Unitary Evolution Between Pure and Mixed States

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Abstract

We propose an extended quantum mechanical formalism that is based on a wave operator \( \hat{\varphi} \), which is related to the ordinary density matrix via \( \rho = \hat{\varphi} \hat{\varphi}^\dagger \). 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 \(\rho\).

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”:

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

(1)

Here, \(Q_n\) are any Hermitian operators and \(h_{nm}\) is c-number hermitian matrix. A sufficient but not necessary condition ensuring the positivity of \(\rho\), is that the matrix \(h\) is positive. Equation (1) does not preserve \(\text{tr}\rho^2\). 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 “micro-environment” is hidden by black-hole horizons and is in principle unobservable. This would render equation (1) a fundamental modification of quantum mechanics, rather than an artifact of interacting with an environment.

Modified evolutions like (1) were applied in various cases. EHNS proposed that the corrections induced might be observed in the ultra-sensitive \(K_0 - \bar{K}_0\) system. Furthermore,
Ellis et. al. [9] and Huet and Peskin [10] examined the possibility that the observed CP violation in the $K_0 - \bar{K}_0$ system is, to some extent, due to non-quantum mechanical corrections. Related modifications where 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 $\rho = \vert \psi \rangle \langle \psi \vert$, let us define the operator $\hat{\rho}$ by [13]:

$$\rho = \hat{\rho} \hat{\rho}^\dagger. \quad (2)$$

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

$$i\hbar \partial_t \hat{\rho} = [H, \hat{\rho}], \quad (3)$$

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

$$\hat{\rho}(t = t_0) = \vert \psi_0 \rangle \langle \psi_0 \rangle. \quad (4)$$

Now we observe that (2) and (3) imply $\rho(t = t_0) = \hat{\rho}(t = t_0)$, 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:

$$\langle A \rangle = \frac{\text{tr} A \rho}{\text{tr} \rho} = \frac{\text{tr} A \hat{\rho}}{\text{tr} \hat{\rho}}. \quad (5)$$

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 $\hat{\rho}$ 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

$$\langle A \rangle = \frac{\text{tr} A \rho}{\text{tr} \rho}. \quad (6)$$

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

The hermiticity and positivity of $\rho$ is automatically ensured by $\rho = \hat{\rho} \hat{\rho}^\dagger$. We need that the modified equation conserve probabilities, i.e, $\partial_t \text{tr} \rho = \partial_t \text{tr} \hat{\rho} \hat{\rho}^\dagger = 0$, but not necessarily purity. The most general linear [15] and local generalization of eq. (3) which satisfies this condition can be written as:

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

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

Eq. (7) implies that the density matrix obeys:

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

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

$$i\hbar \partial_t \hat{\rho} = \tilde{H} \hat{\rho} + g_{ij} K_i \hat{\rho} K_j', \quad (9)$$
where, $\hat{H} = H + L$, $\hat{K}_j = UK'_jU^{-1}$, and $U = \exp\left[-i \int (R - H) dt\right]$. Without the last term this is simply a Schrödinger-like equation for the operator $\hat{\psi}$.

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

$$\langle \hat{\psi}_1, \hat{\psi}_2 \rangle = \text{tr} \hat{\psi}_1^\dagger \hat{\psi}_2,$$

$L$ becomes a Hilbert space. It follows from eq. (9) that this inner product is conserved and hence the generalized dynamics suggested here manifests in $L$ 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 eq. (7) are small, $\langle \hat{\psi}_1, \hat{\psi}_2 \rangle \simeq |\langle \psi_1|\psi_2 \rangle|^2$. Note also that expression (6) for the expectation value of of an observable $A$ can be now re-expressed as:

$$\langle A \rangle = \frac{\langle \hat{\psi}, A \hat{\psi} \rangle}{\langle \hat{\psi}, \hat{\psi} \rangle}.$$

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

The generalized unitarity, namely the conservation of the inner product (11), can be clarified by rewriting eq. (7) in the Hilbert space $L$. 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 $L$ can be spanned by a hermitian basis of $N^2 - 1$ SU(N) matrices and the unit operator:

$$\hat{\psi} = \frac{1}{\sqrt{2}}(\hat{\rho}_0 1 + \hat{\rho}_i T_i),$$

(12)
where $T_i$ are SU(N) generators and $\varrho_a$ are $N^2$ complex numbers. In this basis, the generalized inner product between any two solutions is given by an ordinary vector product in a $N^2$-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:

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

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 ordinary quantum mechanics Schrödinger equation in an $N^2$ dimensional space notwithstanding, we emphasis 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

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

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

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

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 (13) preserves commutation relations. Therefore, an $N$-dimensional representation of SU(N) is mapped into an $N^2$ dimensional representation of SU(N) in $\mathcal{O}_\mathcal{L}$, $T_i \rightarrow T_i$. The linear transformation maps a general observable $A_i = c_{i0} 1 + c_{ia} T_a$ to $\mathcal{A}_i = c_{i0} \mathcal{I} + \sum_a c_{ia} T_a$. 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 $D_j$, which remove the degeneracy of $A_i$ do not correspond to observables. It can be shown that the role of the new terms in eq. (1) or $\delta \mathcal{H}$ in eq. (14) is to generate correlations between $A_i$ and $D_j$, 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 $A \in \mathcal{O}_L$ that is a constant of motion satisfies: $[A, \mathcal{H}] = 0$. Hence the unitary operator $T = \exp(-i\epsilon A/\hbar)$ commutes with the unitary evolution operator $U = \exp(-i\mathcal{H}/\hbar)$, and $A$ 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 $\mathcal{O}_L$ may be mapped back to hermitian operators in the original $N$-dimensional Hilbert space. Therefore, if some hermitian operator $G$ generates a symmetry in $\mathcal{L}$ and its expectation value, $\rho^*_a(t)G_{ab}\rho_b(t)$, 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 2-d Hilbert space and the 4-d Hilbert space $\mathcal{L}$ will be spelled out in detail. Let the “free” Hamiltonian be given by

$$H = E_0 + \frac{1}{2}\hbar \omega \sigma_3. \quad (17)$$

We have seen that the terms $L\hat{\rho}$ and $\hat{\rho}R$ in eq. (7) can be absorbed by a redefinition of $H$ and $K'_j$. Therefore, the modified eq. will be taken as:

$$i\hbar \partial_t \hat{\rho} = [H, \hat{\rho}] + \hat{\rho}K\hat{\rho}, \quad (18)$$

6
where $K$ and $K'$ are functions of the Pauli matrices, and will be assumed to be time independent. Energy conservation, \( \frac{\partial}{\partial t} \langle H \rangle = -\langle \dot{\rho} \rangle + \langle \dot{\rho} \dot{H} \rangle = 0 \), implies that \([\sigma_3, K] = 0\), hence $K = \sigma_3$. This leaves three unknown parameters which determine $K'$:

$$K' = \alpha \sigma_1 + \beta \sigma_2 + \lambda \sigma_3.$$  \hspace{1cm} (19)

When reexpressed in the four dimensional Hilbert space $\mathcal{L}$ the modified dynamics corresponds to eq. (14) with:

$$\delta \mathcal{H} = \begin{pmatrix}
\lambda & i\beta & -i\alpha & 0 \\\n-i\beta & -\lambda & 0 & \alpha \\
+i\alpha & 0 & -\lambda & \beta \\
0 & \alpha & \beta & \lambda \\
\end{pmatrix}.$$  \hspace{1cm} (20)

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

$$\frac{1}{2} \sigma_k \rightarrow (S_k)_{ab} = \frac{1}{2} (\delta_{ak} \delta_{b0} + \delta_{a0} \delta_{bk} + i\epsilon_{abk}).$$  \hspace{1cm} (21)

The $S_i$ are a 4-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, $D_j$, 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. $[S_3, \mathcal{H}^{\text{em}} + \delta \mathcal{H}] = 0$. We also notice that since the energy operator, $E_0 \mathbf{1} + \hbar \omega S_3$, is not the mapped original Hamiltonian: $(\mathcal{H}^{\text{em}})_{ab} = i\hbar \omega \epsilon_{ab3}$, $\mathcal{H}^{\text{em}}$ 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 equation (14) is

$$\varrho_a = \sum_{\mu=0,3} c_\mu \varrho_{\mu a} \exp(-i\lambda_a t),$$  \hspace{1cm} (22)
where $\lambda_a$ and $g_{ab}$ are the (real) eigenvalues and eigenvectors, respectively, of $H_{ab}$.

As an example consider the special case where only $\lambda$ in eq. (20) is non-vanishing, and the spin is found at $t = t_0$ in the state $|\psi_0\rangle = \cos \frac{\eta}{2} \uparrow_z + \sin \frac{\eta}{2} \downarrow_z$. The solution in this case is given by

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

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

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

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

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

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

where $\theta$ is determined by the experimental set up. The expectation value of $A$ is given in our case by

$$\langle A \rangle = \frac{1}{2} \left[ 1 + \sin \eta \left[ \cos^2(\eta/2) \cos((\omega + 2\lambda)t + \theta) + \sin^2(\eta/2) \cos((\omega - 2\lambda)t + \theta) \right] \right]. \quad (26)$$

The correction is indeed oscillatory. This should be contrasted with the exponential $\exp(-2\lambda_{ENHS} t)$ 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 $20A^0$ neutron beam, and the analysis of Pearle [19], to constrains the generic parameter $\lambda$ to $\lambda \sim 10(\text{sec})^{-1} \sim 10^{-23}$ GeV. The constrains 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 \((t_0 \simeq 10^{-2} \text{ sec})\) by
\((1 - 2\lambda_{EHNST}t_0)\). 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 \(K_0 - \bar{K}_0\) system in a similar fashion as in the EHNS model. However, this mixing
predicts a phase of the CP violating parameter \(\epsilon\), which is of by \(\pi/2\) just as in the case
of the EHNS model [10]. Hence our modification can account only for a small part of the
CP violation observed in the \(K_0 - \bar{K}_0\) system. This leads to the generic upper bound of
order \(\sim 10^{-19}\) \(\text{Gev}\), of the same order as \(M^2_K/M_{pl}\) which could be expected on dimensional
grounds if CP and/or CPT violations are due to effects of quantum gravity. The hundred
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 \(\hat{\rho} \hat{\rho}^\dagger\) and \(\hat{\rho}^\dagger \hat{\rho}\) as the reduced density matrices of a sub-
system and an environment, respectively. The generalized Hamiltonian \(\mathcal{H}_{ab}\) in eq. (14) and
the amplitudes \(g_a\) can then be interpreted as the Hamiltonian and wave function of the total
system, while the new terms in eq. (7,9) or (14) as describing an interaction between the
sub-system and the environment. Therefore, the consistency of the proposed equation of
motion follows from quantum mechanics. Nevertheless, postulate (4), \(\hat{\rho}(t = t_0) = |\psi_0\rangle\langle\psi_0|\),
which sets the initial condition for eq. (4) 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 sub-system, 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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References


[7] BPS (ref. 6 above) used this model to examine Hawking’s proposal. They concluded that in a local field theory such a model will imply large observable violations of energy momentum conservation. For recent discussions of this issue see:

[8] For early derivation of eq. (1) see for example:
   Eq. (1) can be derived for the case a “Markovian” environment:
   For detailed derivation for the case of an oscillator coupled to a scalar field see:

    ibid, B293, 37 (1992).


[13] A similar formal relation as in eq. (2) was found in:
B. Reznik and Y. Aharonov, Phys. Rev. A, 52, 2538 (1995). However in that article the operator \( \hat{\rho} \) played the different role of a “two-state” which is determined by a pre and post-selection.

[14] This procedure is not uniquely defined since we could have postulated the initial condition \( \hat{\rho}(t = t_0) = |\psi\rangle\langle u| \), where \( |u\rangle \) is some arbitrary fixed state.

[15] It is interesting to note that (non-linear) odd power of \( \hat{\rho} \) can still be added to eq. (7), which still allow conservation of probability. For example, the most general cubic term with such property has the form \( A\hat{\rho}B\hat{\rho}^\dagger B\hat{\rho}C \) where \( A, B, C \) are hermitian operators. However such terms do no longer conserve the inner product eq. (10) and shall not be discussed further.


[20] Although the oscillatory corrections found in the two-level system are common also in the case of a coupling with some environment, the two cases are distinguishable. The modified equation of motion of the two-level model under consideration can be mapped to an ordinary quantum mechanics spin half sub-system which is coupled to another spin half (the environment). The interaction term is then given by $H_{\text{int}} = \lambda \sigma_1^z \sigma_2^z$. Assuming that a-priori no information about the initial state of $\sigma^2$ is known, we find that quantum mechanics yields a prediction which is identical to $\langle A \rangle$ in eq. (26) only in the special cases of $\eta = n\frac{\pi}{2}$.