Unitary Evolution between Pure and Mixed States

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We propose an extended quantum mechanical formalism that is based on a wave operator $\hat{\varrho}$, which is related to the ordinary density matrix via $\rho = \hat{\varrho}\hat{\varrho}^\dagger$. This formalism allows a (generalized) unitary evolution between pure and mixed states. It also preserves much of the connection between symmetries and conservation laws. The new formalism is illustrated for the case of a two-level system.

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Several proposals motivated by various considerations for generalizing the quantum mechanical formalism have been made to date. In these programs one disposes of a fundamental quantum mechanical principle such as linearity, locality, or unitarity. Weinberg suggested a nonlinear generalization, and proposed precision tests of nonlinear corrections to quantum mechanics [1]. Motivated by the apparent breakdown of unitarity in the black-hole evaporation process, Hawking proposed that a synthesis of quantum mechanics and general relativity requires giving up unitarity [2], and to some extent locality [3]. A model which gives up both properties was constructed by Marinov [4]. As a linear and local phenomenological implementation of Hawking's proposal, Ellis, Hagelin, Nanopoulos, and Srednicki (EHNS) [5], and Banks, Peskin, and Susskind (BPS) [6] suggested a modified Liouville equation for the density matrix ρ.

In particular, BPS showed that the requirements of linearity, locality in time, and conservation of probabilities lead to a modified equation with a "generic form":

$$i\hbar\partial_t\rho = [H,\rho] + i\sum_{n,m} h_{nm}(Q_mQ_n\rho + \rho Q_mQ_n - 2Q_n\rho Q_m). \tag{1}$$

Here, Q_n are any Hermitian operators, and $h_{nm,}$ is a c-number Hermitian matrix. A sufficient but not necessary condition ensuring the positivity of ρ is that the matrix h is positive. Equation (1) does not preserve $\mathrm{tr}\rho^2$. Thus pure states can indeed evolve to mixed states [7].

Similar equations can be obtained from ordinary quantum mechanics for a subsystem interacting with an environment [8]. Nevertheless, when gravity is involved, one can argue that the relevant "microenvironment" is hidden by black-hole horizons and is *in principle* unobservable. This would render Eq. (1) a fundamental modification of quantum mechanics, rather than an artifact of interacting with an environment.

Modified evolutions such as (1) were applied in various cases. EHNS proposed that the corrections induced might be observed in the ultrasensitive K_0-$\overline{K}_0$ system. Furthermore, Ellis, Mavromatos, and Nanopolous [9], and Huet and Peskin [10] examined the possibility that the observed CP violation in the K_0-$\overline{K}_0$ system is, to some extent, due to non-quantum-mechanical corrections. Related modifications were also proposed in connection with the "measurement problem," in order to generate a von Neumann reduction for macroscopic systems [11,12].

In what follows, we propose a different approach. It is also based on the Liouville equation but not for the ordinary density matrix. It constitutes a linear, local, and unitary extension of quantum mechanics. To this end, consider the density matrix in ordinary quantum mechanics and focus first on the case of a pure state. By analogy with the relation $\rho = |\psi\rangle\langle\psi|$, let us define the operator $\hat{\varrho}$ by [13]

$$\rho = \hat{\varrho}\hat{\varrho}^\dagger. \tag{2}$$

If $\hat{\varrho}$ satisfies a Liouville equation

$$i\hbar\partial_t\hat{\varrho} = [H,\hat{\varrho}], \tag{3}$$

it is easy to see that the density matrix $\rho = \hat{\varrho}\hat{\varrho}^\dagger$ also satisfies a Liouville equation with the same Hamiltonian. The initial condition may be specified in terms of the "square root operator" $\hat{\varrho}$, rather than ρ. Thus, if the system is determined at $t = t_0$ by an ordinary complete set of measurements to be in the state $|\psi_0\rangle$ (or $\rho = |\psi_0\rangle\langle\psi_0|$), this sets the initial condition for Eq. (3),

$$\hat{\varrho}(t = t_0) = |\psi_0\rangle\langle\psi_0|. \tag{4}$$

Now we observe that (2) and (4) imply $\rho(t = t_0) = \hat{\varrho}(t = t_0)$, and since both quantities obey the same equation of motion, this relation holds at any subsequent time. The expectation values of any observable A is obtained by the standard expression

$$\langle A\rangle = \frac{\mathrm{tr}A\rho}{\mathrm{tr}\rho} = \frac{\mathrm{tr}A\hat{\varrho}}{\mathrm{tr}\hat{\varrho}}. \tag{5}$$

Hence Eqs. (2)–(5) are equivalent to ordinary quantum mechanics [14].

It is therefore interesting to question whether Eq. (3) can now be used as a new starting point for a quantum mechanical extension. We shall assume that $\hat{\varrho}$ is from now on a general operator (not necessarily a projector) still obeying the initial condition (4), and that expectation values are still obtained by the standard expression

$$\langle A\rangle = \frac{\mathrm{tr}A\rho}{\mathrm{tr}\rho}. \tag{6}$$

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The density matrix, however, is from now on obtained via $\rho = \hat{\varrho}\hat{\varrho}^\dagger$.

The Hermiticity and positivity of ρ is automatically ensured by $\rho = \hat{\varrho}\hat{\varrho}^\dagger$. The modified equation must conserve probabilities, i.e., $\partial_t \mathrm{tr}\rho = \partial_t \mathrm{tr}\hat{\varrho}\hat{\varrho}^\dagger = 0$, but not necessarily purity. The most general linear [15] and local generalization of Eq. (3) which satisfies this condition can be written as

$$i\hbar\partial_t\hat{\varrho} = [H,\hat{\varrho}] + L\hat{\varrho} + \hat{\varrho}R + g_{ij}K_i\hat{\varrho}K_j'. \quad (7)$$

Here, L, R, K_i, and K_j' are any Hermitian operators, g_{ij} are real coefficients, and the summation convention was used.

Equation (7) implies that the density matrix obeys

$$i\hbar\partial_t\rho = [H + L,\rho] + g_{ij}(K_i\hat{\varrho}K_j'\hat{\varrho}^\dagger - \text{H.c.}). \quad (8)$$

The "primary" object $\hat{\varrho}$ cannot be eliminated from Eq. (8) which therefore cannot be rephrased in terms of ρ only. Thus unlike the case of Eq. (1), ρ plays here the role of a "secondary" object. Equation (8) also indicates that the term $L\hat{\varrho}$ in Eq. (7) gives rise to a redefinition of the Hamiltonian, and that the term $\hat{\varrho}R$ can be eliminated. Indeed, the gauge transformation $\hat{\varrho} \rightarrow \hat{\varrho}U$, where U is a unitary operator, does not affect expectation values and can be used to recast Eq. (7) into the form

$$i\hbar\partial_t\hat{\varrho} = \tilde{H}\hat{\varrho} + g_{ij}K_i\hat{\varrho}\tilde{K}_j, \quad (9)$$

where $\tilde{H} = H + L$, $\tilde{K}_j = UK_j'U^{-1}$, and $U = \exp[-i\int^t (R - H)\,dt']$. Without the last term this is simply a Schrödinger-like equation for the operator $\hat{\varrho}$.

To further analyze Eq. (7) we construct a Hilbert space. It is defined as the linear space $\mathcal{L} \equiv \{\hat{\varrho}\}$ of solutions of Eq. (7) with all possible initial conditions at any t_0. With the inner product defined as

$$\langle\hat{\varrho}_1,\hat{\varrho}_2\rangle = \mathrm{tr}\hat{\varrho}_1^\dagger\hat{\varrho}_2, \quad (10)$$

$\mathcal{L}$ becomes a Hilbert space. It follows from Eq. (7) that this inner product is conserved, and hence the generalized dynamics suggested here manifests in $\mathcal{L}$ as a unitary evolution. The inner product (10) may be regarded as an extension of the ordinary quantum mechanical inner product. If the corrections induced after $t = t_0$ by the new terms in the evolution equation (7) are small, $\langle\hat{\varrho}_1,\hat{\varrho}_2\rangle \simeq |\langle\psi_1|\psi_2\rangle|^2$. Note also that expression (6) for the expectation value of an observable A can be now reexpressed as

$$\langle A\rangle = \frac{\langle\hat{\varrho},A\hat{\varrho}\rangle}{\langle\hat{\varrho},\hat{\varrho}\rangle}. \quad (11)$$

Equations (7), (9), (10), and (11) suggest that $\hat{\varrho}$ should be interpreted as a generalized "wave operator." The new feature here, however, is that $\mathrm{tr}\rho^2 = \mathrm{tr}(\hat{\varrho}\hat{\varrho}^\dagger)^2$ is not conserved. This manifests the new aspects of our unitary evolution as a transition between pure and mixed density matrices (ρ).

The generalized unitarity, namely, the conservation of the inner product (10), can be clarified by rewriting Eq. (7) in the Hilbert space $\mathcal{L}$. For simplicity, let us consider a system with a finite, N-dimensional Hilbert space and perform the extension described above. The extended, N^2-dimensional Hilbert space $\mathcal{L}$ can be spanned by a Hermitian basis of $N^2 - 1$ SU(N) matrices and the unit operator,

$$\hat{\varrho} = \frac{1}{\sqrt{2}}(\varrho_0\mathbf{1} + \varrho_i T_i), \quad (12)$$

where T_i are SU(N) generators and ϱ_a are N^2 complex numbers. In this basis, the generalized inner product between any two solutions is given by an ordinary vector product in an N^2-dimensional Hilbert space,

$$\langle\hat{\varrho}_1,\hat{\varrho}_2\rangle = \sum_{a=0}^{N^2-1}\varrho_{1a}^*\varrho_{2a}. \quad (13)$$

We can also express Eq. (7) in this basis as a Schrödinger-like equation,

$$i\hbar\partial_t\varrho_a = \mathcal{H}_{ab}\varrho_b = (\mathcal{H}_{ab}^{(qm)} + \delta\mathcal{H}_{ab})\varrho_b. \quad (14)$$

The condition for conservation of probabilities (and unitarity) is simply that the generalized Hamiltonian $\mathcal{H}_{ab}$ is Hermitian. The deceptive similarity of Eq. (14) and the ordinary quantum mechanics Schrödinger equation in an N^2-dimensional space notwithstanding, we emphasize that the only relevant, physical degrees of freedom are in those of the original (N-dimensional) Hilbert space.

Next, we would like to express the observables A_i as Hermitian operators in $\mathcal{L}$. In general, we have in $\mathcal{L}$ N^4-independent Hermitian operators. Therefore the mapping,

$$A_i \longrightarrow \mathcal{A}_i \in \mathcal{O}_{\mathcal{L}}, \quad (15)$$

of the original (N^2) observables A_i into the set of Hermitian operators $\mathcal{O}_{\mathcal{L}}$ in $\mathcal{L}$ is not one-to-one. This mapping is constrained by demanding that

$$\mathrm{tr}A_i\hat{\varrho}\hat{\varrho}^\dagger = \sum_{a=0}^{N^2-1}\sum_{b=0}^{N^2-1}\varrho_a(\mathcal{A}_i)_{ab}\varrho_b, \quad (16)$$

i.e., that $\langle A\rangle$ is expressible in $\mathcal{L}$ as a "standard" expectation value with respect to the "amplitudes" $\hat{\varrho}_a$. We also require that the mapping (15) preserves commutation relations. Therefore, an N-dimensional representation of SU(N) is mapped into an N^2-dimensional representation of SU(N) in $\mathcal{O}_{\mathcal{L}}$, $T_i \rightarrow \mathcal{T}_i$. The linear transformation maps a general observable $A_i = c_{i0}\mathbf{1} + c_{ia}T_a$ to $\mathcal{A}_i = c_{i0}\mathcal{I} + \sum_a c_{ia}\mathcal{T}_a$. The operator $\mathcal{A}_i \in \mathcal{O}_{\mathcal{L}}$ still has the same eigenvalues as the original operator A_i. However, all the eigenvalues are now N-fold degenerate. Another set of operators, denoted by $\mathcal{D}_j$, which remove the degeneracy of $\mathcal{A}_i$ do not correspond to observables. It can be shown that the role of the new terms in Eq. (7) or $\delta\mathcal{H}$ in Eq. (14) is to generate correlations between $\mathcal{A}_i$ and $\mathcal{D}_j$, which in turn induces the transition to a mixed density matrix.

It was noted by Gross [16] and by Ellis *et al.* [5] that linear modifications of the evolution laws for the density matrix [e.g., Eq. (1)] generally breaks the one-to-one correspondence between symmetries and conservation laws. We now show that in the present formalism this correspondence is partially restored. An observable $\mathcal{A} \in \mathcal{O}_{\mathcal{L}}$ that is a constant of motion satisfies $[\mathcal{A}, \mathcal{H}] = 0$. Hence the unitary operator $T = \exp(-i\epsilon\mathcal{A}/\hbar)$ commutes with the unitary evolution operator $U = \exp(it\mathcal{H}/\hbar)$, and $\mathcal{A}$ generates a symmetry in $\mathcal{L}$. The converse is not generally true. Since $\mathcal{L}$ is N^2 dimensional, not all the Hermitian operators in $\mathcal{O}_{\mathcal{L}}$ may be mapped back to Hermitian operators in the original N-dimensional Hilbert space. Therefore, if some Hermitian operator $\mathcal{G}$ generates a symmetry in $\mathcal{L}$ and its expectation value $\varrho_a^*(t)\mathcal{G}_{ab}\varrho_b(t)$ is conserved, it still may not correspond to an observable.

To illustrate the general discussion above let us consider as an example the simple two-level system (e.g., a spin half particle in a constant magnetic field). The mapping between the original 2D Hilbert space and the 4D Hilbert space $\mathcal{L}$ will be spelled out in detail. Let the "free" Hamiltonian be given by

$$H = E_0 + \tfrac{1}{2}\hbar\omega\sigma_3 . \tag{17}$$

We have seen that the terms $L\hat{\varrho}$ and $\hat{\varrho}R$ in Eq. (7) can be absorbed by a redefinition of H and K_j'. Therefore, the modified equation will be taken as

$$i\hbar\partial_t\hat{\varrho} = [H, \hat{\varrho}] + K\hat{\varrho}K', \tag{18}$$

where K and K' are functions of the Pauli matrices, and will be assumed to be time independent. Energy conservation, $\partial\langle H\rangle/\partial t = \partial(\langle\hat{\varrho}, H\hat{\varrho}\rangle/\langle\hat{\varrho},\hat{\varrho}\rangle)/\partial t = 0$, implies that $[\sigma_3, K] = 0$, hence $K = \sigma_3$. This leaves three unknown parameters which determine K':

$$K' = \alpha\sigma_1 + \beta\sigma_2 + \lambda\sigma_3 . \tag{19}$$

When re-expressed in the four-dimensional Hilbert space $\mathcal{L}$ the modified dynamics corresponds to Eq. (14) with

$$\delta\mathcal{H} = \begin{pmatrix} \lambda & i\beta & -i\alpha & 0 \\ -i\beta & -\lambda & 0 & \alpha \\ +i\alpha & 0 & -\lambda & \beta \\ 0 & \alpha & \beta & \lambda \end{pmatrix}. \tag{20}$$

The observables in this model are combinations of σ_i and the unit operator. The mapping $\sigma_i \longrightarrow S_i \in \mathcal{O}_{\mathcal{L}}$ is

$$\tfrac{1}{2}\sigma_k \longrightarrow (S_k)_{ab} = \tfrac{1}{2}(\delta_{ak}\delta_{b0} + \delta_{a0}\delta_{bk} + i\epsilon_{abk}). \tag{21}$$

The S_i are a four-dimensional representation of SU(2), preserving the commutation relation $[S_i, S_j] = i\epsilon_{ijk}S_k$. The mapping (21) was constructed so as to satisfy Eq. (16). The operators $\mathcal{D}_j$ which remove the degeneracy of S_i have also been explicitly constructed. The latter indeed do not correspond to observables.

It can now be verified that S_3 is a constant of motion, i.e., $[S_3, \mathcal{H}^{qm} + \delta\mathcal{H}] = 0$. We also notice that since the energy operator, $E_0\mathbf{1} + \hbar\omega S_3$, is not the mapped original Hamiltonian, $(\mathcal{H}^{qm})_{ab} = i\hbar\omega\epsilon_{ab3}$, $\mathcal{H}^{qm}$ does not correspond to an observable in $\mathcal{L}$.

The present model differs qualitatively from the model of BPS or EHNS: While Eq. (1) yields, in general, exponentially decaying (or exponentially increasing) solutions, our modifications are oscillatory. Indeed the general solution of Eq. (14) is

$$\varrho_a = \sum_{\mu=0,3} c_\mu\varrho_{\mu a}\exp(-i\lambda_a t), \tag{22}$$

where λ_α and $\varrho_{a\alpha}$ are the (real) eigenvalues and eigenvectors, respectively, of $\mathcal{H}_{ab}$.

As an example, consider the special case where only λ in Eq. (20) is nonvanishing, and the spin is found at $t = t_0$ in the state $|\psi_0\rangle = \cos(\eta/2)|\uparrow_{\hat{z}}\rangle + \sin(\eta/2) \times |\downarrow_{\hat{z}}\rangle$. The solution in this case is given by

$$\hat{\varrho}(t) = \begin{pmatrix} \cos^2(\eta/2)e^{-i\lambda t} & \frac{1}{2}\sin(\eta)e^{-i(\omega-\lambda)t} \\ \frac{1}{2}\sin(\eta)e^{i(\omega+\lambda)t} & \sin^2(\eta/2)e^{-i\lambda t} \end{pmatrix}. \tag{23}$$

The resulting density matrix, $\rho = \hat{\varrho}\hat{\varrho}^\dagger$, oscillates periodically between a pure and mixed state. For example, in the simple case $\eta = \pi/2$

$$\rho(t) = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\omega t}\cos(2\lambda t) \\ e^{i\omega t}\cos(2\lambda t) & 1 \end{pmatrix}, \tag{24}$$

and $\mathrm{tr}\rho^2 = \frac{1}{2} + \frac{1}{2}\cos^2(2\lambda t)$.

Observable effects due to these modifications can, in principle, be searched for in neutron interferometry experiments [17]. In such interference experiments, one typically measures an observable of the form

$$A(\theta) = \frac{1}{2}\begin{pmatrix} 1 & e^{i\theta} \\ e^{-i\theta} & 1 \end{pmatrix}, \tag{25}$$

where θ is determined by the experimental setup. The expectation value of A is given in our case by

$$\langle A\rangle = \tfrac{1}{2}\big(1 + \sin\eta\{\cos^2(\eta/2)\cos[(\omega + 2\lambda)t + \theta] + \sin^2(\eta/2)\cos[(\omega - 2\lambda)t + \theta]\}\big). \tag{26}$$

The correction is indeed oscillatory. This should be contrasted with the exponential $\exp(-2\lambda_{\mathrm{EHNS}}t)$ decay of the interference obtained by EHNS.

What are the present experimental bounds pertinent to the three new parameters of the two-level system? We can use the two slit experiments of Zeilinger *et al.* [18] with a 20 Å neutron beam, and the analysis of Pearle [19], to constrain the generic parameter λ to $\lambda \sim 10\ \mathrm{sec}^{-1} \sim 10^{-23}$ GeV. The constraint of the same experiment on the corresponding parameters in the EHNS model is $\sim$100 times stronger ($\sim 10^{-25}$ GeV). The exponential factor modifies the interference contrast during the short flight time ($t_0 \simeq 10^{-2}$ sec) by $(1 - 2\lambda_{\mathrm{EHNS}}t_0)$. In the present case the extra oscillation can be subsumed into slow "beating" $\sim\cos(2\lambda t_0) \simeq 1 - 2(\lambda t_0)^2$, causing a much weaker reduction of the contrast in the interference pattern.

We found that our modification induces $K_L K_S$ mixing generating CP violation in the two-level K_0-$\overline{K}_0$ system in a similar fashion as in the EHNS model. However, this mixing predicts a phase of the *CP* violating parameter ϵ, which is of $\pi/2$ just as in the case of the EHNS model [10]. Hence our modification can account for only a small part of the *CP* violation observed in the K_0-$\overline{K}_0$ system. This leads to the generic upper bound of order $\sim 10^{-19}$ GeV, of the same order as $M_K^2/M_{\rm pl}$ which could be expected on dimensional grounds if *CP* and/or *CPT* violations are due to effects of quantum gravity. The 100-fold larger parameter allowed by the neutron interference experiment in our model could be important. In particular, this renders smaller, yet experimentally detectable, *CPT* violations more likely in the present framework.

We have constructed a formalism based on an operator generalization of the wave function which is linear, local, and unitary. As a consistency check of this proposal we note that to some extent the proposed formalism can be embedded in the framework of ordinary quantum mechanics. We can interpret $\hat{\varrho}\hat{\varrho}^\dagger$ and $\hat{\varrho}^\dagger\hat{\varrho}$ as the reduced density matrices of a subsystem and an environment, respectively. The generalized Hamiltonian $\mathcal{H}_{ab}$ in Eq. (14) and the amplitudes ϱ_a can then be interpreted as the Hamiltonian and wave function of the total system, while the new terms in Eqs. (7), (9), or (14) as describing an interaction between the subsystem and the environment. Therefore, the consistency of the proposed equation of motion follows from quantum mechanics. *Nevertheless,* postulate (4), $\hat{\varrho}(t = t_0) = |\psi_0\rangle\langle\psi_0|$, which sets the initial condition for Eq. (7) goes beyond any ordinary quantum mechanical scheme. It would amount in quantum mechanics to an additional requirement that, after carrying a complete set of measurements on the subsystem, the wave function of the environment becomes identical to that of the system. This additional constraint is not satisfied in quantum mechanics. Therefore the predictions of this formalism will generally differ from that of a quantum mechanical system with an environment [20].

Finally, we note that the proposed formalism may also be relevant to the information problem in black-hole evaporation and to the measurement problem. In the latter case, for large systems the modified evolution might, under appropriate conditions, give rise to loss of coherence which amounts to a measurement.

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