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# A reconstruction of quantum theory for nonspinning particles

Ulf Klein

Institute for Theoretical Physics, University of Linz,  
Altenberger Strasse 69, Linz, A-4040, Austria .

Corresponding author(s). E-mail(s): [ulf.klein@jku.at](mailto:ulf.klein@jku.at);

## Abstract

This work is based on the idea that the classical counterpart of quantum theory (QT) is not mechanics but probabilistic mechanics. We therefore choose the theory of statistical ensembles in phase space as starting point for a reconstruction of QT. These ensembles are described by a probability density  $\rho(\mathbf{q}, \mathbf{p}, \mathbf{t})$  and an action variable  $\mathbf{S}(\mathbf{q}, \mathbf{p}, \mathbf{t})$ . Since the state variables of QT only depend on  $\mathbf{q}$  and  $\mathbf{t}$ , our first step is to carry out a projection  $\mathbf{p} \Rightarrow \mathbf{M}(\mathbf{q}, \mathbf{t})$  from phase space to configuration space. We next show that instead of the momentum components  $\mathbf{M}_k$  one must introduce suitable potentials as dynamic variables. The quasi-quantal theory resulting from the projection is only locally valid. To correct this failure, we have to perform as a second step a linearization or randomization, which ultimately leads to QT. In this work we represent  $\mathbf{M}$  as an irrotational field, where all components  $\mathbf{M}_k$  may be derived from a single function  $\mathbf{S}(\mathbf{q}, \mathbf{t})$ . We obtain the usual Schrödinger equation for a nonspinning particle. However, space is three-dimensional and  $\mathbf{M}$  must be described by  $\mathbf{3}$  independent functions. In the fourth work of this series, a complete representation of  $\mathbf{M}$  will be used, which explains the origin of spin. We discuss several fundamental questions that do not depend on the form of  $\mathbf{M}$  and compare our theory with other recent reconstructions of QT.

**Keywords:** Quantum theory, Projection to Configuration Space, Linearization, Randomization, Derivation of Schrödinger's equation, Quantum-classical relation

**MSC Classification:** 81P05 , 81S99 , 81Q20 , 70H99 , 37A60

# 1 Introduction

Among the many different interpretations of the quantum theoretical formalism, there is one that does not require any additional philosophical assumptions. This is the so-called statistical interpretation or ensemble interpretation of quantum theory (QT) preferred by Einstein [1]. From his point of view, the Schrödinger equation does not describe individual (one or several) particles, but only statistical ensembles of (one or several) particles. In fact, there is no doubt that the predictions of QT are probabilities - even if the quantum probabilities cannot be described by standard classical probability theory. In this minimalist interpretation there is no unsolvable measurement problem, no controversial reduction of the wave packet, and no mysterious nonlocality. On the other hand, one has to do without the highly honored principle of reductionism. The more widespread individuality interpretation is in agreement with this principle.

By the very nature of the term the truth or falseness of an interpretation cannot be proven. Nonetheless, one can give facts that speak for or against a particular interpretation. If it would be possible to derive QT in a convincing manner from a classical probabilistic (ensemble) theory, then that would be a fact favoring the ensemble interpretation of QT. On top of that, such a derivation might lead to a better understanding of QT and eliminate some or all of the strange features mentioned above.

The present paper is the third in a series of works which are based on Einstein's point of view; the previous works will be referred to as I [2] and II [3]. Of course, these papers are not the first using this point of view; a number of relevant quotations may be found in II. In I and II an attempt has been undertaken to derive QT from a minimal number of reasonable postulates. The first postulate is that it must be possible to derive QT from the theory of classical statistical ensembles. From this most fundamental assumption and the fact that QT uses space-time variables as independent variables, most of the subsequent steps in the derivation of QT follow more or less automatically. The theory reported in II was named "Hamilton-Liouville-Lie-Kolmogorov theory" (HLLK) quoting some of the great scientists who made this work possible. We continue to use this acronym for the present theory, which shares with I and II the same basic assumptions and the same aim, but uses a different method.

Let us briefly recall the ideas on which works I, II are based. In contrast to previous ensemble theories in configuration space, see e.g. [4–7], the works I, II start from the most fundamental level, namely from phase space. A classical statistical ensemble in phase space is defined as the uncountable set of all solutions of the canonical equations

$$\dot{q}_k = \frac{\partial H(q, p)}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H(q, p)}{\partial q_k}. \quad (1)$$

The state of each member of the ensemble, at each instant of time  $t$ , is described by  $2n$  numbers, namely  $n$  coordinates  $q = q_1, \dots, q_n$  and  $n$  conjugate momenta

$p = p_1, \dots, p_n$ . The dependence of the state  $q, p$  on time  $t$  is ruled by the time-independent Hamiltonian  $H(q, p)$ . The solutions of (1) are written in the form

$$q_k = Q_k(t, t^0, q^0, p^0), \quad p = P_k(t, t^0, q^0, p^0), \quad (2)$$

where  $(q^0, p^0)$  is the state at the initial time  $t^0$ ; the dependence on  $t_0$  will often be suppressed. The ensemble is given by the infinite set of solutions (2) with  $(q^0, p^0)$  taking all possible values in the  $2n$ -dimensional phase space  $\Omega = \mathbb{R}_q^n \times \mathbb{R}_p^n$ .

The variables  $q, p$  are ‘‘Lagrangian coordinates’’ describing properties of *particles*. Such a ‘‘particle-like’’ description of an ensemble is unwieldy. In the more convenient ‘‘Eulerian description’’, which corresponds to the usual field-theoretical formulation, the same symbols  $q, p$  are used to denote points of *space*, in this case points of  $\Omega$ . The distinction is important despite the fact that the mathematical range of values is the same in both cases. The relation between both descriptions is discussed in more detail in II. The most important Eulerian dynamic variable is the probability density  $\rho(q, p, t)$ , describing the distribution of possible trajectories in phase space, which obeys the Liouville equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial \rho}{\partial p_k} \frac{\partial H}{\partial q_k} = 0. \quad (3)$$

This partial differential equation is the counterpart of Newton’s law [or its reformulation (1)] for probabilistic ensembles of trajectories. If  $\rho(q, p, t)$  is known, all of the observable output (expectation values) of such a probabilistic theory may be calculated.

The differences between classical mechanics (CM) and the theory of probabilistic ensembles, which is referred to as probabilistic mechanics (PM), are important in particular in view of a transition to QT: A state of CM (at fixed time) is a point in  $\Omega$ , a state of PM is a point in an appropriately defined function space. Observable results in a state of CM are given by values of observables  $A(q, p, t)$ , observable results in a state of PM are given by expectation values

$$\bar{A}_\rho(t) = \int dq dp \rho(q, p, t) A(q, p, t). \quad (4)$$

This listing of obvious facts shows that the structural similarity between PM and QT is much stronger than that between CM and QT. It is also clear that PM is more realistic than CM because there are no experiments with unlimited accuracy, as pointed out by Born [8]. Let us also make a comment on the limit of individual particles in the ensemble theory. It is well-known that solutions of the Liouville equation for arbitrary initial conditions may be constructed with the help of the solutions of the particle equations (1). In particular, particle-like solutions of the Liouville equation exist, where the probability is concentrated entirely on the trajectories. The question arises as to whether the probabilistic description and the description with individual trajectories are equivalent in

this limit. It turns out that this is *not* the case. We refer to the literature for arguments in favor of the probabilistic description [9].

The dynamical variable  $\rho(q, p, t)$  is all we need in order to calculate time-dependent expectation values of arbitrary classical observables  $A(q, p, t)$ ; no further dynamical variables are required, in principle, to define a “state” of PM. Nevertheless, we introduce, as in I,II, the classical action

$$S = \int_{t_0}^t dt' L(q(t'), \dot{q}(t'), t'), \quad (5)$$

evaluated at the real paths  $q(t')$ , as a second dynamical variable. The action integral (5), formulated here as a function  $S(q, p, t)$  on phase space, plays an indispensable role in the transition from PM to QT. In I, II it has been shown that  $S(q, p, t)$  obeys the differential equation

$$\frac{\partial S}{\partial t} + \frac{\partial S}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial S}{\partial p} \frac{\partial H}{\partial q} = \bar{L}, \quad (6)$$

which will be referred to as action equation. The quantity  $\bar{L}$  (the Lagrangian) is defined by

$$\bar{L} = \bar{L}(q, p, t) = p \frac{\partial H(q, p)}{\partial p} - H(q, p). \quad (7)$$

The left-hand-sides of (3) and (6) may be interpreted as total derivatives with respect to time, with a velocity field  $V = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q})$ . Arbitrary “Lagrangian” functions, describing the distribution of certain particle properties may be transformed to “Eulerian” functions describing corresponding fields. This is a general method [10] frequently applied in 3–dimensional fluid mechanics [11] and applied here to  $2n$ –dimensional phase space; in section 2.2.2 we will apply it to  $n$ –dimensional configuration space  $\Sigma = \mathbb{R}_q^n$ .

Note that there is no coupling between the basic differential equations (3) and (6); in particular  $\rho(q, p, t)$  does not occur in the differential equation (6) for  $S(q, p, t)$ . This is a triviality in classical probabilistic physics: the dynamical laws remain intact while all the uncertainty is due to the initial states. Adding the law (6) to PM offers the possibility to construct an indeterministic theory (like QT), where a *coupling* between the corresponding variables occurs.

In I and II Schrödinger’s equation was derived from PM by means of two simple steps. In the first step, the state variable  $\rho$  was replaced by a complex-valued state variable  $\psi$  which depends in a suitable manner (Madelung form) on  $\rho$  and  $S$ . The resulting evolution equation for  $\psi$  is the counterpart of Schrödinger’s equation in phase space. In the second step, this equation was projected onto  $\Sigma$ . This leads to the standard quantization rules and to Schrödinger’s equation. Furthermore, in II the structures described by Eqs. (1), (3), (6) have been defined in an analogous way not only for the Hamiltonian function  $H(q, p)$  but for any observable  $A(q, p)$ . In this way the most important relations of QT, namely the form of operators, Schrödinger’s equation, eigenvalue equations, commutation relations, expectation values, and

Born's rule have been derived in II. The simplicity of the derivation in II is a consequence of the fact that mathematical structures exist in phase space which are very similar to those of quantum theory; these structures belong to the framework of PM and are "invisible" if CM is considered as the classical counterpart of QT.

Let us extract now from this overview the general structure of HLLK. We start from PM, which is a theory of ensembles of point particles with  $2n + 1$  independent variables  $q, p, t$ , and construct a theory of type QT, with  $n + 1$  independent variables  $q, t$ . Such a construction must contain at least two essential steps, namely

- a linearization, and
- a projection from  $\Omega$  to  $\Sigma$ .

Let us discuss these two requirements in more detail.

- The property of *linearity* for a fundamental law of physics (this means: a law containing only fixed parameters like mass and universal constants like Planck's constant, the velocity of light, or the unit of charge) is a necessary requirement if we want this law to describe a large number of well-defined processes. This follows from the fact that almost all solutions of nonlinear evolution equations become singular outside some (small) time interval. We shall use the term "locally valid" to characterize this restricted validity of solutions of nonlinear equations. On the other hand, linearity implies that all solutions of the initial value problem exist not only locally but on a global scale; this is of course a consequence of the superposition principle, which facilitates enormously the construction of solutions with prescribed initial values. We shall use the term "globally valid" to characterize the almost unrestricted validity of solutions of linear equations.
- The requirement of *having space-time coordinates as independent variables* is also very reasonable. Space coordinates are more fundamental than momentum coordinates; the latter can only be determined if a continuous set of the former is available. All fundamental fields of physics represent properties which vary as a function of space-time and not as a function of space-momentum-time (if several particles are considered each one may have its own space coordinates). There is of course an infinite number of coordinate systems in  $\Omega$  and  $\Sigma$ , all of which are mathematically equivalent. However, the systems  $q, p, t$  in  $\Omega$  and  $q, t$  in  $\Sigma$  are the simplest and the only ones that allow intuitive access.

In the version of HLLK reported in I and II the linearization was performed first, followed by a projection to  $\Sigma$  as a second step. As a result, in II we were able to derive the most important relations of QT very quickly. There is, however, a disadvantage here because we lost the quasi-classical theory in the course of this quick derivation. This failure may be responsible for the fact that the phenomenon of *spin* is not predicted by the version of the HLLK reported in II. We know today that all structureless particles with non-zero mass have

spin one-half. The HLLK is a (probabilistic) theory of structureless (point) particles, and should therefore predict the phenomenon of spin, in particular the universal number one-half.

In the present and the following work, to be referred to as IV [12], we carry out the transition from PM to QT in a more complete way by simply reversing the order of the above two steps. Thus, we first carry out the transition from  $\Omega$  to  $\Sigma$  - in this way we are able to gain insight into the structure of the momentum field - and perform afterwards the linearization or randomization of the resulting equations. We restrict ourselves to the study of a single observable, namely Hamilton's function  $H$ . Thus, in a first step, to be carried out in section 2, a momentum field  $M(q, t)$  is assigned to each point of  $\Sigma$ , at each instant of time  $t$ . In section 3 we show that  $M(q, t)$  is conveniently described in terms of a special kind of potentials originally introduced by Clebsch as a mathematical tool of fluid mechanics [13]. There is no reason to assume that  $M(q, t)$  is irrotational. In fact it turns out that its rotational part is responsible for spin, as will be shown in detail in IV. However, in the present work we cover only the very basics of the spin theory, as our primary aim here is to understand the interface between classical physics and QT. The essential properties of this interface as well as related questions of interpretation become much more transparent when spin is neglected. Thus we restrict ourselves in the present paper, despite its artificial nature, to an irrotational momentum field, which is described by a single Clebsch potential  $S$ . Using  $\rho$  and  $S$  as new dynamic variables we obtain a theory which will be referred to as "quasi-quantal approximation" (QA) of PM. This theory is closely related to the well-known quasi-classical approximation of the Schrödinger equation for spin-less particles. In section 5 we carry out the transition from QA to QT by means of two methods, a linearization and a randomization. In section 6 questions of interpretation and the relation between QT and the classical theory are discussed; we examine, in particular, the role of Dirac's "families of classical solutions" [14] as seen from the point of view of the ensemble interpretation. In section 7 we discuss the relationship of the present theory to other recent theories based on similar concepts. The final section 8 contains a list of conclusions.

## 2 Projection to configuration space

In this section our basic equations (1), (3), (6) will be projected to configuration space. This first step of HLLK means defining appropriate momentum fields which replace the independent variables  $p$ . The phase space variables  $\rho(q, p, t)$  and  $S(q, p, t)$  will be replaced by appropriate configuration space variables, which depend on  $q, t$  only, and the equations of motion for these new dynamical variables will be derived. The theory obtained this way is not realized in nature but plays a very important role as an intermediate step from PM to QT.

## 2.1 Projection of particle equations

We associate with each point  $q$  of configuration space (at each instant of time  $t$ ) a particle momentum by replacing the variable  $p$  by a  $n$ -component momentum field  $M$ :

$$p_k \rightarrow M_k(q, t). \quad (8)$$

Thus,  $2n$ -dimensional phase space is projected to a  $n$ -dimensional surface parameterized by the configuration space coordinates  $q_k$  [15]. We may also say that we restrict our considerations from now on to a  $n$ -dimensional subspace  $\mathbb{M}$  of phase space, which is defined, suppressing time for the moment, by  $\mathbb{M} = \{(q, p) \in \Omega \mid p = M(q)\}$ . A large part of the following considerations is devoted to a study of  $\mathbb{M}$  and its various transformed versions.

Of course, the momentum field  $M_k(q, t)$  should be chosen in such a way that the original structure of the canonical equations (1) is preserved as far as possible. Following Rund [16] and Kozlov [17], we introduce fields  $V(q, p, t)$ ,  $v(q, t)$ ,  $h(q, t)$ , defined by

$$V_k(q, p, t) = \frac{\partial H(q, p, t)}{\partial p_k}, \quad (9)$$

$$v_k(q, t) = V_k(q, M(q, t), t), \quad (10)$$

$$h(q, t) = H(q, M(q, t), t). \quad (11)$$

Then, given that the trajectory  $q_k(t)$  is a solution of the first member of (1),

$$\dot{q}_k = v_k(q, t), \quad (12)$$

the corresponding momentum  $p_k(t) = M_k(q(t), t)$  must be a solution of the second member of (1). This requirement leads to the following equation for the momentum field  $M(q, t)$ :

$$\frac{\partial M_i(q, t)}{\partial t} + \left[ \frac{\partial M_i(q, t)}{\partial q_l} - \frac{\partial M_l(q, t)}{\partial q_i} \right] v_l(q, t) = -\frac{\partial}{\partial q_i} h(q, t). \quad (13)$$

This nonlinear partial differential equation (recall that  $v$  and  $h$  depend on the unknown variables) will be referred to as canonical condition. Thus, we obtain, as a result of the projection to configuration space, new equations for the particle trajectories, namely  $n$  partial differential equations (13) for  $M$  and  $n$  ordinary differential equations (12) for the positions  $q$ . These new equations replace (1).

These equations can still be used to calculate trajectories. One has to perform the following steps:

1. Assign an initial value  $M_0(q)$ , at  $t = t_0$ , to the momentum field  $M(q, t)$ .
2. Find a solution  $M(q, t)$  of (13) for this initial value.
3. Solve the ordinary differential equations (12) to obtain the trajectory coordinates  $q(t)$ .



4. Use these coordinates to obtain the corresponding momenta  $p(t) = M(q(t), t)$ .

While trajectories still exist they are only locally valid as a consequence of the nonlinearity of the dynamical equations (13). A more detailed discussion of the modifications the concept of trajectories undergoes, when transforming from phase space to configuration space, will be given in section 4.

Momentum fields also appear in the theory of canonical transformations in phase space. However, these are by definition irrotational, in contrast to the fields  $M(q, t)$  above. The difference between the two types of fields **A** is discussed in the appendix.

For  $n = 3$  Eq. (13) agrees with the evolution equation for the velocity field of a barotropic ideal fluid; in this context it is sometimes referred to as Lamb equation [17]. In the present work we will encounter several other formal similarities between our probabilistic theory and fluid mechanics. Despite such similarities, the different physical meaning of the basic variables should be born in mind. In particular, in fluid mechanics the density  $\rho(q, t)$  is a directly measurable “material” quantity. In the present theory  $\rho(q, t)$  is a rather abstract quantity, a probability density which may, for example, be measured by performing a large number of individual experiments with arbitrary large time-intervals in between.

## 2.2 Projection of ensemble equations

In this section we project the Liouville equation (3) and the action equation (6) to the subspace defined by a solution  $M(q, t)$  of the canonical condition (13). The resulting partial differential equations represent an essential step on our way from PM to QT.

### 2.2.1 Projection of Liouville equation

The projection of the Liouville equation to configuration space is a standard process which is, in a three-dimensional fluid-dynamical context, sometimes referred to as “hydrodynamical substitution”. We rewrite (3) as a continuity equation in phase space:

$$\frac{\partial \rho(q, p, t)}{\partial t} + \frac{\partial}{\partial q_k} \rho(q, p, t) \frac{\partial H(q, p, t)}{\partial p_k} - \frac{\partial}{\partial p_k} \rho(q, p, t) \frac{\partial H(q, p, t)}{\partial q_k} = 0. \quad (14)$$

In order to make sure that  $\rho(q, p, t)$  vanishes everywhere except on the surface  $p = M(q, t)$  we write  $\rho(q, p, t) = \rho(q, t) \delta(p - M(q, t))$ , where  $\rho(q, t)$  is the new probability density in configuration-space, and  $\delta$  is the  $n$ -dimensional delta function. Using this expression, the integration with respect to the momentum variables may be performed, assuming non-singular behavior of the relevant quantities. Then the contribution of the last term on the l.h.s. of (14) vanishes

and we obtain the desired continuity equation in configuration-space

$$\frac{\partial \rho(q, t)}{\partial t} + \frac{\partial}{\partial q_k} \rho(q, t) V_k(q, M(q, t), t) = 0, \quad (15)$$

which may be interpreted as a probabilistic conservation law with  $\rho v(q, t)$  as probability current. The same result may also be obtained from the reasonable requirement that the measure defined by  $\rho(q, t)$  is invariant under the flow defined by (12).

### 2.2.2 Projection of action equation

It is also necessary to consider the projection of the action equation (6) to configuration space, as the (classically redundant) quantity  $S(q, p, t)$  will play an important role in the transition to QT. We define a configuration space field  $s(q, t)$  according to

$$s(q, t) = S(q, M(q, t), t). \quad (16)$$

We omit an index  $M$  but bear in mind that this field depends by definition on the momentum field  $M$ . We may replace in (6) the partial derivatives of  $S(q, p, t)$  with respect to  $q$  and  $t$  by partial derivatives of  $s(q, t)$  with respect to the same variables. After performing several such manipulations, Eq. (6) takes the form

$$\frac{\partial s}{\partial t} - \frac{\partial S}{\partial p_k} \Bigg|_{p=M} \left[ \frac{\partial M_k}{\partial t} + \left( \frac{\partial M_k}{\partial q_i} - \frac{\partial M_i}{\partial q_k} \right) v_i + \frac{\partial}{\partial q_k} h \right] + v_k \left( \frac{\partial s}{\partial q_k} - M_k \right) + h = 0. \quad (17)$$

As  $M_k(q, t)$  is a solution of (13) the bracket vanishes and Eq. (17) takes the form

$$\frac{\partial s}{\partial t} + v_k \left[ \frac{\partial s}{\partial q_k} - M_k(q, t) \right] + h = 0. \quad (18)$$

This is the projection of Eq. (6) to configuration space derived in a straightforward way. There is an alternative derivation of this equation which makes its physical meaning more transparent. Starting from the phase space action (5), the derivation of (18) was performed in two steps. The first step was a Lagrangian to Eulerian transition in phase space leading to Eq. (6). The second step, performed above, was a projection to configuration space. It should be possible to change the order of these steps. If we start from (5) and project this quantity to configuration space, we obtain the ‘‘Lagrangian’’ quantity

$$S_M(q_0, t) = \int_{t_0}^t dt' [M_i(q(q_0, t'), t') v_i(q(q_0, t'), t') - h(q(q_0, t'), t')]. \quad (19)$$

Performing now a Lagrangian to Eulerian transition (see II for details) for the action integral in configuration space (19) we obtain

$$\frac{Ds}{Dt} := \frac{\partial s}{\partial t} + v_k \frac{\partial s}{\partial q_k} = M_k(q, t)v_k - h, \quad (20)$$

in agreement with (18). The left hand side of (20) is the total derivative along the particle trajectories defined by (12) and the right-hand-side is the projection of the Lagrangian to the subspace  $\mathbb{M}$ .

The projection of the canonical equations (1) to configuration space has led us to Eqs. (12) and (13). These relations, together with the continuity equation (15), define a theory which suffers from two shortcomings. The first, mentioned already in section 2.1, is given by the fact that trajectories are only locally well-defined. The second is given by the fact that the  $n$  components  $M_1(q, t), \dots, M_n(q, t)$  of the momentum field may not be *functionally independent* from each other.

### 3 Introducing potentials

In this section we show that the next step in the development of the HLLK has to be a replacement of the dynamical variables  $M_i$  by potentials. First we consider arbitrary particle numbers  $N$ , but later specialize to  $N = 1$  and to an irrotational momentum field, which may be described by a single scalar potential  $S$ . The general (correct) treatment of the case  $N = 1$  requires 3 independent potentials and is will be reported in IV.

If we consider a system of  $N$  free particles in phase space, the  $3N$  components of the particle momentum are not subject to any restrictions. It seems unlikely that this freedom will be maintained for the  $3N$  fields  $M_k$  after projection to  $\mathbb{M}$ . To examine this question more closely, we need a mathematical theory that tells us how to eliminate redundancy from a set of fields. This question was studied by the mathematician Pfaff in 1815 (see [18] for references and background information). Pfaff's problem may be formulated as follows:

Given  $n$  fields  $M_1(q, t), \dots, M_n(q, t)$  not necessarily functionally independent from each other. What is the minimal number  $L$  of fields  $F_1(q, t), \dots, F_L(q, t)$  required to derive the  $M_i(q, t)$ , and which relations exist between the fields  $M_i(q, t)$  and the "potentials"  $F_i(q, t)$  ?

This problem is equivalent to a "complete reduction" of the 1-form, or Pfaffian form  $\omega = M_i(q) dq_i$  i.e. to a transformation of the Pfaffian form into an equivalent form with a minimal number of terms. The number  $L$  is referred to as "class" of the vector field  $M = \{M_1, \dots, M_n\}$ . A detailed treatment of Pfaff's problem may be found, e.g., in Caratheodory's book [10].

The number  $L$  may be determined (by finding the rank of a certain matrix [10]) if the functional form of  $M(q, t)$  is known. As  $M(q, t)$  is not known to us we cannot take advantage of this mathematical result. Rather, we have

to treat  $L$ , or the integer  $m$  introduced below, as a kind of "adjustable parameter". The part of Pfaff's solution which is most interesting for us is the form of the expansion. For momentum fields of odd class there is an integer  $m$  given by  $L = 2m + 1$ . In this case  $M$  may be written in the form

$$M_k(q, t) = \frac{\partial S(q, t)}{\partial q_k} + P_\alpha(q, t) \frac{\partial Q_\alpha(q, t)}{\partial q_k}, \quad (21)$$

where  $S(q, t)$ ,  $P_\alpha(q, t)$ ,  $Q_\alpha(q, t)$  are  $2m + 1$  independent functions of  $q_1, \dots, q_n, t$  (Greek indices  $\alpha, \beta, \dots$  run from 1 to  $m$  and double occurrence of these indices entails a summation from 1 to  $m$ ). The functions  $S(q, t)$ ,  $P_\alpha(q, t)$ ,  $Q_\alpha(q, t)$  are referred to as Clebsch potentials [13]. For fields of even class there is an integer  $m$  given by  $L = 2m$  and  $M$  may be written in the form

$$M_k(q, t) = P_\alpha(q, t) \frac{\partial Q_\alpha(q, t)}{\partial q_k}, \quad (22)$$

with  $m$  pairs of functions  $P_\alpha(q, t)$ ,  $Q_\alpha(q, t)$ . We should note that the above expansions are only locally valid. This is a serious limitation for many tasks in physics but not for the present one. The reason is that the global validity of the present theory has already been lost (by projecting to configuration space) *before* the elimination of redundancy is implemented.

Two questions now arise, namely (i) which one of the above two expansions is suitable for our purposes, and (ii) is there really redundancy or may we continue to use  $M_k$  as our dynamical variables? Both of these questions can be answered in a simple way, just by considering the form of the expansions (21) and (22). We use the fact that the concept of constraints makes only sense in macroscopic physics. This means we can identify the coordinates of the configuration space with the Cartesian coordinates of one or several particles. In other words, if we have  $N$  particles then we have  $n = 3N$  spatial degrees of freedom, and a change in  $n$  is always a consequence of a change in  $N$ ; in particular  $n = 3, 6, 9, 12, \dots$  if  $N = 1, 2, 3, 4, \dots$

From the fact that the structure of our (future) theory can not depend on the number of particles, we conclude first of all that only one of the two representations (21) and (22) can be true for all  $N$ . Then, only (21) survives. In fact, the representation (22) leads to an even number of fields and fails to describe the single particle case,  $N = 1$ , which requires three fields. Thus, in the three-dimensional space of nonrelativistic physics, which is considered throughout the present study, we have to use the odd representation, Eq. (21), with non-vanishing Clebsch potential  $S(q, t)$ . On the other hand, for the four-dimensional space-time of relativistic physics the even representation (22) with  $S(q, t) = 0$  is appropriate, as has been shown by Rund [16], [19].

To answer the second question we first assume that there is no redundancy, that is,  $L = n = 3N$ . Since  $L$  is alternately odd and even with increasing  $N$ , this assumption leads to a contradiction. Thus, there must be redundancy, at least for some  $N$  the number  $L$  of independent components of  $M$  will be less

than  $n$ . This leads to the important conclusion that we have to use *potentials* as dynamic variables instead of momentum fields. We have derived a fundamental structural property of QT, whose origin is seldom asked for.

We know now that only (21) can be used, i.e. the class is given by  $L = 2m + 1$ . Secondly, we know that  $L$  cannot be equal to  $n$  for all  $n$ ; i.e. a relation of the form  $L = n - k$ , where  $1 \leq k \leq n - 1$ , will exist at least for some  $n$  ( $k$  is the number of functional relations between the  $M_i$ ). Combining both relations we have

$$n - k = 2m + 1. \quad (23)$$

Since  $n, k, m$  are all integers we have a countable number of solutions for  $k$  and  $m$ . There is a solution of maximal redundancy for arbitrary  $n$  which is given by  $m = 0$  and  $k = n - 1$ . For  $N = 1$  there is no redundancy, the relation  $3 - k = 2m + 1$  can only be true for  $k = 0$  and  $m = 1$  (excluding here the case of maximal redundancy). For  $N = 2$  we have necessarily redundancy; the relation  $6 - k = 2m + 1$  can only be true for nonzero  $k$ ; the possible pairs  $(k, m)$  are from the set  $\{(1, 2), (3, 1)\}$ . For  $N = 3$  the possible pairs  $(k, m)$  are from the set  $\{(0, 4), (2, 3), (4, 2), (6, 1)\}$ , etc. Inspecting the various possible solutions for each  $N$  one finds that only a single "regular" solution for  $k$  and  $m$  exists, namely the linear solution  $k = N - 1$ ,  $m = N$ . Only for this "regular" solution the increase in the total number  $2m + 2$  of dynamical variables (taking  $\rho$  into account) is the same for all  $N$ , namely 2. For all other solutions this number changes in an irregular way; examples for such solutions (for  $N = 1, 2, 3, 4, \dots$ ) are  $2m + 2 = 4, 4, 6, 4, \dots$  or  $2m + 2 = 4, 6, 4, 8, \dots$ . These irregular solutions, are, although not impossible from a logical point of view, obviously unacceptable, and can be excluded. Let us summarize the results of our analysis for  $n = 3N$ .

- To expand the momentum fields  $M_1, \dots, M_n$  only the odd representation, Eq. (21) can be used, i.e.  $L = 2m + 1$ . As regards the number  $m$  two possibilities exist:
- Either the case of maximal redundancy is realized, i.e.  $m = 0$  for all  $N$ . In this case the momentum field  $M$  is the gradient of a scalar function  $S(q_1, \dots, q_n)$ .
- Or  $m = N$  and  $N - 1$  relations exist among the  $3N$  momentum field components. In this case  $M$  can be expanded in  $2m + 1$  Clebsch potentials, where  $m = N$ . Thus, a  $N$ -particle ensemble is described by a function  $S$  and  $N$  pairs of dynamic variables  $P_\alpha, Q_\alpha$ .

The most important conclusion of this section is that the momentum fields *have to be replaced by potentials*. This conclusion is only correct for theories with a variable number of particles. For theories like fluid mechanics, where the number of degrees of freedom is always 3 (corresponding to  $N = 1$ ), both the three components of the momentum (the velocity) and the three Clebsch potentials may equivalently be used as dynamic variables. For  $N = 1$  it is also possible to rewrite QT with the help of both types of variables [20, 21]. However, for our present task of reconstructing QT for arbitrary  $N$ , only potentials are appropriate.

In the present work we restrict ourselves to the case  $m = 0$ , where only a single potential  $S$  occurs. The case  $m = 1$ , which leads to the spin of a single particle, will be treated in IV.

### 3.1 Irrotational momentum fields

It is useful to introduce a quantity which characterizes the purely rotational (or vortical) part of the momentum field  $M$ . An appropriate quantity is the vorticity tensor  $\Omega_{ik}$ , defined by

$$\Omega_{ik}(q, t) := \frac{\partial M_k(q, t)}{\partial q_i} - \frac{\partial M_i(q, t)}{\partial q_k}. \quad (24)$$

The evolution equation for  $\Omega_{ik}$ , which may be derived from the canonical condition (13), expresses the fact that the Lie derivative of  $\Omega_{ik}$  with respect to the velocity field  $v_l$  vanishes. Roughly speaking the tensor  $\Omega_{ik}$  moves with the flow defined by the particle equations of motion; in particular,  $\Omega_{lj}(q, 0) = 0$  implies  $\Omega_{ik}(q, t) = 0$  for all future times [16].

A momentum field obeying  $\Omega_{ik} = 0$  is referred to as irrotational momentum field. It corresponds to the case  $m = 0$  and is, according to (21), given by the  $n$ -dimensional gradient of a single Clebsch potential  $S$ ,

$$M_k(q, t) = \frac{\partial S(q, t)}{\partial q_k}. \quad (25)$$

For such a field there are  $n - 1$  functional relations between the  $M_i$  no matter how large the number of particles. A physical reason for such strong dependencies between the momentum components cannot be seen. In particular, it would be reasonable to assume that for  $N = 1$  the number of independent components is not 1 but equal to the maximal possible number 3, as there is no restriction in principle for momenta in three-dimensional space. In spite of this unsatisfactory situation, which will be discussed further in IV, the case of the irrotational momentum field is important because it leads to Schrödinger's equation.

For irrotational momentum fields the change of dynamical variables from  $M_i$  to  $S$  is very simple. As a consequence of Eq. (25) the bracket in the canonical condition (13) vanishes. The latter reduces to the Hamilton-Jacobi equation if an unspecified function  $f(t)$  is eliminated by means of a redefinition of  $S(q, t)$ . If we add the particle equation (12) and the continuity equation (15), we obtain the three basic differential equations

$$\dot{q}_k = V_k(q, \frac{\partial S(q, t)}{\partial q}, t), \quad (26)$$

$$\frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}, t) = 0, \quad (27)$$

$$\frac{\partial \rho(q, t)}{\partial t} + \frac{\partial}{\partial q_k} \rho(q, t) V_k(q, \frac{\partial S}{\partial q}, t) = 0. \quad (28)$$

Thus, the irrotational case may be described by only two dynamical field variables,  $S(q, t)$  and  $\rho(q, t)$  no matter how large  $n$ . These equations have to be solved as initial value problems; the steps required to calculate trajectories are similar to the ones listed in section 2.1.

The physical interpretation of the new dynamical variable  $S(q, t)$  may easily be found by comparing (27) with the projected action equation in the form (18). The variable  $s(q, t)$  is defined in terms of the phase space action  $S(q, p, t)$ , which is denoted by the same symbol  $S$  but depends on  $2n + 1$  variables, as follows:

$$s(q, t) = S \left( q, \frac{\partial S}{\partial q}, t \right). \quad (29)$$

Inserting (25) in the projected action equation (18) and using (27) shows that  $S(q, t)$  differs from  $s(q, t)$  by a function which is constant along the trajectories defined by the velocity field  $v(q, t) = V(q, \frac{\partial S}{\partial q}, t)$ :

$$\frac{D}{Dt}(s - S) = 0. \quad (30)$$

Thus, the potential  $S(q, t)$  is closely related to the projected action integral  $s(q, t)$ ; the simplest solution of (30) is the trivial solution  $s - S = 0$ .

Equations (27) and (28) represent the basic equations of the "quasi-quantal approximation" (QA) to PM, because (27) and (28) have been obtained here, in the framework of HLLK, as a first step to QT starting from classical physics. A linearization of these equations leads to Schrödinger's equation, as will be shown in section 5. The same equations (27) and (28) constitute also the basis of the so-called quasi-classical approximation of QT. Although both theories share the same basic equations, they differ in the additional conditions that also decisively determine the form of the solutions. In the QA the differential equations are to be solved with given initial values, as is the case in QT. In the quasi-classical approximation the solutions are mostly constructed with the help of complete solutions of the Hamilton-Jacobi equation using a phase space method that goes back to van Vleck [22]; this method will be discussed in more detail in section 6.

## 4 The structure of the quasi-quantal approximation

The basic equations (26), (27), (28) of the QA represent the result of the first of the two essential steps of the HLLK. They describe the simplest version of an ensemble theory projected onto configuration space  $\Sigma$ . Let us ask now whether or not this theory makes sense from a physical point of view. If not, we ask what further steps are required to construct a physically meaningful theory in  $\Sigma$ .

Our starting point was the physically meaningful theory PM of statistical ensembles in phase space  $\Omega$ . The fact that this theory makes physical sense is reflected in its mathematical structure. The Cauchy problem for systems of first-order ordinary differential equations is well-defined for rather weak mathematical conditions [23]. This implies that (almost) all solutions of PM are globally valid and that, consequently, these solutions define an invertible map

$$l_t : \Omega \rightarrow \Omega, \quad q = Q(t, q_0, p_0), \quad p = P(t, q_0, p_0), \quad (31)$$

of phase space onto itself. Actually, a continuous family of maps (31), parametrized by the time  $t$ , exists corresponding to the fact that, at each instant of time, each point of phase space belongs to a single trajectory. The existence of this family implies the validity of the Liouville equation (3) which is, like all fundamental laws of nature, a *linear* differential equation. Linearity is a necessary and sufficient condition for "global validity" of a physical law as mentioned already in section 1. The global validity of the Liouville equation and the global validity of the canonical equations are closely related to each other.

During the transition from PM to QA the manifold of independent variables has been reduced from  $\Omega$  to  $\Sigma$ . An invertible map, analogous to (31) but now for the reduced manifold of QA, would be given by

$$l_t^c : \Sigma \rightarrow \Sigma, \quad q = Q^c(q_0, t). \quad (32)$$

If such a map existed, it would imply a globally valid, linear "Liouville equation" in configuration space, which would then be the universal law, we were looking for. Such a map does not exist, as mentioned already. From the solution of the initial-value problem of the Hamilton-Jacobi equation (27) the associated momentum field  $M(q, t)$ , with initial value  $M_0(q)$ , may be calculated with the help of relation (25). Then, particle trajectories  $q(t)$ ,  $p(t) = M(q(t), t)$  on the (irrotational) momentum surface  $\mathbb{M}$  are obtained as solutions of Eqs. (26). These trajectories are locally well-defined, in a certain vicinity of  $t_0$ , but the momentum surface  $\mathbb{M}$  defined by  $M_0(q)$  immediately starts deforming during its movement through phase space. As a consequence, the map from configuration space to the (deformed) momentum hypersurface  $\mathbb{M}$  becomes multivalued and the concept of trajectories breaks down in QA. This breakdown is closely related to the nonlinearity of Eq. (27). Clearly, we cannot cover the whole of phase-space by means of a single momentum surface (we would need an infinite number as in the "complete solutions" of the theory of canonical transformations).

The breakdown of the concept of particle trajectories is not related to the introduction of potentials; this also happens in the earlier theory, with hydrodynamic variables, reported in section 2. However, in the QA, as derived from QT, the singularities that occur when the concept of trajectories collapses have been carefully studied, see e.g. [24–26]. Thus, the concept of trajectories - which represents the "deterministic part" of our probabilistic theory - is still



present in the QA but has been seriously "weakened", due to its loss of global validity. This is the price we have to pay for the enormous reduction in the number of degrees of freedom brought about by the projection.

This discussion leads us to suspect that we cannot construct a globally valid probabilistic theory for particles in configuration space, while keeping at the same time the concept of particle trajectories intact. This raises several fascinating philosophical questions (concerning "reality", "completeness", and others) which lie outside of the scope of the present paper. A probabilistic particle theory makes predictions of a probabilistic nature (predictions to be verified by means of statistical ensembles) about particles. This definition, which is based on the physical principle of verification by observation, does not require that deterministic laws for particle trajectories are part of a probabilistic theory. Theories of this kind, where not only the initial values are uncertain (as in PM) but also the laws of movement themselves are "uncertain" or "unknown" (or possibly "nonexistent", whatever that may mean exactly) have been called "Type 3 theories" in a recent work of the present author [27].

This discussion also leads us to suspect that QT is a globally valid modification of the QA. In order to test if this working hypothesis is true we have to *linearize* the partial differential equations (27), (28). This will be done in section 5; an alternative way of deriving the resulting linear equations will also be described in section 5. There is no other way to restore the former global validity (of PM in phase space) in configuration space. We have to accept that this step will completely eliminate the deterministic concept of particle trajectories.

## 5 Transition to quantum theory

In this section the second essential step of the HLLK is carried out, which leads from the QA to the final QT. Two different variants of this step are reported which lead to the same result, but illuminate the nature of QT from two different angles. Furthermore, we examine the relationship between Kelvin's theorem and the condition for uniqueness of the wave function.

### 5.1 Transition by linearization

The linearization of the spinless version of the QA, which we consider in this work, can be carried out in a relatively simple way. As a first step we introduce a quasiquantal wave function which is defined in an analogous way as in II:

$$\psi = \sqrt{\rho} e^{\frac{i}{\hbar} S}. \quad (33)$$

However, the quantities  $S$  and  $\rho$  satisfy now (27) and (28). In order to be able to carry out a comparison with the original equations (6) and (3) in phase space, we use the explicit functional form of the Hamilton function  $H(q, p) = p_k p_k / 2m + V(q)$  and write equations (27) and (28) in the following

form:

$$D_t S = \bar{L}, \quad (34)$$

$$\hat{\mathbb{L}}_{\frac{1}{2}} \rho^{\frac{1}{2}} = 0, \quad (35)$$

where the Lagrangian  $\bar{L}$  and the operator  $\hat{\mathbb{L}}_{\frac{1}{2}}$  are defined by  $\bar{L} = \frac{1}{2} v_k M_k - V(q)$  and  $\hat{\mathbb{L}}_{\frac{1}{2}} = \partial_t + v_k \partial_k + \frac{1}{2} (\partial_k v_k)$ . We introduced here the abbreviations  $\partial_t$ ,  $\partial_k$  for the derivatives with respect to  $t$ ,  $q_k$  and the abbreviation  $D_t$  for the total derivative as defined in Eq. (20). Comparing (34), (35) with the phase space relations (6) and (3) we find that the following properties that are valid in phase space are no longer valid in configuration space: (1) the divergence of the velocity field vanishes, (2) the probability density moves with the flow, and (3) the operator  $v_k \partial_k$  multiplied by the imaginary unit is self-adjoint.

In the next step we evaluate the expression  $-\frac{\hbar}{i} \hat{\mathbb{L}}_{\frac{1}{2}} \psi$ . Using the basic Eqs. (34), (35) we obtain the relation  $(-\frac{\hbar}{i} \hat{\mathbb{L}}_{\frac{1}{2}} + \bar{L}) \psi = 0$  which is equivalent to (27) and (28), and has some similarity to the generalized Koopmann-von Neumann equation derived in I. We have to transform this equation, which takes the form

$$\left[ -\frac{\hbar}{i} \partial_t - \frac{\hbar}{i} v_k \partial_k - \frac{1}{2} \frac{\hbar}{i} (\partial_k v_k) + \frac{1}{2} v_k (\partial_k S) - V(q) \right] \psi = 0, \quad (36)$$

when written out, into an equation (not necessarily linear) for the complex variable  $\psi$ . According to the definition of  $\psi$  it is possible to replace the derivatives of  $S$  by the derivatives of  $\psi$  and  $\rho$ . This may be done with the help of the relation

$$(\partial_k S) \psi = \frac{\hbar}{i} \left[ \partial_k \psi - \frac{1}{2\rho} (\partial_k \rho) \psi \right], \quad (37)$$

whose validity is easily verified with the help of the definition (33). We replace the fourth term of (36) with the help of (37) and write the third term of (36) in the form

$$-\frac{1}{2} \frac{\hbar}{i} (\partial_k v_k) \psi = -\frac{1}{2} \frac{\hbar}{i} \partial_k v_k \psi + \frac{1}{2} \frac{\hbar}{i} v_k \partial_k \psi. \quad (38)$$

Using (37) again, the equation of motion (36) takes the form

$$\left[ -\frac{\hbar}{i} \partial_t + \frac{\hbar^2}{2m} \left( \partial_k + \frac{1}{2\rho} (\partial_k \rho) \right) \left( \partial_k - \frac{1}{2\rho} (\partial_k \rho) \right) - V(q) \right] \psi = 0. \quad (39)$$

A few further elementary manipulations finally lead to the nonlinear differential equation

$$\left[ -\frac{\hbar}{i} \partial_t + \hat{H} \right] \psi + \frac{\hbar^2}{2m} \frac{1}{\sqrt{\rho}} (\partial_k \partial_k \sqrt{\rho}) \psi = 0, \quad (40)$$

where  $\hat{H} = \frac{1}{2m} \hat{p}_k \hat{p}_k + V(q)$ ,  $\hat{p}_k = \frac{\hbar}{i} \partial_k$ , and  $\rho = \psi^* \psi$ . The “quantum-like” differential equation (40) for the complex variable  $\psi$  is essentially equivalent to

the relations (27) and (28), apart from certain uniqueness conditions [28] for  $\psi$  which are not important in the present context (see however section 5.3). The classical equation (40) has been reported several times before in the literature (see e.g. [27, 29–31]), what is new here is the derivation from first principles.

Two steps have always to be carried out in the HLLK, a linearization and a projection onto configuration space. If the vortical component of the momentum field is neglected, as is done here, the order of these two steps does not matter. In order to illustrate this point it is instructive to compare the quasi-classical equation (40) with the quantum-like classical (phase space) equation

$$\left[ \frac{\hbar}{i} \frac{\partial}{\partial t} - \frac{\hbar}{i} \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} + \frac{\partial H}{\partial p_k} \left( \frac{\hbar}{i} \frac{\partial}{\partial q_k} - p_k \right) + H \right] \psi^{(c)} = 0. \quad (41)$$

This extension of the Koopman-von Neumann equation [32] is useful when studying the relation between classical physics and QT (see I,II) or when investigating the problem of quantum-classical coupling [33], [34]. The classical wave function  $\psi^{(c)}$  is defined as in (33) but with  $\rho$  and  $S$  depending on  $q, p, t$ . The classical equation (41) is the result of a suitable linearization in phase space, which was carried out in I as a first step. The second step in I, the projection onto the configuration space was realized by implementing the quantization rules

$$\frac{\partial}{\partial p_k} = 0, \quad p_k = \frac{\hbar}{i} \frac{\partial}{\partial q_k} \quad (42)$$

which may easily be read off from (41). On the other hand, the quasi-classical equation (40) is obtained by performing a suitable projection onto configuration space in a first step. Roughly speaking, this first step corresponds to the first of the above quantization rules. The linearization is now the second step; it may be carried out very easily by omitting the nonlinear term in (40). The second, more familiar quantization rule in (42) is described by equation (37), where the second term on the right-hand side has to be omitted as a consequence of the linearization. The final result is the same in both cases, namely Schrödinger's equation

$$\left[ \frac{\hbar}{i} \frac{\partial}{\partial t} + H \left( q, \frac{\hbar}{i} \frac{\partial}{\partial q_k} \right) \right] \psi(q, t) = 0. \quad (43)$$

In I we referred to (41) as classical counterpart of Schrödinger's equation. In the same sense, we might now refer to equation (40) as quasi-classical counterpart of Schrödinger's equation.

An interesting question is how the basic equations of the QA are modified in the transition to QT. A brief calculation, first performed by Madelung [35], shows that the continuity equation (28) remains unchanged

while the Hamilton-Jacobi equation (27) takes the following form:

$$\frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}) = \frac{\hbar^2}{2m} \frac{1}{\sqrt{\rho}} (\partial_k \partial_k \sqrt{\rho}). \quad (44)$$

Thus, the transition from QA to QT leads to an additional term  $T_Q = (\hbar^2/(2m\sqrt{\rho}))(\partial_k \partial_k \sqrt{\rho})$  on the right-hand side of (27). Due to its derivation, this term is a quantum correction to the kinetic energy, as could have been guessed from the form of its prefactor. Clearly, the term  $T_Q$  introduces a coupling between the action variable  $S$  and the probability density  $\rho$ . What does that mean exactly?

Let us recall that in the QA the action variable  $S$  defines a particle momentum at every point of configuration space. The solutions  $S$  of the Hamilton-Jacobi equation define, in combination with the particle equation (26), particle trajectories - even if these trajectories are only locally well-defined as discussed in section 4. Clearly, the coupling term  $T_Q$  destroys this quasiclassical concept of a local particle momentum. Let us recall at this point that equations (28) and (44) are to be solved as an initial value problem. From the very beginning, all particle trajectories and momenta are “mixed together”, depending on the specification of  $S$  and  $\rho$  at time  $t = 0$ . As a result, the particle equation (26) loses its meaning in QT. Only the two partial differential equations (44) and (28) survive the transition to QT. These two relations, which are equivalent to Schrödinger’s equation (43), determine the time-development of an object, which may be described as a new kind of *ensemble where no separation of deterministic and probabilistic properties is possible*.

Using the nomenclature of reference [27], we may say that, starting from PM and arriving at QT, we performed a transition from a type 2 theory to a type 3 theory. In a type 2 theory there are deterministic laws for trajectories, while the initial conditions must be described by probabilities [27]. In a type 3 theory only probabilities and expectation values may be obtained, which, however, may be of an unusual form. The peculiar (operator) form of the observables in QT indicates that a clear separation, in a classical sense, between “observables” and “states” is no longer possible.

In summary, it can be said that a randomization took place during the transition from PM to QT, and that the remaining elements of determinism, still present in PM, were eliminated. In the forthcoming paper IV it will be shown that this basic structure is retained in the framework of a more realistic description of the momentum field.

## 5.2 Transition by randomization

The above derivation of Schrödinger’s equation is based on the idea that a fundamental law of nature must permit a large variety of solutions. This leads to the requirement of linearity. The resulting theory is purely probabilistic - without deterministic laws for particle trajectories. In this sense, the physical effect of the formal process of linearization may be interpreted as a randomization.

In this section we try to understand the transition to the new probabilistic theory in more detail. The following developments represent an improved version of earlier work [7, 27] of the present author.

Our task is to construct a theory in which the deterministic equation (26) is no longer included, but which is otherwise as similar as possible to the basic equations (27) and (28) of QA. Therefore, we continue to use  $\rho$  and  $S$  as our basic variables. Furthermore, we assume that the fundamental conservation law of probability (28) remains unchanged. Another reasonable assumption is that the particle equations of motion (1) “survive” in a statistical sense, i.e. hold true not for particle variables but for the corresponding expectation values,

$$\frac{d}{dt}\overline{q_k} = \frac{\overline{p_k}}{m}, \quad \frac{d}{dt}\overline{p_k} = \overline{F_k}. \quad (45)$$

Here, the expectation values in configuration space  $\overline{q_k}$ ,  $\overline{p_k}$ ,  $\overline{F_k}$  are defined as follows:

$$\overline{q_k} = \int dq \rho(q, t) q_k, \quad (46)$$

$$\overline{p_k} = \int dq \rho(q, t) \frac{\partial S}{\partial q_k}, \quad (47)$$

$$\overline{F_k} = - \int dq \rho(q, t) \frac{\partial V}{\partial q_k}. \quad (48)$$

The assumption that the deterministic equations of QA may be replaced during the transition to QT by a statistical version is quite natural and has been mentioned several times in the literature. However, as will soon become clear, it is not sufficient to establish the structure of QT unambiguously; further plausible assumptions, concerning the probabilistic structure of QT, must be made to achieve this.

Using the second of the Ehrenfest-like relations (45) and the continuity equation (28) we derive the following integrodifferential equation:

$$\int dq \frac{\partial \rho}{\partial q_k} \left[ \frac{\partial S}{\partial t} + \frac{1}{2m} \sum_j \left( \frac{\partial S}{\partial q_j} \right)^2 + V \right] = 0. \quad (49)$$

In accordance with our general strategy of constructing a theory that is as similar as possible to Eqs. (27) and (28) we try to replace the integrodifferential equation (49) with a differential equation of standard form

$$\bar{L}(q, t) - L_0 = 0, \quad (50)$$

which differs from (27) only by an additional term  $L_0$  which may depend, in principle, on the variables  $S$  and  $\rho$  as well as their derivatives. The quantity

$\bar{L}$  in (50) is an abbreviation for the square bracket in Eq. (49),

$$\bar{L} := \frac{\partial S}{\partial t} + \frac{1}{2m} \sum_j \left( \frac{\partial S}{\partial q_j} \right)^2 + V. \quad (51)$$

We see that the statistical condition (45) is not sufficient to determine the form of the basic equations. The unknown function  $L_0$  must obviously [see Eq. (49)] obey the constraint

$$\int dq \frac{\partial \rho}{\partial q_k} L_0 = 0, \quad (52)$$

which is not sufficient to determine its functional form. Further constraints of a statistical nature are required to fix  $L_0$ .

A statistical constraint that is in agreement with our general strategy is the following. We require that the space-time average of the difference between  $\bar{L}$  and  $L_0$  is minimal. This leads to the variational problem

$$\delta \int dt \int dq \rho (\bar{L} - L_0) = 0. \quad (53)$$

In order to write down the Euler-Lagrange equations for  $\mathcal{L} = \rho (\bar{L} - L_0)$  in a compact way, we introduce the two-component field  $\chi_\alpha$ , with  $\chi_1 = \rho$  and  $\chi_2 = S$ . If derivatives up to first order with respect to  $t$  and second order with respect to  $q_k$  are taken into account, the Euler-Lagrange equations of the variational problem (53) are given by

$$\frac{\partial \mathcal{L}}{\partial \chi_\alpha} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial (\partial_t \chi_\alpha)} - \frac{\partial}{\partial q_k} \frac{\partial \mathcal{L}}{\partial (\partial_k \chi_\alpha)} + \frac{\partial}{\partial q_k} \frac{\partial}{\partial q_l} \frac{\partial \mathcal{L}}{\partial (\partial_k \partial_l \chi_\alpha)} = 0. \quad (54)$$

For the “correct”  $L_0$ , the Euler-Lagrange equations, with regard to  $\rho$  and  $S$ , must agree with the new field equations and the function  $\rho (\bar{L} - L_0)$  must agree with the Lagrangian density. On the other hand, we have already determined the form of these field equations; they are given by (50) and (28) and do *also* depend on  $L_0$ . The field equations are therefore overdetermined if both the conditions (50) and (28) and the variational equations (54) are implemented. Thus, these conditions can be used to determine, or at least restrict, the unknown function  $L_0$ , which must be a solution of the four equations (54), (50), (28).

As for the functional form of  $L_0$ , we assume that  $L_0$  does not depend on the derivatives of  $\rho$  and  $S$  with respect to time  $t$ ; such a dependency would change the basic structure of the evolution equations. Further, if  $L_0$  depends on  $S$  and its derivatives, the validity of the continuity equation requires, as a consequence of (54), a complicated dependence of  $L_0$  on the momentum distribution of the considered system. The simplest and at the same time most general  $L_0$  (not depending on the considered system) can only depend on  $\rho$  and its derivatives with respect to  $q_k$ ,  $L_0 = L_0(\rho, \partial_k \rho, \partial_k \partial_l \rho)$ . Then, we find

from Eqs. (54), (50), (28) that  $L_0$  must obey the condition

$$\rho \frac{\partial L_0}{\partial \rho} - \frac{\partial}{\partial q_k} \rho \frac{\partial L_0}{\partial (\partial_k \rho)} + \frac{\partial}{\partial q_k} \frac{\partial}{\partial q_l} \rho \frac{\partial L_0}{\partial (\partial_k \partial_l \rho)} = 0. \quad (55)$$

The second order derivatives in  $L_0$  must be taken into account but should not lead to contributions of higher order in the variational equations. The simplest nontrivial solution of (55) that satisfies this requirement is given by

$$L_0 = B_0 \left[ -\frac{1}{2\rho^2} \sum_k (\partial_k \rho)^2 + \frac{1}{\rho} \sum_k \partial_k \partial_k \rho \right], \quad (56)$$

where  $B_0$  is a constant. The second term in the square bracket, multiplied by  $\rho$ , is a “Null-Lagrangian”, which means that it does not contribute anything to the Euler-Lagrange equations [see (55)]. It is easy to verify that this  $L_0$  also fulfills condition (52). If  $\rho$  is replaced by the amplitude  $\sqrt{\rho}$  and the constant  $B_0$  is replaced by  $\hbar^2/4m$ , then one obtains the simpler expression

$$L_0 = \frac{\hbar^2}{2m} \frac{1}{\sqrt{\rho}} (\partial_k \partial_k \sqrt{\rho}). \quad (57)$$

Thus, the term  $L_0$  agrees with the term  $T_Q$  defined earlier, and the randomized field equation (50) agrees exactly with the modified Hamilton-Jacobi equation (44) obtained by linearization. This means that Schrödinger’s equation may be derived either by linearizing equations (27), (28) according to section 5.1, or by “randomizing” these equations in the sense of condition (53).

If the term  $\rho L_0$  is integrated over the configuration space, the second term in the square brackets of (56) gives no contribution and one obtains

$$\int dq \rho L_0 = -\frac{B_0}{2} I[\rho], \quad (58)$$

where  $I[\rho]$  is the Fisher information functional, defined by

$$I[\rho] = \int dq \rho \sum_k \left( \frac{\partial_k \rho}{\rho} \right)^2. \quad (59)$$

While the second term in the square brackets of (56) gives no contribution to the variation it is nevertheless indispensable, because without it condition (52) could not be fulfilled. Fortunately, the same term is generated again when the first term of (56), i.e. the Fisher functional, is varied. The same final result is therefore obtained by adding the integrand of the Fisher functional to the Lagrangian density  $\rho \bar{L}$  of the original system and performing the variation. In this way Schrödinger’s equation was derived by Reginatto [4], see also [36].

The importance of the concept of Fisher information for the construction of the field equations of physics has been particularly emphasized by Frieden [37, 38]. The Fisher functional (59) takes its smallest value zero for spatially constant probability densities. Physically meaningful results are obtained if the requirement for minimal Fisher information is combined with suitable constraints. The situation is basically the same as with the entropy functional, which is written in configuration space as

$$S[\rho] = - \int dq \rho(q) \ln \rho(q), \quad (60)$$

where a proportionality constant has been omitted. If, as the simplest case, one considers discrete probabilities and only requires as an additional condition that the sum of all probabilities is 1, then one obtains the most fundamental result of probability theory from the requirement of maximum entropy, namely that all probabilities must be equal. Other constraints lead to the well-known probability distributions of statistical physics.

In contrast to the Boltzmann-Shannon entropy (60), the Fisher information (59) contains the first derivatives of the probability density. While varying  $S[\rho]$  yields algebraic equations, varying  $I[\rho]$  yields differential equations. One can view the Fisher information as a local variant of the global Boltzmann Shannon entropy. It defines what form the terms of a differential equation must have, so that passing from one point in the state space to the next, one is in accordance with the laws of probability theory.

This interpretation of the Fisher information is confirmed by a comparison with the “relative entropy” or Kullback-Leibler entropy [39], defined by

$$G[\rho, \chi] = - \int dq \rho(q) \ln \frac{\rho(q)}{\chi(q)}, \quad (61)$$

where  $\chi(q)$  is the initial, “prior”, probability density relative to which  $\rho$  is to be determined. We identify  $\chi(q)$  with the probability distribution  $\rho(q_1, \dots, q_k + \Delta q, \dots, q_n)$  obtained from  $\rho$  by shifting the  $k$ -th coordinate  $q_k$  by an amount  $\Delta q$ , and denote the resulting relative entropy by  $\Delta G_k[\rho]$ . For small  $\Delta q$  one obtains in leading order the result

$$\Delta G_k[\rho] = -\frac{1}{2}(\Delta q)^2 \int dq \rho(q) \left( \frac{\partial_k \rho}{\rho} \right)^2, \quad (62)$$

Thus, the Fisher information (59) is obtained, apart from a proportionality constant, by adding up the contributions  $\Delta G_k[\rho]/(\Delta q)^2$  from all coordinates.

The transition from the unphysical theory QA to the physically meaningful theory QT may thus be performed using two methods motivated by quite different physical ideas but leading to the same final result; either way seems plausible and almost inevitably. We will see in IV that this duality persists if a complete representation of the momentum field is used. The second method,



the derivation of QT by means of a randomization, is longer than the first, but also more detailed. It gives maximal insight into the structure of QT - in relation to PM - because both essential steps, the projection and the linearization, are not treated as discontinuous processes but are resolved into their components. The second method is also useful in view of a comparison with other attempts to derive QT from a deeper structure (see section 7).

### 5.3 Poincaré invariant and quantization condition

The physically meaningful solutions of the Schrödinger equation must meet two additional conditions. First, the total probability of finding the particle(s) anywhere must be equal to one. This condition is also present in the classical theory from which QT was derived and needs no further explanation. Naturally, its influence on the form of the solutions is relatively strong for confined systems, that are located in a bounded spatial area. Second, the quantum mechanical state variable  $\psi$ , as defined by (33), must be a single-valued function in configuration space (at each instant of time). This allows for multi-valued functions  $S/\hbar$  whose values differ from each other by multiples of  $2\pi$ . This single-valuedness condition is especially important for the determination of the spectra of atomic systems and was called “quantization condition” in the old quantum theory. The question arises whether or not an analogous structure exists in the field of classical physics. A more complete discussion will be given in IV where the  $\hbar$ -dependence of the vortical terms of the momentum field will also be taken into account.

Such a structure can be found in the concept of integral variants. Let us briefly recapitulate this concept. For our purposes it is useful to consider non-autonomous dynamical systems, with velocity field  $V(x, t)$ , whose basic equations are given by

$$\dot{x}_k = V_k(x, t). \quad (63)$$

Here,  $x = (x_1, \dots, x_m)$  denotes a point in a  $m$ -dimensional space  $\mathbb{A}$ . Let us consider an arbitrary closed contour  $C_0$  in  $\mathbb{A}$  at a fixed time  $t_0$ . The solutions of (63) transform each point of the contour  $C_0$  to a different point at a later (fixed) time  $t$ . The totality of all transformed points forms again a closed contour  $C_t$ , at time  $t$ , as a consequence of continuity. The contour may change its form but remains a contour if transformed according to the flow; adopting a term from fluid mechanics we may say that the contour is “moving with the fluid”. The solutions of (63) may be written as  $x_k(t, u)$  where  $u$  is a parameter varying, say, in the interval  $[0, 1]$ . For fixed  $t$  the points  $x_k(t, u)$  trace out a closed contour (with  $x_k(t, 0) = x_k(t, 1)$ ), for fixed  $u$  the points  $x_k(t, u)$  describe trajectories. The totality of all trajectories is referred to as tube.

Consider now a vector field  $G(x, t)$  on  $\mathbb{A}$ , which may also parametrically depend on time  $t$ . The contour integral

$$I(t) = \oint_{C_t} G_i(x, t) dx_i \quad (64)$$

depends for given  $C_0$  on the time  $t$  and on the analytical form of the field  $G(x, t)$ . Evaluating the derivative of (64) with respect to time, one obtains the following necessary and sufficient condition for the invariance of  $I(t)$  along the considered tube [40]:

$$\oint_{C_t} dx_i \left\{ \frac{\partial G_i}{\partial t} + \left( \frac{\partial G_i}{\partial x_k} - \frac{\partial G_k}{\partial x_i} \right) V_k \right\} = 0. \quad (65)$$

If  $G(x, t)$  fulfills condition (65) the contour integral (64) is referred to as a (linear, relative) “integral invariant”.

Let us start in phase space and specialize this formalism to autonomous systems of Hamiltonian type. We have  $\mathbb{A} = \Omega$ ,  $m = 2n$ ,  $x = (q_1, \dots, q_n, p_1, \dots, p_n) = (q, p)$  and

$$V(q, p, t) = \left( \frac{\partial H(q, p)}{\partial p}, -\frac{\partial H(q, p)}{\partial q} \right), \quad (66)$$

which means that (63) agrees with the canonical equations. The latter may also be written in the form  $\dot{x} = Z \frac{\partial H}{\partial x}$  where  $Z$  is an antisymmetric  $2n \times 2n$  matrix with constant elements (the matrix  $Z$  is sometimes referred to as symplectic matrix). It can be shown that essentially only a single integral invariant of type (64) exists, which is defined by  $G(q, p, t) = (p_1, \dots, p_n, 0, \dots, 0)$ . The corresponding line integral

$$\oint_{C_t} p_i dq_i, \quad (67)$$

whose invariance is easily verified, is referred to as Poincaré integral invariant. The antisymmetric matrix in (65), which is the  $2n$ -dimensional counterpart of the rotation of a vector in three dimensions, agrees with the constant matrix  $Z$

$$\frac{\partial G_i}{\partial x_k} - \frac{\partial G_k}{\partial x_i} = Z_{ik}. \quad (68)$$

Thus, the “vorticity tensor” of the vector field  $G(q, p, t)$  is the same for all points of phase space, as a consequence of its simple (linear in  $q$  and  $p$ ) structure. The Poincaré invariant cannot be used to characterize individual systems, but rather describes certain structural properties of the theory; the same applies to the conceptually similar but more general Poincaré-Cartan invariant, which may be used as an axiomatic basis for the whole theory [41].

This situation changes if the replacement  $p_k \rightarrow M_k(q, t)$  is performed. After projection to the  $n$ -dimensional subspace defined by  $M$ , the Poincaré integral invariant takes the form

$$I_{\bar{C}}(t) = \oint_{\bar{C}_t} M_i(q, t) dq_i. \quad (69)$$

Comparing the canonical condition (13) with the invariance condition (65) one sees immediately that the latter is fulfilled if  $h(q, t)$  is a single-valued function.

In phase space arbitrary closed paths were allowed. Now, the allowed closed paths, denoted here by  $\vec{C}_t$ , as well as the tube formed by the solutions of (12), must lie in the subset  $(q, M(q, t))$  of  $\Omega$ . As a consequence, the Poincaré invariant may now be used to characterize individual systems, it depends not only on the considered path but also on the initial value  $M_0(q)$ . The vorticity tensor  $\Omega_{ik}(q, t)$ , as defined by (24), is not a constant anymore but varies in configuration space in a way depending on the considered momentum surface. This means that vorticity for individual physical systems does not exist in phase space but only arises through the projection onto the configuration space. This is remarkable in view of the fact that vorticity is the (quasi-)classical [more precisely: the quasi-quantal] counterpart of quantum spin, as will be shown in IV.

The tensor  $\Omega_{ik}(q, t)$  is the  $n$ -dimensional generalization of the fluid-dynamical “vorticity”, which is given by  $\vec{\nabla} \times \vec{u}$  where  $\vec{u}$  is the velocity field. The constant  $I_{\vec{C}}$  is also referred to as “circulation”. For  $n = 3$  several of the above relations agree - after a proper reinterpretation of the variables - with the dynamic equations for an ideal barotropic fluid. In this fluid-dynamical context the invariance of the circulation is referred to as Kelvin’s theorem.

In the next step we specialize to irrotational momentum fields (25). In this case the circulation (69) vanishes for arbitrary  $\vec{C}$  given that  $S(q, t)$  is single-valued. The invariance condition (65) takes the form

$$\oint_{\vec{C}_t} dq_i \frac{\partial h(q, t)}{\partial q_k} = 0, \quad (70)$$

if the derivative of  $M$  with respect to time is replaced with the help of the Hamilton-Jacobi equation (27). This condition, the single-valuedness of  $h(q, t)$ , is the same as for general momentum fields. Vorticity and circulation vanish by definition, except in the presence of topological singularities of  $S(q, t)$ . In the present formalism QA there are, however, no natural causes for such topological singularities. We may say that Kelvin’s theorem holds true in the QA (We remind the reader at this point that the theory QA is generally unstable, as discussed in section 4; we are considering a possibly small period of time in which stability prevails).

If we carry out the transition to QT as a last step, we obtain an unchanged continuity equation (28), and a modified Hamilton-Jacobi equation (44). These two differential equations are to be solved taking the above multi-valuedness condition for  $S$  into account; if required by the considered physical system. The particle-like Eq. (26) played no role in the transition to QT; according to our discussion in section 5.1 this equation has no independent physical meaning in QT anymore. The validity of Kelvin’s theorem in QA, as expressed by the validity of Eq. (70), is an indication of the fact that the concept of particle motion is still valid in QA. We can test Eq. (26) in this regard by seeing whether or not a conservation law of the type of Kelvin’s theorem still exists

in the QT. Using (44) the invariance condition (65) takes the form

$$\oint_{\tilde{C}_t} dq_i \frac{\partial}{\partial q_i} \left[ h(q, t) - \frac{\hbar^2}{2m} \frac{1}{\sqrt{\rho}} (\partial_k \partial_k \sqrt{\rho}) \right] = 0. \quad (71)$$

At first glance, this equation looks similar to (70), since the integrand is given by a gradient in both cases. Due to the coupling between the phase  $S$  and the probability density  $\rho$  in Eq. (44), however, there is now a natural source for singularities, since  $S$  is undefined at the zeros of  $\rho$  and may become discontinuous there. This happens quite often in QT and leads to a multivaluedness of  $S$ , which is characterized by an integer  $n$  different from zero. The question is if this  $n$  remains the same if the path  $\tilde{C}_t$  changes as a function of time according to the differential equation (26). Damski and Sacha have shown that this is generally not the case by examining several simple physical systems [42]. Vortices in the quantum mechanical probability fluid are rather unstable. Vortices in many-particle systems (superfluid phases), which are described by non-linear field equations, are more stable.

This means that Kelvin's theorem does not hold true in the QT. There is no support, from this point of view, for the idea that Eq. (26) describes the motion of real particles. The analogy between Kelvin's theorem and the quantization condition is of a formal nature. Kelvin's theorem is of dynamical origin, while the quantization condition has a topological cause, namely the uniqueness of the state variable  $\psi$ . The need to introduce a new state variable is ultimately due to the requirement for *linearity* of the basic equations - which is one of the two fundamental requirements of the HLLK.

## 6 Concerning the interpretation

The vast number of different interpretations of the quantum theoretical formalism is closely related to the poorly understood relationship between QT and classical physics. In this section we examine what the theory developed in the present series of works, the HLLK, can contribute to a better understanding of this relationship. When we speak of the relationship between QT and classical physics, we should more precisely distinguish the theory of the individual classical particles CM from the probabilistic description of classical particle ensembles PM. We speak of classical physics when a distinction between CM and PM is not necessary.

Let us consider the following three points that seem plausible at first glance. (1) We know that QT is suitable for describing microscopic reality while classical physics fails in this area. (2) A concept that has evolved over time and describes sometimes successfully the relationship between individual areas of physics is the principle of reductionism. Put simply, it means that the better theory - in the area under consideration - "contains" the worse theory. It is also said that the better theory "reduces" itself to the worse theory. In physics, this is understood to mean that the better theory changes into the worse one if the additional structure that is present in the better theory is "switched off"

(example: let the speed of light become infinite). (3) The additional structure that exists in QT, relative to classical physics, is associated with a new natural constant  $\hbar$ . If we consider these three points together - without a more detailed analysis - we arrive at the conclusion that classical physics must be the limiting case of QT in the limit of small  $\hbar$ .

This leads to the further question, which part of classical physics, CM or PM, arises for  $\hbar \rightarrow 0$ ? Depending on the answer, QT is either a theory of individual particles or of statistical ensembles. This question was one of the central points of disagreement between Bohr and Einstein [43]. This rhetorical battle was lost by Einstein, who advocated the ensemble theory. This was partly due to the fact that Einstein's physical arguments were not distinguished clearly from his metaphysical demand for a more complete theory. Basically, disregarding the rhetoric skills, one can say that the question remains undecided to this day.

## 6.1 Formal versus empirical reduction

Let us now take a closer look at the above three points. What exactly does it mean when we say that the better theory (QT) is reduced to the worse (CM or PM)? In order to answer this question we have to fall back on some very elementary facts. A physical theory is defined by a certain number of fundamental *equations*, mostly differential equations. With the help of the solutions of the fundamental equations (of a successful theory) one can describe a certain range of processes in nature. It is the *solutions* that decide whether a theory is successful or not.

The first clearly defined meaning of the term *reduction* is obtained when one considers the relationship between the fundamental equations. This means, for example, that the QT is reduced (in this sense) to the CM or to the PM if Schrödinger's equation in the limit of small  $\hbar$  merges into the canonical equations or into the Liouville equation. An important point is, that this kind of reduction has nothing to do with the question of the truth or falsity of the theories in question. For example, if the Liouville equation could be reduced to Schrödinger's equation, that would not mean that the Liouville equation is the better theory. Following Rosaler [44], we refer to this kind of reduction as *formal reduction*.

It is unsatisfactory to characterize the relationship between two theories solely on the basis of the formal relationship between their fundamental equations; the question which one of the two theories describes nature correctly, is of course of paramount importance and must also be taken into account. In order to introduce a meaningful concept of reduction from this point of view, one must compare the solutions of the corresponding theories - and the associated experimental results - with one another: The successful theory A is reduced to theory B, in a certain area, if the results of B are reproduced at least approximately in this area. Clearly, the concept of reduction has a slightly different meaning here and, due to the large number of possible solutions (systems), is by far not as sharply defined as in the formal case.

Using again the notation of Rosaler [44] we refer to this kind of reduction as *empirical reduction*.

## 6.2 The quantum-classical interface

The relationship between QT and classical physics has not been analytically investigated for an astonishingly long period of time; one can say that the majority approach was dominated by a philosophical principle, the principle of reductionism. In particular, no distinction was made between formal reduction and empirical reduction. However, we should also note that a considerable number of works exist that deviate from the majority view; several of these works are quoted in previous papers of the present author, see e.g. [7].

Let us start with the question of formal reduction, which is the one studied in the present work. The first systematic investigation of this question [45] led to the conclusion that, contrary to common belief, QT is not formally reducible to CM. A second recent study, reported in II, which took into account all the theoretical results obtained during the past decades, led to the stronger conclusion that QT can neither be reduced to CM nor can it be reduced to the probabilistic version PM of classical mechanics. In II it was shown that, to the contrary, PM may be reduced to QT. In the present work we arrived at the same conclusion, using a different method that allows us to study the details of the transition. This represents a radical change as compared to the common view. The projection method used in the present work can still be called a reduction, since phase space is larger than configuration space. However, this type of formal reduction is not associated with a vanishing  $\hbar$ , but to the contrary with the *creation* of this new fundamental constant. Its finite numerical value is a consequence of the randomization, or linearization, following the projection.

Let us proceed now to the question of empirical reduction. There are several systems in which an empirical reduction of QT to classical physics can be observed. The historically oldest case concerns transitions between highly excited atomic states. Here, an analogy to classical oscillators exists which is described by Bohr's correspondence principle. If the characteristic dimensions of a system are much larger than the De Broglie wavelength, then a classical approximation is often allowed. Generally speaking, the influence of typical quantum mechanical effects decreases when a characteristic quantity of the dimension of an action can be defined, whose numerical value is much larger than  $\hbar$ . In more complex systems, high particle numbers and high temperature have a similar effect. While all these effects have only an approximate character, they are undoubtedly real, so it is justified to speak of an empirical reduction of QT to classical physics.

Thus, there are two interfaces between QT and classical physics, a formal and an empirical one. Both interfaces are associated in a natural way with a direction. The formal interface is associated with the direction from classical physics (PM) to QT, the empirical interface is associated with the direction from QT to classical physics. In both cases we have transitions from a more

complicated structure to a simpler one, that is why we can speak of a reduction in both cases. For the formal reduction, the direction points from the phase space to the lower dimensional configuration space. For the empirical reduction the direction points from QT to (quasi-) classical systems, in which the fine structure of the complicated quantum effects is “smeared out”.

### 6.3 Which systems can be described by QT

Let us return to the question, asked at the beginning of this section, whether QT is able to describe the behavior of individual particles or whether sensible statements can only be made about statistical ensembles. (note that the original question, the one which played a central role in the discussions between Bohr and Einstein, is now asked from a different point of view). With the help of the above derivation of QT, performed in the framework of the HLLK, we are now able to answer this question.

Our starting point was the classical probabilistic theory PM. This theory still contains both probabilistic and deterministic elements. In a first step, this theory was projected onto the configuration space. This did not change the basic character of the theory, even if, as discussed in sections 2 and 4, the deterministic element was weakened. In a second decisive step, the deterministic relations were completely eliminated and an unavoidable inaccuracy - not only with regard to the initial values, but also with regard to the determination of the orbits of the particles - was introduced. This fundamental uncertainty was indicated by the occurrence of a new natural constant  $\hbar$ . In the theory derived this way there are no longer any individual particles. This does not mean that individual particles cannot *exist*; we just have no theory to describe them (and do not believe that such a theory exists). Instead of particle trajectories, there are measurement values, probabilities and expectation values. The answer to the above question is therefore that QT is not a single particle theory but is only able to describe statistical ensembles. It is well-known that the ensembles occurring in QT cannot be described by standard probability theory but this does not change the fundamental conclusion. Remarkably, Schrödinger already arrived at the same conclusion when analyzing the equation he had derived: “... the true laws of quantum mechanics do not consist of definite rules for the single path ...” [46].

This conclusion is at variance with the reductionistic view formulated at the beginning of this section, that the classical limit of QT must be CM. The formal considerations that have been undertaken, in order to support this historically evolved view, must be flawed somewhere if the present conclusion is to be correct.

If one examines the behavior of Schrödinger’s equation for small  $\hbar$ , one obtains the Hamilton-Jacobi equation and the continuity equation as leading terms of an asymptotic expansion. These differential equations agree with Eqs. (27) and (28), which were obtained by projection and subsequent introduction of potentials. On the other hand, the Hamilton-Jacobi equation also occurs in the theory of canonical transformations [see Eqs. (A1)-(A3)]. If

a complete solution  $F_1(q_1, \dots, q_n, a_1, \dots, a_n)$ , which depends on  $n$  parameters  $a_1, \dots, a_n$ , is known, the trajectories of all particles can be calculated. It was believed that this fact marked the transition from QT to CM. A complete solution with fixed numerical values of the parameters  $a_1, \dots, a_n$  was interpreted as (quasi-)classical counterpart of the quantum mechanical state vector. Pauli wrote in his “General principles of quantum mechanics” ([47], chapter VI, p. 91, bracket mine):

If in the solution  $S_0$  of ...[the Hamilton-Jacobi equation] no further parameter is present, it is one mechanical path and in the general case giving special numerical values to parameters  $a_1, \dots, a_n$ , ...occurring in  $S_0$  corresponds to a definite trajectory”.

In fact, a fixed choice of the parameters  $a_1, \dots, a_n$  does not correspond to a single trajectory but to an  $n$ -fold infinite set - a “family” - of trajectories, as equation (A2) shows. This leads to a contradiction to the idea that the wave function describes a single particle. Dirac expressed this contradiction in the following frequently quoted statement [14]:

The family does not have any importance from the point of view of Newtonian mechanics; but it corresponds to one state of motion in the quantum theory, so presumably the family has some deep significance in nature, not yet properly understood.

This contradiction persists to this day as one of the many contradictions that exist in the individuality interpretation of QT [48]. Similar contradictions are encountered when examining the behavior of wave packets in the limiting case of small  $\hbar$  [45]

This line of argument is flawed as a consequence of the fact that the solutions of Schrödinger’s equation are determined by their initial values. Therefore, the Hamilton-Jacobi equation (27), which is obtained for small  $\hbar$ , has also to be solved as an initial value problem and not as a complete solution problem. As a consequence, it is not immediately possible to set the quasi-classical limit of Schrödinger’s equation in correspondence to classical mechanics. In order to make it possible, Pauli and Dirac considered special solutions, which are obtained by assigning fixed numerical values to the  $n$  parameters  $a_1, \dots, a_n$  of a complete solution, as solutions to the initial value problem. However, this is not mathematically consistent. As is known from the theory of partial differential equations, one can construct arbitrary solutions to initial value problems if a complete solution is known [49, 50]. However, this requires the calculation of the envelope of a whole family of solutions with different values of the parameters  $a_1, \dots, a_n$ ; it is not possible to describe arbitrary initial conditions by simply assigning numerical values to the parameters. This is the error in the assertion that CM is the limiting case of QT for small  $\hbar$ . Let us mention once again that Eqs. (27) and (28) have to be solved as initial value problems. Thus, the quasi-classical limit of Schrödinger’s equation fully agrees with the present theory QA.

As far as Dirac’s statement is concerned, it is in the context of the ensemble interpretation obviously true (by construction) that a whole ensemble of



classical trajectories corresponds to a single quantum state. Dirac's ensemble has no special significance in the present theory, since here the ensembles are defined by initial conditions and not by complete solutions; the "deep significance" may of course be seen in the general validity of this correspondence. The ensemble interpretation is seldom able to answer the questions posed by the individuality interpretation and vice versa [51]. When making the transition from one interpretation to the other, it is the questions that are exchanged and not the answers.

## 7 Discussion

This series of works is based on the fact that there are mathematical structures in phase space that are very similar to mathematical structures of QT. This similarity becomes fully visible only when statistical ensembles of particles, instead of single particles, are considered.

Many of these structures are described in Sudarshan and Mukunda's outstanding book on analytical mechanics [52]. The solutions of the canonical equations for any observable  $A(q, p)$ , which takes the place of Hamilton's function, form a one-parameter group of canonical transformations in phase space (a realization of a corresponding one-parameter Lie group). These transformations are the classical counterparts of the unitary transformations in Hilbert space; the observables  $A(q, p)$  correspond to the self-adjoint operators that are the generators of these unitary transformations. The vanishing of the Poisson bracket of two observables  $A$  and  $B$  implies mutual invariance under the transformations generated by the other observable. As is well-known, the Poisson bracket of two observables is the classical counterpart of the commutator of the corresponding operators in QT. Each observable  $A$  creates a statistical ensemble with the help of a velocity field  $V_A$ , a probability density  $\rho_A$ , and a corresponding Liouville equation. In this work we have identified  $A$  with the Hamiltonian function  $H$ . The present method may, however, be used for any observable and leads to the same results as in II.

This summary shows that the mathematical and physical analogy between functions in phase space (describing states of ensembles) and vectors in Hilbert space is much stronger than the corresponding analogy for points in phase space (describing states of particles). Accordingly, only a few simple and natural additional assumptions have to be made, in the framework of HLLK, in order to derive QT from the above classical probabilistic structure PM. The first assumption is the introduction of a new dynamical variable  $S(q, p, t)$  that describes the purely deterministic content of the canonical equation in a compact way. A second fundamental assumption is that a projection to configuration space must be performed. This is plausible from a physical point of view; it is downright trivial if one considers the simplest formulation of QT, on the level of differential equations, and looks at the independent variables. The final result of the HLLK is a construction of QT that provides not

only the basic differential equation, but also most of the other structural elements of QT, such as the probability interpretation of the wave function, the explanation of why observables become operators, the eigenvalue equations for measurable values of operators, and Born's rule. A more complete list of structural elements of QT may be found in II. In the following work IV this list will be completed and to a certain extent closed, by showing that the HLLK also provides an explanation for the spin of QT. Anticipating this point, we may say that QT as a whole "emerges" from PM, if the assumptions of the HLLK are implemented. Of course, if the transition from CM to PM is included as first step of the theory, we may also say that QT emerges from CM. The HLLK brings together numerous known results and some new considerations under a common idea, which was essentially formulated by Einstein. It provides a new conceptual foundation for QT that seems to be simpler, and at the same time more complete, than any other attempt in this direction.

The need to find a new basis for understanding QT was felt by many physicists. The question of whether QT is a "complete" theory plays a central role in all of these discussions. Let us ask what the term "completeness" means exactly (as we did in section 6.1 with the term "reduction"). In section 6 we discussed the question of whether QT is able to describe the behavior of individual particles, and we arrived at the conclusion that this is not the case. In this sense, QT is incomplete. To describe this kind of (in)completeness more precisely, one could say that QT is "empirically (in)complete". Does empirical incompleteness imply that there must be a more "complete" theory, that also describes the behavior of individual particles? This second concept of "(in)completeness" is evidently quite different from the empirical one used above. This question cannot be decided empirically, in the absence of empirical data it is a matter of philosophical belief. Let us use the term "metaphysical (in)completeness" to characterize this kind of (in)completeness.

To illustrate the difference, Einstein, Podolski and Rosen (EPR) have *shown* in their famous work that QT is empirically incomplete; at the end of their paper they expressed their *belief* that QT is metaphysically incomplete [53]. These authors understood perfectly the difference between the two meanings of the term "completeness". Most of the papers criticizing this work try to refute EPR's (nonexisting) claim that QT is metaphysically incomplete. However, the fact that there are experimental observations that we cannot explain does not automatically imply that a better theory must exist.

## 7.1 Comparison of HLLK with the theories of Adler and 't Hooft

More recently, some authors assume that QT is metaphysically incomplete and that a deeper deterministic (complete) theory exists, from which it can be derived. Two theories of this kind are due to Adler [54] and 't Hooft [55]. Both constructions, that are otherwise quite different, aim to enable a synthesis of QT and general relativity by means of abstract deterministic structures, which are totally different from CM. Quantum theory is then obtained as a statistical

variant of this deterministic theory, assuming that the initial states are not exactly known; this randomization is of course associated with an enormous loss of information. Thus, these theories try to confirm Einstein’s *belief* that a determinism beneath QT exists; just as deterministic equations of motion exist beneath classical statistical physics. In theories of this kind, the principle of reductionism requires that nature, when one goes to short distances, first sets up a limit for the accuracy of measurements, which it then cancels again, when going to even smaller distances of the order of the Planck length.

In comparison, the present theory is very simple from a conceptual point of view. We know that QT is an empirically incomplete theory and try to derive it, together with all its structural properties, from a number of reasonable assumptions. We do not accept the universal validity of the principle of reductionism and do not discuss the question of metaphysical completeness. The present theory may also be built on the basis of a deterministic theory, but this is the most familiar theory of its kind, namely CM; we only have to include the transition from the canonical equations to Liouville mechanics as the first step of HLLK. Then, QT as derived in the present work can also be interpreted as a “statistical version” of CM. However, this concept needs to be generalized in an appropriate manner. The statistical theory used in the (enlarged) HLLK has to be implemented as a two-step process. In the first step, from the canonical equations to Liouville mechanics, the uncertainty of the initial values is taken into account. This is done with the help of the standard formalism of probability theory. In the second step, which is described in detail in section 5.2, the law of motion itself is randomized. In contrast to the physics of uncertain initial values, which is ruled by the principle of maximal entropy, the physics of uncertain dynamics is ruled by the principle of minimum Fisher information. This second step, in which the new constant  $\hbar$  is introduced, can either be performed as a linearization or alternatively, as the implementation of a new statistical concept. Both steps together form, so to speak, the complete randomization. The associated loss of information is also a two-step process.

The fact that not only the uncertainty of the initial values but also the indeterminacy of dynamic processes may be included in the formalism represents a fundamental generalization of the idea of statistics. Moyal called classical statistical physics a “cryptodeterministic” theory, since the uncertainty exists only in the initial values and not in the dynamics [56]. He has already recognized that QT may be understood as a form of general statistics that also includes dynamics.

## 7.2 Comparison of HLLK with the theory of Spekkens

The difference between the two types of completeness defined above has often been overlooked. It is, however, taken into account in the classification of possible models of QT formulated by Spekkens and Harrigan [57, 58]. Spekkens distinguishes between ontic and epistemic states. Ontic states are points in

phase space or configuration space, epistemic states are probability distributions over these spaces. In other words, CM is ontic and PM (Liouville dynamics) is epistemic; the latter is based on the former. In recent years an increasing number of researchers are realizing that QT is more similar to Liouville dynamics than to CM. At the beginning of paper II a number of well-known facts supporting this claim have been listed. This list is not complete. For example, Mauro has shown that the Hilbert space of QT may be embedded in the Koopman-von Neumann Hilbert space spanned by phase space functions [59]. Let us also note at this point that only Liouville dynamics shares the property of no-cloning with QT [60].

In Spekkens scheme, the HLLK belongs to the class of “ $\psi$ -epistemic” models of QT. A detailed explanation of this term as well as an interesting analysis, suggesting a reassessment of Einstein’s position, may be found in [58]. The starting point of Spekkens’ theory is the same as in the present work, namely Liouville dynamics (which is, in the present notation, PM restricted to Hamilton’s function). A constraint on the allowed statistical distributions of Liouville dynamics is referred to as an *epistemic restriction*. The fundamental postulate of Spekkens’ theory is the following: if epistemic restrictions are implemented large parts of the quantum theoretical formalism may be reproduced. A number of epistemic restrictions are constructed, based on a classical version of the uncertainty principle, a classical version of complementarity, and others [57]. If Poisson-commuting classical observables are taken into account, one arrives at the conclusion that a  $2n$ -dimensional phase space can at most be restricted to  $n$ -dimensional subspaces (maximally isotropic subspaces, or Lagrangian subspaces). It is indeed possible to understand various aspects QT by implementing such restrictions. However, it is not possible to derive the entire formalism of QT; the theory is therefore called a quasi-quantization method. Another disadvantage is, of course, that no explanation is given why epistemic restrictions should be introduced.

The projection from phase space onto configuration space is the first and most important step of the HLLK, since the further steps more or less inevitably follow from it. The reasons for such a projection were discussed in section 1. In this first step, the variety of possible states is restricted to an  $n$ -dimensional subspace of  $2n$ -dimensional phase space. This projection can therefore be interpreted as an epistemic restriction; here we find punctual agreement with Spekkens’ theory. The  $n$ -dimensional subspace is defined by the momentum variable under consideration. As explained in II, the projection must be carried out for all observables of interest, each one defining its own momentum field. Thus, there is a multitude of epistemic restrictions in the HLLK, but all of them have the same structure. With the exception of Hamilton’s function which describes the dynamics, all other observables lead to eigenvalue equations after performing the linearization (see II for details).

## 8 Conclusions

The HLLK is based on the assumption that QT can be derived from classical probabilistic mechanics by means of a projection and a linearization. This concept has been confirmed in the present work; we have performed the same steps as in I and II, just in different order, and reached the same result. In I and II we gave a complete derivation of all fundamental properties of QT for a single spinless particle. In the present work we have derived only Schrödinger's equation although preliminary calculations indicate that all aspects of QT may be derived using the present method. We consider the calculations performed in I and II and in the present work as two versions of one and the same theory, each allowing different insights. In this paper, the emphasis is on a deeper understanding of the classical-quantum interface and on laying the groundwork for the treatment of spin in the following work. We note the following specific points.

- Performing the projection first only a single fundamental assumption must be implemented, namely that the theory can be formulated using the independent variables  $q, t$ . The second step, the subsequent linearization or randomization, can be interpreted as a correction of the instability of the QA, i.e. as a necessary consequence of the first step.
- One of the important conclusions of the present work is that the four real fields contained in the true (spinorial) wave function are closely related to the probability density and the three components of the momentum field. However, to avoid non-existing dependencies between the components, it is necessary to introduce potentials. It is only the potentials and not the components that can be used to formulate the dynamic variables of QT.
- A second important insight that can already be gained in the present spinless theory is that massive spinless particles cannot occur in nature. This conclusion of our non-relativistic theory is a straightforward consequence of the three-dimensionality of space combined with the requirement that the three components of the momentum field must be functionally independent from each other.
- The principle of minimal coupling states that external influences can be described by means of a simple modification of certain (irrotational) potentials. So there is a close connection between this fundamental principle and the introduction of momentum fields.
- In this work, only the case of a single irrotational momentum field has been treated in detail. Although unrealistic, this model is very useful for many questions because of its simplicity. This is especially true for the second step, which can be performed either as a linearization or as a randomization.
- The linearization is a discontinuous process which allows a very rapid derivation of Schrödinger's equation, but whose physical meaning is not immediately obvious. Its meaning is a randomization of the statistical theory QA, in the sense that the concept of particle trajectories is completely removed from the emerging QT.

- This randomization has been made explicit by starting from QA (in which locally valid particle trajectories still exist) and constructing a higher-level "statistical version" of QA in which the concept of particle trajectories no longer plays any role.
- This construction is based on two plausible assumptions. First, we assume that only statistical versions (Ehrenfest's theorem) of particle trajectories exist. Second, we formulate a variational problem that can be viewed as the microscopic equivalent of macroscopic Boltzmann-Shannon entropy, leading to the concept of Fisher information. This construction shows that QT is the simplest and most reasonable randomized version of QA.
- As for the interface between QT and classical physics, we have confirmed the results of I and II in this paper, insofar as we have shown that QT cannot be reduced to either CM or PM.
- We consider the present derivation as a strong argument in favor of the ensemble interpretation of QT. We have critically discussed some of Pauli's and Dirac's arguments in favor of the individuality interpretation, in particular Dirac's famous "families of solutions".

In the following fourth paper in this series of works, building on the results of this paper, we will address the phenomenon of spin.

## Appendix A Comparison with phase-space momentum fields

It is interesting to study the relation between the momentum fields  $M(q, t)$  and the more familiar momentum fields in phase space that occur in the theory of canonical transformations. Let us consider a canonical transformation that leads from old coordinates  $q, p$  and the old Hamiltonian  $H(q, p)$  to new coordinates  $Q, P$  and the new Hamiltonian  $K(Q, P) = 0$ . We assume that we have a complete set of Poisson-commuting classical observables, which is seldom the case in practice. Furthermore, we consider non-degenerate canonical transformation, for which the variables  $q, Q$  may be used as phase space coordinates. A generating function  $F_1(q, Q, t)$  is then determined by the equations

$$p_i(q, Q, t) = \frac{\partial F_1}{\partial q_i}(q, Q, t), \quad (\text{A1})$$

$$P_i(q, Q, t) = -\frac{\partial F_1}{\partial Q_i}(q, Q, t), \quad (\text{A2})$$

$$H(q, p(q, Q, t), t) = -\frac{\partial F_1}{\partial t}(q, Q, t), \quad (\text{A3})$$

where  $Q$  stands for a set of  $n$  arbitrary constants. As shown by Jacobi, the general solution of the equations of motion (1) may be calculated if a "complete solution"  $F_1(q, Q, t)$  of the Hamilton-Jacobi equations is known.

The fields  $p(q, Q, t)$  defined by (A1) are referred to as momentum fields in phase space. More precisely, we have a whole family of fields, each value

of the  $n$ -component quantity  $Q$  determines a field. The crucial point is that all these fields are irrotational; the second term on the left-hand side of the canonical condition [the vorticity tensor (24)] vanishes by definition. On the other hand, the momentum fields on configuration space  $M(q, t)$ , defined as solution of Eq. (13), are *not* subject to this restriction; explicit expressions for  $M(q, t)$  with non-vanishing vorticity tensor (corresponding to spin  $1/2$ ) will be reported in IV. We know that the theory of canonical transformations provides a complete description of particle motion. How can it be that the momentum fields  $M(q, t)$ , satisfying Eq. (13), are more general than the momentum fields in phase space  $p(q, Q, t)$ , satisfying the formalism of canonical transformations?

The reason is that the theory of canonical transformations describes the detailed structure of the trajectories in phase space. There can be no “vorticity” in the continuous set of these exactly defined trajectories. However, this is possible for the momentum fields  $M(q, t)$  that have been forced to live in a subspace (configuration space) of phase space. The fields  $M(q, t)$  are obtained as solutions of an initial value problem, while the fields  $p(q, Q, t)$  are obtained from complete solutions of the Hamilton-Jacobi equation. An important but sometimes overlooked point is that the solutions of Schrödinger’s equation are defined by an *initial value problem*. The fields  $M(q, t)$  are therefore much better suited for a transition to (or from) QT than the fields  $p(q, Q, t)$  (we shall come back to this point in section 3.1). As a matter of fact, the possible existence of momentum fields with vorticity is a consequence of our projection to configuration space. In other words, it is a consequence of the first step of HLLK in the transition from PM to QT.

The complete solutions of the Hamilton-Jacobi equation provide a most general solution to the problem of particle motion. With their help one can construct the general solution of the equations of motion and Hamilton’s principal function as well as the general solution of the initial value problem of the Hamilton-Jacobi equation [50, 61]. However, the momentum fields on configuration space  $p(q, t)$  obtained in this way (by means of the method of envelopes [49]) are again irrotational, just like the original momentum fields on phase space  $p(q, Q, t)$  (the present author is not aware of a theory that allows to solve initial value problems within the framework of the theory of *degenerate* canonical transformations [52]).

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