that in the classical limit the uncertainty product is in general different from zero; a detailed comparison has been reported by Devi and Karthik [4]. Almost all states of PHJ will show uncertainties;

the equality sign in (31) just indicates that the transition to the deterministic limit (as performed in section 4) is not forbidden.

The classical limit plays an important role in the prolonged discussion about the proper interpretation of QT. In the years after discovery of QT a number of dogmas have been established, which have been repeated since then so many times that they are considered today as 'well-established' scientific facts. One of these dogmas states that "QT provides a complete description of individual particles". It is hard to understand how a probabilistic theory could provide a 'complete' description of individual events. But one should first analyze the possible meanings of the term 'complete'. A detailed analysis shows that this term is ambiguous [14]. It may mean 'no better theory exists' (metaphysical completeness) or 'all facts that can be observed can be predicted' (predictive completeness). The still prevailing (Copenhagen) standard interpretation claims that QT is complete in both respects. Einstein, Podolsky, and Rosen (EPR), showed that QT is predictive incomplete [7]. In the last paragraph of their paper [7], the authors expressed their *belief* that QT is metaphysical incomplete. EPR's proof of predictive incompleteness was correct and could not be attacked, so metaphysical incompleteness was attacked instead. The EPR paper was misinterpreted as if the authors had claimed they had proven metaphysical incompleteness. Further consequences of this misinterpretation will not be discussed here. The important point to note is that metaphysical completeness is a philosophical term; physics can only test predictive completeness (by comparison with observation). Thus, let us concentrate on the question of predictive completeness of QT; in the remaining part of this section the term completeness will be used in this sense.

The fact that NM disagrees with the $\hbar \to 0$ limit of QT presents a painful obstacle to the completeness dogma. Every statistical theory, no matter whether classical or quantum, is unable to predict individual events and is therefore, by its very definition, incomplete. How can quantum theory be complete if its classical limit is incomplete? In order to eliminate this problem, Bohr created the 'correspondence principle'. It postulates, that quantum states become similar to states of NM for large values of $S/\hbar$. However, this principle is not in agreement with the structure of Schrödinger's equation. For large $S/\hbar$ the quantum term in Eq (9) becomes negligibly small and QT becomes similar to PHJ and not to NM; similarity with NM requires *in addition* a sharply-peaked ρ. The breakdown of Bohr's correspondence principle in concrete situations has been reported many times in the literature; see e.g. Cabrera and Kiwi [2] and Diamond [5].

What might our bright student - whose incisive question has triggered this investigation - say at this point (if he is still listening) ? Maybe he says "O.K, so far. But is not my reasoning necessarily correct, even without reference to Dirac's statement ?". Again, one can imagine a variety of possible answers. From the point of view of the present author, the answer is: "Nothing is wrong with your reasoning; considered as a logical implication it is perfectly correct. But the conclusion need not be true because the premise is wrong: QT does not describe a single electron nor does it describe any other single particle; it is a statistical theory whose predictions refer to statistical ensembles only".

9 Conclusion

In this work we compared the predictions of QT for vanishing $\hbar$ with the predictions of NM. Generally, the predictions of a physical theory are a logical consequence of (a) the mathematical form of its basic equations, and (b) the set of initial values. Both aspects have been studied in this work, in order to take into account all possible ways to create predictions of NM from QT in the limit $\hbar \to 0$. This comparison has been performed for the simplest and most significant situation of single particles in external potentials. Our conclusion is that NM cannot be identified with the limit $\hbar \to 0$ of QT. This mathematical result should be taken into account in considerations about the interpretation of QT.

10 Appendix

Using the theory of generalized functions [17] the integral equation (30) can be solved quickly. We discuss for simplicity the one-dimensional integral equation,

$$f(x) = \int \mathrm{d}x\, k(x-y) f(y), \tag{32}$$

where $k(x)$ is a normalized gaussian. Introducing the Fourier-transforms $F(k)$ and $K(k)$ of $f(x)$ and $k(x)$, Eq. (32) takes the form

$$\int \mathrm{d}k\, F(k) \left[1 - \sqrt{2\pi} K(k)\right] = 0. \tag{33}$$

Non-trivial solutions for $F(k)$ [and $f(x)$] can only exist if the term in brackets has zeros. This is the case since the Fourier-transform of a normalized gaussian is again a normalized gaussian and therefore the bracket vanishes at $k = 0$ with a leading quadratic term. Thus, the Fourier transform of every solution of (32) must obey

$$F(k)k^2 = 0. \tag{34}$$

for all k. This implies that the Fourier-transform of $k^2F(k)$, which is proportional to the second derivative $f''(x)$ of $f(x)$, vanishes too. This implies $f(x) = a + bx$, in agreement with a theorem by Titchmarsh [26]. [The solution for $F(k)$ is a linear combination of $\delta(k)$ and $\delta'(k)$].

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