

Entanglement and the factorization-approximation

J. Gemmer^a and G. Mahler^b

Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Received 8 June 2001

Abstract. For a bi-partite quantum system defined in a finite dimensional Hilbert-space we investigate in what sense entanglement change and interactions imply each other. For this purpose we introduce an entanglement-operator, which is then shown to represent a non-conserved property for any bi-partite system and any type of interaction. This general relation does not exclude the existence of special initial product states, for which the entanglement remains small over some period of time, despite interactions. For this case we derive an approximation to the full Schrödinger-equation, which allows the treatment of the composite systems in terms of product states. The induced error is estimated. In this factorization-approximation one subsystem appears as an effective potential for the other. A pertinent example is the Jaynes-Cummings model, which then reduces to the semi-classical rotating wave approximation.

PACS. 03.65.Yz Decoherence; open systems; quantum statistical methods – 42.50.Ct Quantum description of interaction of light and matter; related experiments – 03.65.Ud Entanglement and quantum nonlocality (e.g. EPR paradox, Bell’s inequalities, GHZ states, etc.)

1 Introduction

During the last decades entanglement has been investigated under various aspects. The famous EPR-paradox, for example, has led to a discussion of the most basic principles of quantum physics [1]. The Gedanken experiment based on “Schrödinger’s Cat” may be seen as an attempt to challenge the consistency of quantum mechanics: it has been argued that this situation could only be understood by allowing for entanglement between the atom and the cat which, on the other hand, should be considered a classical object [2]. But, by definition, a classical object cannot become entangled with any other system.

Since it has been shown, that quantum algorithms have the potential to outperform corresponding classical computing [3–5], considerable efforts have been made to implement gates like the so-called quantum controlled NOT-gate (QCNOT). Performing a QCNOT generically results in preparing an entangled state. Meanwhile various experimental schemes to prepare entangled states have been developed [6, 7].

In all these approaches entanglement has been in the very center of interest. The question was always either how to interpret the state of two systems being entangled, or how to deliberately produce entanglement and detect it, once it has been produced.

Rather neglected seems to have been the question of entanglement as an unavoidable “waste product” of quantum mechanical dynamics. Little attention has been paid to the fact that it cannot be taken for granted that any two

interacting systems will remain in a product state, even if they have been in one in the beginning [11, 14]. This means that there is always the possibility for them to entangle. And if they are entangled, it is impossible to assign two separate wavefunctions to the subsystems. Nevertheless this is typically done in standard “textbook level” quantum mechanics: the particle in a box, *e.g.*, is always described by a wavefunction although it definitely interacts with the box that necessarily consists of a many particle-quantum-system itself and therefore could become entangled with it. There is no discussion of the electron going through the double slit being possibly entangled with the material defining the slit itself.

But since these approximations typically lead to excellent results, it should be possible to point out why. In which situations is it reasonable to neglect entanglement and treat whole complicated systems as effective potentials for another quantum-system?

Apart from the rather academic desire to understand the basis of this “classical limit”, there is also a good practical reason to address such questions.

An important prerequisite of all quantum computer designs suggested so far is the possibility of so-called local unitary transformations. These should be performed selectively on each effective spin (q-bit) through potentials that are supposed to be controllable in time [15]. But again, in reality, those potentials can only be implemented by means of other complicated quantum-systems that could possibly entangle with those spins: this would inevitably lead to decoherence. But quantum computers need to be coherent. In that sense the problem of entanglement through interaction (as required by external

^a e-mail: jochen@theo1.physik.uni-stuttgart.de^b e-mail: mahler@theo1.physik.uni-stuttgart.de

control) could even challenge the implementation of any real quantum computer.

Our paper is organized as follows: we first specify a theorem relating some purity measure P (as an entanglement test) to inter-subsystem interactions (Sect. 2). For the proof of this theorem (Sect. 3) we proceed as follows.

Starting from the von-Neumann-equation, which describes the dynamics of the density operator, we proceed by inserting an expansion of the density operator into this equation. The result is an equation only in terms of the expansion coefficients that has exactly the form of the Schrödinger-equation and will therefore be called “quasi-Schrödinger-equation”. It is now possible to define a linear operator in the space of those coefficients which has an expectation value equal to P , and will therefore be called “purity operator”. Since the dynamics of those coefficients are controlled by an equation that is formally identical with the Schrödinger-equation (including a “quasi-Hamiltonian”), it is possible to reduce the question of P being conserved or not, to the problem whether the commutator of the purity operator and quasi-Hamiltonian will vanish or not.

Thus, the mathematical scheme used here is essentially the same as used in standard quantum mechanics to identify conserved quantities. Only the space of the state vector and the interpretation of the considered quantities, are different.

The last step will be to show, that the above commutator becomes nonzero whenever the full Hamiltonian involves any kind of interaction.

However, even in the presence of interactions the system may remain “almost” unentangled. In Section 4 we use our quasi-Schrödinger formulation to derive the factorization-approximation with its effective potentials for this case. In Section 5 the induced error is estimated to lowest order. In Section 6 we apply the results to the Jaynes-Cummings-model.

2 Theorems

There is a still ongoing debate on entanglement measures [9]. A lot of propositions have been made, but it seems still rather difficult to introduce a general entanglement measure that satisfies all conditions that have been imposed on such a measure and, at the same time, is applicable for any number of subsystems and any case (pure and mixed states of the whole system). And it seems even more difficult to construct a measure in such a way that it could actually be calculated (or measured!) for reasonably complicated situations.

Fortunately, it is possible to introduce a simple measure under specific conditions: if the state of the whole system is a pure state, and the full system is being regarded as divided into two subsystems, a convenient entanglement measure is $1 - P$, where

$$P = \text{Tr}_I \left\{ \left(\hat{\rho}^I \right)^2 \right\} = \text{Tr}_{II} \left\{ \left(\hat{\rho}^{II} \right)^2 \right\}; \quad (2.1)$$

here $\hat{\rho}^I, \hat{\rho}^{II}$ are the reduced density matrices of the corresponding subsystems.

Entanglement between to subsystems originating from unitary quantum evolution, can only result from interactions¹. If two systems do not interact they can be treated without even taking the other one into account. So, if they are both in pure states at the beginning, which means they are in a product state with respect to the whole system, they will remain so forever under these conditions.

One may ask now whether two systems that interact might remain entanglement-free, depending for example on the kind of systems that interact, or on the kind of interaction that is considered.

Concerning this question we are aware of only rather vague statements in the literature. A typical formulation due to d’Espagnat reads:

Theorem A – “In general it is impossible to describe systems that interacted in the past by separate wavefunctions” [11].

But does this always have to be the case? To address this problem we will prove the following theorem for finite discrete Hilbert-spaces.

Theorem B – “There exists no interaction what so ever between arbitrary systems, such that the entanglement measure $(1 - P)$ remains conserved”.

This theorem does not imply that there cannot be initial states, starting from which the system might remain in a product state, though it can be shown that those states, if they exist at all, only play a negligible role in typical larger systems. But it definitely means, that there must be initial states that lead to entanglement, even between the particle and the box-system, or between the electron and the slit-system.

Further consequences of theorem B can most conveniently be assessed from an approximation-scheme that is valid as long as the systems remain approximately unentangled, as will be shown in Sections 4, 5 and 6.

3 Proof of theorem B

3.1 Basis operators

The operators into which the density matrix will be expanded here, are products of the generators of the respective $SU(n)$ groups, where one set of generators corresponds to one subsystem [8].

The basis operators for the different subsystems are defined in the following way:

$$\hat{Q}_{i\nu} := \begin{cases} \frac{1}{\sqrt{n_\nu}} \hat{1}^\nu: & i = 0 \\ \frac{1}{\sqrt{2}} \hat{\lambda}_i^\nu: & i \neq 0 \end{cases} \quad (3.1)$$

¹ Non-unitary transformations can do without direct interactions: this phenomenon has become known as entanglement swapping [16].

where, ν denotes the index of the subsystem, n_ν the number of levels of subsystem ν (dimension) and $\hat{\lambda}_i^\nu$ the i th generator of the $SU(n_\nu)$ group, $i = 1, 2, \dots, n_\nu^2 - 1$.

The basis operators of the full system are defined as dyadic products of the basis operators of the subsystems,

$$\hat{Q}_i := \prod_{\nu=0}^N \otimes \hat{Q}_{i_\nu} \quad (3.2)$$

where N is the number of subsystems.

Thus any basis operator is defined by a sequence of N indices i_ν (abbreviated as \mathbf{i}), each index specifying, which generator i should be applied to the corresponding subsystem ν . The operators constructed according to these rules form a complete and orthonormal set in the following sense:

$$\text{Tr}\{\hat{Q}_i \hat{Q}_j\} = \delta_{\mathbf{i}\mathbf{j}} := \prod_{\nu=1}^N \delta_{i_\nu j_\nu} \quad \hat{A} = \sum_{\mathbf{i}} \hat{Q}_i \text{Tr}\{\hat{Q}_i \hat{A}\} \quad (3.3)$$

where \hat{A} is an arbitrary operator.

Representing the density matrix in the case of only two subsystems as

$$\hat{\rho} = \sum_{i,j} q_{ij} \hat{Q}_i \otimes \hat{Q}_j \quad (3.4)$$

where the index i corresponds to subsystem I and the index j to subsystem II, we find

$$\hat{\rho}^I = \sqrt{n_{II}} \sum_i q_{i0} \hat{Q}_i \quad P = n_{II} \sum_i q_{i0}^2. \quad (3.5)$$

The objects we are going to examine are thus specified in terms of their expansion coefficients.

3.2 Quasi-Schrödinger-equation

The von-Neumann-equation reads:

$$i\hbar \frac{d}{dt} \hat{\rho} = [\hat{H}, \hat{\rho}]. \quad (3.6)$$

Inserting the expansion (3.4) yields:

$$i\hbar \sum_{\mathbf{i}} \frac{d}{dt} q_i \hat{Q}_i = \sum_{\mathbf{j}} [\hat{H}, \hat{Q}_j] q_j. \quad (3.7)$$

After multiplying by \hat{Q}_m , taking the trace and applying some trace theorems, we get:

$$i\hbar \frac{d}{dt} q_m = \sum_{\mathbf{j}} \mathcal{H}_{m\mathbf{j}} q_j \quad \mathcal{H}_{m\mathbf{j}} := \text{Tr}\{\hat{H} [\hat{Q}_j, \hat{Q}_m]\} \quad (3.8)$$

This equation (hereafter called quasi-Schrödinger-equation) has evidently the Schrödinger-form. The

hermiticity of \mathcal{H} is easily shown by examining the corresponding matrix elements,

$$\begin{aligned} \mathcal{H}_{m\mathbf{j}}^* &= \text{Tr}\{\hat{H} [\hat{Q}_j, \hat{Q}_m]\}^* = \text{Tr}\left\{\left(\hat{H} [\hat{Q}_j, \hat{Q}_m]\right)^\dagger\right\} \\ &= \text{Tr}\{\hat{H} [\hat{Q}_m, \hat{Q}_j]\} = \mathcal{H}_{\mathbf{j}m}. \end{aligned} \quad (3.9)$$

We can even define a formal bracket notation: for this purpose we re-arrange the multiple indices \mathbf{j} as a simple index s and introduce a set of real orthogonal basis vectors

$$|s\rangle = |s\rangle^* \quad (3.10)$$

with

$$\langle s|s'\rangle = \delta_{ss'} \quad \hat{1} = \sum_s |s\rangle\langle s| \quad (3.11)$$

such that

$$\mathcal{H}_{ss'} = \langle s|\mathcal{H}|s'\rangle \quad q_s = \langle s|q\rangle. \quad (3.12)$$

Inserting (3.12) into (3.8) yields:

$$i\hbar \frac{d}{dt} |q\rangle = \mathcal{H}|q\rangle \quad (3.13)$$

with the infinitesimal solution

$$|q(dt)\rangle = \left(1 + \frac{1}{i\hbar} \mathcal{H} dt\right) |q(0)\rangle. \quad (3.14)$$

On the basis of this formal equivalence it is now possible to investigate the conservation of some quantity \mathcal{A} in the space of the vectors $|q\rangle$ ($\langle q|\mathcal{A}|q\rangle = \sum_{s,s'} q_s \mathcal{A}_{ss'} q_{s'}$), by evaluating the commutator of \mathcal{A} with \mathcal{H} .

3.3 Purity operator

We first note that our purity measure, P , can be given the mathematical form of an expectation value:

$$\langle q|\mathcal{P}|q\rangle = P. \quad (3.15)$$

To find \mathcal{P} , we go back to the explicit multi-index notation (for two subsystems),

$$P = \sum_{s,s'} q_s \mathcal{P}_{ss'} q_{s'} = \sum_{i,j,u,v} q_{ij} \mathcal{P}_{ijuv} q_{uv}. \quad (3.16)$$

If we require (see (3.5))

$$\langle q|\mathcal{P}|q\rangle = n_{II} \sum_i q_{i0}^2 \quad (3.17)$$

it follows that

$$P_{ijuv} = n_{II} \delta_{iu} \delta_{jv} \delta_{0j} \quad (3.18)$$

i.e., up to a normalization factor \mathcal{P} is a projector, projecting out the components of $|q\rangle$ that refer locally to subsystem I, those components that would read q_{i0} in multi-index notation for a bi-partite system. Using the bracket notation \mathcal{P} reads:

$$\mathcal{P} = n_{\text{II}} \sum_w |w^{\text{I}}\rangle\langle w^{\text{I}}|. \quad (3.19)$$

Adding the complementary projector that projects out all the other components, that is all those that do not refer locally to subsystem I, we can write the unity operator as:

$$\hat{1} = \sum_w |w^{\text{I}}\rangle\langle w^{\text{I}}| + \sum_k |k^{\text{R}}\rangle\langle k^{\text{R}}|. \quad (3.20)$$

Using this representation, \mathcal{H} , which controls the complete dynamics, can be split up into:

$$\mathcal{H} = \mathcal{L}^{\text{I}} + \mathcal{R} + \mathcal{W} \quad (3.21)$$

where

$$\begin{aligned} \mathcal{L}^{\text{I}} &:= \sum_{l,m} \mathcal{L}_{lm}^{\text{I}} |l^{\text{I}}\rangle\langle m^{\text{I}}| \\ \mathcal{R} &:= \sum_{i,j} \mathcal{R}_{ij} |i^{\text{R}}\rangle\langle j^{\text{R}}| \\ \mathcal{W} &:= \sum_{l,j} \left(\mathcal{W}_{lj} |l^{\text{I}}\rangle\langle j^{\text{R}}| + \mathcal{W}_{jl} |j^{\text{R}}\rangle\langle l^{\text{I}}| \right). \end{aligned}$$

One easily convinces oneself, that

$$[\mathcal{P}, \mathcal{L}^{\text{I}}] = 0 \quad \text{and} \quad [\mathcal{P}, \mathcal{R}] = 0. \quad (3.22)$$

Finally, the commutator $[\mathcal{P}, \mathcal{W}]$ reads:

$$[\mathcal{P}, \mathcal{W}] = n_{\text{II}}^2 \sum_{w,j} \left(\mathcal{W}_{wj} |w^{\text{I}}\rangle\langle j^{\text{R}}| - \mathcal{W}_{jw} |j^{\text{R}}\rangle\langle w^{\text{I}}| \right). \quad (3.23)$$

We now convince ourselves that not all matrix-elements \mathcal{W}_{wk} can be identically zero in the presence of interactions. For this purpose we define “interaction” operationally: two subsystems are said to interact, if the dynamics of one subsystem, at least for some initial state (but generically for any initial state) depend on the state of the other subsystem.

The state of subsystem I at time dt is completely described by the projection

$$|q^{\text{I}}(dt)\rangle := \sum_w |w^{\text{I}}\rangle\langle w^{\text{I}}|q(dt)\rangle. \quad (3.24)$$

Substituting $|q(dt)\rangle$ according to the evolution equation (3.14) with \mathcal{H} given by (3.21) we obtain

$$\begin{aligned} |q^{\text{I}}(dt)\rangle &= |q^{\text{I}}(0)\rangle \\ &+ \frac{1}{i\hbar} dt \left(\sum_{w,m} L_{wm}^{\text{I}} |w^{\text{I}}\rangle\langle m^{\text{I}}|q(0)\rangle + \sum_{w,j} \mathcal{W}_{wj} |w^{\text{I}}\rangle\langle j^{\text{R}}|q(0)\rangle \right). \end{aligned} \quad (3.25)$$

As only the components $\langle j^{\text{R}}|q\rangle$ carry information about subsystem II not all W -matrix-elements can be zero for interacting subsystems.

Since the two terms that are summed over in (3.23) obviously belong to different (off diagonal) parts of \mathcal{H} , they cannot cancel each other. Thus we conclude,

$$[\mathcal{P}, \mathcal{H}] \neq 0, \quad (3.26)$$

for any sort of interaction, which completes the proof of theorem B.

4 Factorization-approximation and effective potentials

As we have shown, there is, *a priori*, no reason to assume that two interacting systems remain in pure states. Nevertheless, as we will argue now, it is a reasonable approximation to treat one subsystem as if it was in a pure state, and the other one as an effective potential for the former, as long as $1 - P$ remains small over the period of time under investigation.

4.1 Factorization-approximation

We start with the quasi-Schrödinger-equation (3.8) for two subsystems,

$$i\hbar \frac{d}{dt} q_{ij} = - \sum_{l,m} \text{Tr} \left\{ \hat{H} \left[\hat{Q}_{ij}, \hat{Q}_{lm} \right] \right\} q_{lm} \quad (4.1)$$

and consider only those equations which refer to the two subsystems locally, not to the correlations. We thus need to study:

$$\begin{aligned} \text{I: } i\hbar \sqrt{n_{\text{II}}} \frac{d}{dt} q_{i0} &= - \sum_{l,m} \text{Tr} \left\{ \hat{H} \left[\frac{\hat{\lambda}_i}{\sqrt{2}}, \hat{Q}_{lm} \right] \right\} q_{lm} \\ \text{II: } i\hbar \sqrt{n_{\text{I}}} \frac{d}{dt} q_{0j} &= - \sum_{l,m} \text{Tr} \left\{ \hat{H} \left[\frac{\hat{\lambda}_j}{\sqrt{2}}, \hat{Q}_{lm} \right] \right\} q_{lm} \end{aligned} \quad (4.2)$$

i.e., we have to examine the relation between “local” (q_{i0}, q_{0j}) and “global” (q_{ij}) coefficients. We define a tensor M in the following way:

$$M_{ij} := \langle \hat{Q}_i \otimes \hat{Q}_j \rangle - \langle \hat{Q}_i \rangle \langle \hat{Q}_j \rangle \quad (4.3)$$

or, according to (3.4) and (3.3):

$$M_{ij} = q_{ij} - \sqrt{n_{\text{I}} n_{\text{II}}} q_{i0} q_{0j}. \quad (4.4)$$

Obviously, for a product state all M_{ij} 's have to vanish. If the two subsystems get correlated (entangled), the M_{ij} 's will take on nonzero values, so that

$$\beta := \sum_{i,j} M_{ij}^2 \quad (4.5)$$

can be considered as an alternative entanglement measure. It is indeed possible to derive a relation between β and P [10]:

$$\beta < 1 - P^2. \quad (4.6)$$

If we now solve (4.4) for q_{ij} and insert the result into (4.2) we get for subsystem I:

$$\begin{aligned} i\hbar\sqrt{n_{\text{II}}}\frac{d}{dt}q_{i0} = & \\ & - \sum_{l,m} \text{Tr} \left\{ \hat{H} \left[\frac{\hat{\lambda}_i}{\sqrt{2}}, \hat{Q}_{lm} \right] \right\} \left(\sqrt{n_{\text{I}}n_{\text{II}}}q_{l0}q_{0m} + M_{lm} \right). \end{aligned} \quad (4.7)$$

Using (3.5) and (4.6) we find

$$n_{\text{I}}n_{\text{II}} \sum_{l,m} q_{l0}^2 q_{0m}^2 = P^2 \quad \sum_{l,m} M_{lm}^2 < 1 - P^2, \quad (4.8)$$

so that it seems reasonable to neglect the M_{lm} -term and only keep the $\sqrt{n_{\text{I}}n_{\text{II}}}q_{l0}q_{0m}$ -term in (4.7), as long as P stays close to 1. The error that occurs if this approximation is used over a period of time instead of the true Schrödinger-equation, will be estimated later.

With the above approximation we get after performing the sum over m :

$$i\hbar\sqrt{n_{\text{II}}}\frac{d}{dt}q_{i0} = - \sum_l \text{Tr} \left\{ \hat{H} \left[\frac{\hat{\lambda}_i}{\sqrt{2}}, \sqrt{\frac{n_{\text{II}}}{2}}\hat{\lambda}_l \right] \otimes \hat{\rho}^{\text{II}} \right\} q_{l0}. \quad (4.9)$$

The latter is a quasi-Schrödinger-equation for subsystem I with a quasi-Hamiltonian depending on the momentary local state of subsystem II. It is easy to check that the quasi-Hamiltonian of this equation, although depending on time, will always be Hermitian. This means that in this approximation $\sqrt{n_{\text{II}}}\sum_i q_{i0}^2 = P$ is a conserved quantity. Both subsystems will remain in pure states and unentangled if the initial state was a product state.

Performing the sum over l and taking the partial trace with respect to subsystem II yields:

$$i\hbar\sqrt{n_{\text{II}}}\frac{d}{dt}q_{i0} = -\text{Tr}_{\text{I}} \left\{ \text{Tr}_{\text{II}} \left\{ \hat{H}\hat{\rho}^{\text{II}} \right\} \left[\frac{\hat{\lambda}_i}{\sqrt{2}}, \hat{\rho}^{\text{I}} \right] \right\}. \quad (4.10)$$

Since $\hat{\rho}_1$ and $\hat{\rho}_2$ always represent pure states in this case, we can use separate wavefunctions to re-express local expectation values, such as:

$$\text{Tr}_{\text{II}} \left\{ \hat{H}\hat{\rho}^{\text{II}} \right\} = \left\langle \psi^{\text{II}} | \hat{H} | \psi^{\text{II}} \right\rangle. \quad (4.11)$$

Attention should be paid to the fact that this expectation value is still an operator with respect to subsystem I, if \hat{H} contains interactions.

Following the standard trace theorems, we get:

$$i\hbar\sqrt{n_{\text{II}}}\frac{d}{dt}q_{i0} = \text{Tr}_{\text{I}} \left\{ \frac{\hat{\lambda}_i}{\sqrt{2}} \left[\left\langle \psi^{\text{II}} | \hat{H} | \psi^{\text{II}} \right\rangle, \hat{\rho}^{\text{I}} \right] \right\}. \quad (4.12)$$

Multiplying the i th equation by $\hat{\lambda}_i/\sqrt{2}$, summing over i , exploiting the completeness of the $\hat{\lambda}_i/\sqrt{2}$'s and using (3.5) leads to:

$$i\hbar\frac{d}{dt}\hat{\rho}^{\text{I}} = \left[\left\langle \psi^{\text{II}} | \hat{H} | \psi^{\text{II}} \right\rangle, \hat{\rho}^{\text{I}} \right]. \quad (4.13)$$

This equation is of the same form as the von-Neumann-equation. Since the reduced density operators $\hat{\rho}_1, \hat{\rho}_{\text{II}}$ represent pure states we can change to the corresponding Schrödinger-equation, without loss of generality:

$$i\hbar\frac{\partial}{\partial t}|\psi^{\text{I}}\rangle = \left\langle \psi^{\text{II}} | \hat{H} | \psi^{\text{II}} \right\rangle |\psi^{\text{I}}\rangle. \quad (4.14)$$

After splitting the Hamiltonian \hat{H} into local ($\hat{L}_1, \hat{L}_{\text{II}}$) and interaction (\hat{W}) parts and adding the corresponding equation of subsystem II, we find the complete system of equations:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi^{\text{I}}\rangle &= \left(\hat{L}_1 + \left\langle \psi^{\text{II}} | \hat{L}_{\text{II}} | \psi^{\text{II}} \right\rangle + \left\langle \psi^{\text{II}} | \hat{W} | \psi^{\text{II}} \right\rangle \right) |\psi^{\text{I}}\rangle \\ i\hbar\frac{\partial}{\partial t}|\psi^{\text{II}}\rangle &= \left(\hat{L}_{\text{II}} + \left\langle \psi^{\text{I}} | \hat{L}_1 | \psi^{\text{I}} \right\rangle + \left\langle \psi^{\text{I}} | \hat{W} | \psi^{\text{I}} \right\rangle \right) |\psi^{\text{II}}\rangle. \end{aligned} \quad (4.15)$$

4.2 Gauge

Since the overall phases of both subsystems are arbitrary and can be chosen freely, a method, which is completely analogous to the Lorentz gauge in classical electrodynamics, can be used to simplify these equations even further.

Applying the substitutions

$$e^{i\alpha_{\text{I}}(t)}|\phi^{\text{I}}\rangle := |\psi^{\text{I}}\rangle \quad e^{i\alpha_{\text{II}}(t)}|\phi^{\text{II}}\rangle := |\psi^{\text{II}}\rangle \quad (4.16)$$

and choosing the phases as

$$\begin{aligned} \left\langle \psi^{\text{II}} | \hat{L}_{\text{II}} | \psi^{\text{II}} \right\rangle + \hbar\dot{\alpha}_{\text{I}}(t) &= 0 \\ \left\langle \psi^{\text{I}} | \hat{L}_1 | \psi^{\text{I}} \right\rangle + \hbar\dot{\alpha}_{\text{II}}(t) &= 0 \end{aligned} \quad (4.17)$$

transforms the system of equations into:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\phi^{\text{I}}\rangle &= \left(\hat{L}_1 + \left\langle \phi^{\text{II}} | \hat{W} | \phi^{\text{II}} \right\rangle \right) |\phi^{\text{I}}\rangle \\ i\hbar\frac{\partial}{\partial t}|\phi^{\text{II}}\rangle &= \left(\hat{L}_{\text{II}} + \left\langle \phi^{\text{I}} | \hat{W} | \phi^{\text{I}} \right\rangle \right) |\phi^{\text{II}}\rangle. \end{aligned} \quad (4.18)$$

This is a coupled set of nonlinear first-order differential equations which, although it does not necessarily create unitary dynamics, keeps the absolute values of the wavefunctions of both subsystems fixed. Instead of the $(n_{\text{I}}n_{\text{II}})$ dimensions of the exact treatment, this approximation has only $(n_{\text{I}} + n_{\text{II}})$ dimensions (number of equations).

Each of these equations can be considered as an ‘‘ordinary’’ Schrödinger-equation of one system, in which the influence of the other one appears as an effective potential. This approach may be termed ‘‘quasi-classical’’ with

respect to interactions. It underlies, *e.g.* the potential for the particle in a box.

Similar equations are well-known in the theory of many particle systems (for example the Hartree-equation [12]). But in those cases they are basically justified by their success. We are now going to derive a criterion for their applicability.

5 Error estimation

We will now examine the deviation of the solution in factorization-approximation $|\phi(t)\rangle$ from the solution of the full Schrödinger-equation $|\psi(t)\rangle$, under the condition that $|\phi(0)\rangle = |\psi(0)\rangle$. We will expand this deviation in terms of an effective interaction which will allow us to connect the resulting error with the purity P .

The Schrödinger-equation reads:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = (\hat{L}_I + \hat{L}_{II} + \hat{W}) |\psi\rangle. \quad (5.1)$$

With $|\phi\rangle := |\phi^I\rangle \otimes |\phi^{II}\rangle$, the factorization-approximation reads:

$$i\hbar \frac{\partial}{\partial t} |\phi\rangle = (\hat{L}_I + \hat{L}_{II} + \langle \phi^I | \hat{W} | \phi^I \rangle + \langle \phi^{II} | \hat{W} | \phi^{II} \rangle + \alpha) |\phi\rangle \quad (5.2)$$

where α denotes an insignificant overall phase, and

$$|\phi\rangle := |\phi^I\rangle \otimes |\phi^{II}\rangle. \quad (5.3)$$

Introducing the deviation $|\theta\rangle$ as

$$|\psi\rangle = |\theta\rangle + |\phi\rangle, \quad (5.4)$$

and the abbreviation

$$\hat{V} := \hat{W} - \langle \phi^I | \hat{W} | \phi^I \rangle - \langle \phi^{II} | \hat{W} | \phi^{II} \rangle - \alpha \quad (5.5)$$

we can write a differential equation for this deviation $|\theta\rangle$ just in terms of $|\phi\rangle$ and $|\theta\rangle$ as

$$\frac{\partial}{\partial t} |\theta\rangle = \frac{1}{i\hbar} (\hat{H}|\theta\rangle + \hat{V}|\phi\rangle). \quad (5.6)$$

Defining

$$|\theta'\rangle := e^{\frac{i\hat{H}t}{\hbar}} |\theta\rangle \quad (5.7)$$

we can rewrite (5.6) as

$$\frac{\partial}{\partial t} |\theta'\rangle = \frac{1}{i\hbar} e^{\frac{i\hat{H}t}{\hbar}} \hat{V} |\phi\rangle. \quad (5.8)$$

The exponential may be written as

$$e^{\frac{i\hat{H}t}{\hbar}} = \sum_n |\psi_n(0)\rangle \langle \psi_n(t)| = \sum_n |\phi_n(0)\rangle (\langle \phi_n(t)| + \langle \theta_n(t)|). \quad (5.9)$$

Here the $|\phi_n(0)\rangle = |\psi_n(0)\rangle$ are chosen to form a complete orthonormal set. The $|\phi_n(t)\rangle$ as solutions in factorization approximation form a complete orthonormal set at all times if they did so at $t = 0$, so they will be used as a basis. Since they all obey (5.8) we get, using (5.9):

$$|\theta'_i(t)\rangle = \frac{1}{i\hbar} \sum_n |\phi_n(0)\rangle \times \int_0^t (\langle \phi_n(t')| + \langle \theta_n(t')|) \hat{V} |\phi_i(t')\rangle dt'. \quad (5.10)$$

Transforming back to the unprimed quantities, we find

$$|\theta_i(t)\rangle = \frac{1}{i\hbar} \sum_n (|\phi_n(t)\rangle + |\theta_n(t)\rangle) \times \int_0^t (\langle \phi_n(t')| + \langle \theta_n(t')|) \hat{V} |\phi_i(t')\rangle dt'. \quad (5.11)$$

By iterating this equation we can produce an expansion of $|\theta_i(t)\rangle$ in terms of time integrals over matrix elements of the effective interaction \hat{V} . As long as those matrix elements remain small, a truncation scheme can be applied, which gives to first order:

$$|\theta_i(t)\rangle = \frac{1}{i\hbar} \sum_n |\phi_n(t)\rangle \int_0^t \langle \phi_n(t') | \hat{V} | \phi_i(t') \rangle dt'. \quad (5.12)$$

We return now to the double-index notation

$$|\phi_{ij}\rangle := |\phi_i^I\rangle \otimes |\phi_j^{II}\rangle, \quad \langle \phi_i^I | \phi_{i'}^I \rangle = \delta_{i'i}, \quad \langle \phi_j^{II} | \phi_{j'}^{II} \rangle = \delta_{j'j} \quad (5.13)$$

and take $|\psi_{00}\rangle (|\phi_{00}\rangle)$ as the solution (approximation) under consideration. We use the $|\phi_{ij}\rangle$'s as a basis to write the full solution

$$|\psi_{00}\rangle = \sqrt{1 - \sum_{i,j} |\theta_{ij}|^2} |\phi_{00}\rangle + \sum_{i,j} \theta_{ij} |\phi_{ij}\rangle, \quad \theta_{00} := 0. \quad (5.14)$$

Its overlap of this solution with the solution in factorization-approximation (“fidelity”) is exactly given by

$$|\langle \psi_{00} | \phi_{00} \rangle|^2 = 1 - \sum_{i,j} |\theta_{ij}|^2. \quad (5.15)$$

On the other hand, the square-root of the purity of either subsystem of the state $|\psi_{00}\rangle$ to first order in $|\theta_{ij}|^2$ is given by

$$\sqrt{P} \approx 1 - \sum_{i \neq 0, j \neq 0} |\theta_{ij}|^2. \quad (5.16)$$

Obviously the two quantities are the same except for the θ_{i0} 's and the θ_{0j} 's. Computing the θ_{ij} 's from equation (5.12) yields:

$$\theta_{ij} = \frac{1}{i\hbar} \int_0^t (\langle \phi_{ij} | \hat{W} | \phi_{00} \rangle - \langle \phi_{0j} | \hat{W} | \phi_{00} \rangle \delta_{i0} - \langle \phi_{i0} | \hat{W} | \phi_{00} \rangle \delta_{0j} + \alpha \delta_{i0} \delta_{0j}) dt'. \quad (5.17)$$

Choosing $\alpha := \langle \phi_{00} | \hat{W} | \phi_{00} \rangle$ to satisfy the definition $\theta_{00} := 0$ from (5.14) we get

$$\theta_{i0}(t) = 0 \quad \theta_{0j}(t) = 0 \quad (5.18)$$

so that

$$|\langle \psi_{00} | \phi_{00} \rangle|^2 = \sqrt{P} \quad (5.19)$$

as long as the small deviation of \sqrt{P} from 1 is dominated by the lowest order term in the effective interaction strength, as it is the case in the example in Section 6.

This means that no “local” errors are generated in first order, any deviation occurring due to the factorization-approximation leads to entanglement and therefore reduces purity.

6 Application to the Jaynes-Cummings-model

6.1 The model

The factorization-approximation will now be applied to the Jaynes-Cummings-model. This choice is motivated by the fact that this model can be solved exactly, hence it can be tested whether the approximation is really applicable. Furthermore, both methods of treating this system, the fully quantum mechanical and the semi-classical one, are well-known, thus the result of applying the factorization-approximation can easily be interpreted.

The Jaynes-Cummings-model [13] describes a spin in a magnetic field, interacting with some monochromatic electromagnetic field. A good example is a typical NMR experiment of any sort.

The model in rotating wave approximation is defined by the Hamiltonian:

$$\hat{H} = Bg\mu\frac{1}{2}\hat{\sigma}_z + \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \hbar\gamma\left(\hat{a}^\dagger\hat{\sigma}^- + \hat{a}\hat{\sigma}^+\right), \quad (6.1)$$

where B denotes the magnetic field, g the gyromagnetic relation, μ Bohr’s magneton, $\hat{\sigma}_z$ the operator of the z -component of the spin, γ the coupling constant, $\hat{\sigma}^+$, $\hat{\sigma}^-$ are the creation and annihilation operators of the spin system, ω is the frequency of the electromagnetic field and \hat{a}^\dagger , \hat{a} are the creation and annihilation operators of the electromagnetic field.

The second term describes the monochromatic electromagnetic field, the first term the spin in the magnetic field and the third term their mutual interaction.

6.2 Application of the factorization-approximation

Applying the scheme (4.18) to this system yields:

$$i\hbar\frac{\partial}{\partial t}|\phi^S\rangle = \left(Bg\mu\frac{1}{2}\hat{\sigma}_z + \hbar\gamma\left(\langle\phi^L|\hat{a}^\dagger|\phi^L\rangle\hat{\sigma}^- + \langle\phi^L|\hat{a}|\phi^L\rangle\hat{\sigma}^+\right)\right)|\phi^S\rangle \quad (6.2)$$

$$i\hbar\frac{\partial}{\partial t}|\phi^L\rangle = \left(\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \hbar\gamma\left(\langle\phi^S|\hat{\sigma}^-|\phi^S\rangle\hat{a}^\dagger + \langle\phi^S|\hat{\sigma}^+|\phi^S\rangle\hat{a}\right)\right)|\phi^L\rangle \quad (6.3)$$

where S indicates the spin system and L the system of the electromagnetic field. The absolute values of the expectation values $\langle\phi^S|\hat{\sigma}^-|\phi^S\rangle$, $\langle\phi^S|\hat{\sigma}^+|\phi^S\rangle$ are always limited by:

$$\left|\langle\phi^S|\hat{\sigma}^-|\phi^S\rangle\right|, \left|\langle\phi^S|\hat{\sigma}^+|\phi^S\rangle\right| \leq 1. \quad (6.4)$$

The influence of the coupling terms on the evolution of the electromagnetic field is thus negligible, if $\gamma \ll \omega$ and/or the system of the electromagnetic field is in a highly excited state. Thus, for example, a coherent state $|\alpha\rangle$ with a large parameter α is a valid solution to the equation controlling the dynamics of the electromagnetic field.

Inserting this solution into the equation for the spin systems leads to:

$$i\hbar\frac{\partial}{\partial t}|\phi^S\rangle = \left(Bg\mu\frac{1}{2}\hat{\sigma}_z + \hbar\gamma\left(\langle\alpha|\hat{a}^\dagger|\alpha\rangle\hat{\sigma}^- + \langle\alpha|\hat{a}|\alpha\rangle\hat{\sigma}^+\right)\right)|\phi^S\rangle = \left(Bg\mu\frac{1}{2}\hat{\sigma}_z + \hbar\gamma\sqrt{2}|\alpha|\left(\cos(\omega t)\hat{\sigma}_x + \sin(\omega t)\hat{\sigma}_y\right)\right)|\phi^S\rangle. \quad (6.5)$$

This is exactly the semi-classical approach, which often produces excellent results, such as the correct Rabi-frequency, etc.

It remains to be shown, that it was indeed justified to use the factorization-approximation for some time τ .

6.3 Estimation of P

If the spin and electromagnetic field are in resonance, an exact solution of the Jaynes-Cummings-model can be found:

$$|n^+\rangle := \frac{1}{\sqrt{2}}(|0\rangle \otimes |n\rangle + |1\rangle \otimes |n-1\rangle) \\ |n^-\rangle := \frac{1}{\sqrt{2}}(|0\rangle \otimes |n\rangle - |1\rangle \otimes |n-1\rangle), \quad (6.6)$$

which satisfies the following eigenvalue equations:

$$\hat{H}|n^+\rangle = (\hbar\omega n + \hbar\gamma\sqrt{n})|n^+\rangle \\ \hat{H}|n^-\rangle = (\hbar\omega n - \hbar\gamma\sqrt{n})|n^-\rangle. \quad (6.7)$$

Considering the initial product state

$$|\psi(0)\rangle = \left(\sum_n A_n |n\rangle\right) \otimes |0\rangle, \quad (6.8)$$

we then find for the components of the Bloch vector of the spin system:

$$\begin{aligned} \langle \hat{\sigma}_x \otimes \hat{1} \rangle &= \sum_n -\text{Im} \left(A_n^* A_{n+1} e^{-i\omega t} \right) \left(\sin(\gamma(\sqrt{n} + \sqrt{n+1})t) \right. \\ &\quad \left. - \sin(\gamma(\sqrt{n} - \sqrt{n+1})t) \right) \\ \langle \hat{\sigma}_y \otimes \hat{1} \rangle &= \sum_n \text{Re} \left(A_n^* A_{n+1} e^{-i\omega t} \right) \left(\sin(\gamma(\sqrt{n} + \sqrt{n+1})t) \right. \\ &\quad \left. - \sin(\gamma(\sqrt{n} - \sqrt{n+1})t) \right) \\ \langle \hat{\sigma}_z \otimes \hat{1} \rangle &= \sum_n |A_n|^2 \cos(2\sqrt{nt}). \end{aligned} \quad (6.9)$$

From these components we find P as:

$$\text{Tr}_S \{ \hat{\rho}_S^2 \} = P = \frac{1}{2} \left(1 + \langle \hat{\sigma}_x \rangle^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2 \right). \quad (6.10)$$

For the initial state we again choose a coherent state (for simplicity with a real parameter α), which means:

$$A_n = e^{-\frac{1}{2}|\alpha|^2} \frac{\alpha^n}{\sqrt{n!}}. \quad (6.11)$$

Now we want to simplify the terms in (6.9). Consider:

$$\begin{aligned} A_n^* A_{n+1} &= e^{-|\alpha|^2} \frac{\alpha^n}{\sqrt{n!}} \frac{\alpha^{n+1}}{\sqrt{(n+1)!}} \\ &= \left(e^{-|\alpha|^2} \frac{\alpha^{2n}}{n!} \right) \left(\frac{\alpha}{\sqrt{(n+1)}} \right). \end{aligned} \quad (6.12)$$

The first factor describes a Poisson-distribution which is characterized by the mean value α^2 and the standard deviation α . Since the main weight of such a distribution is concentrated near its mean value (98% within 3 standard deviations), it is a reasonable approximation to keep only contributions from this range. The second factor can be estimated using its respective value at the boundaries of this range:

$$\frac{\alpha}{\sqrt{(\alpha^2 + \alpha + 1)}} \leq \frac{\alpha}{\sqrt{(n_{\text{rel}} + 1)}} \leq \frac{\alpha}{\sqrt{(\alpha^2 - \alpha + 1)}} \quad (6.13)$$

where n_{rel} denotes the n 's from within this relevant range. If we now again only consider highly excited coherent states, that means the limit $\alpha \rightarrow \infty$, the upper as well as the lower bound converges against 1. Hence in this limit:

$$\frac{\alpha}{\sqrt{(n_{\text{rel}} + 1)}} \approx 1. \quad (6.14)$$

In the same limit we also find:

$$\sqrt{n} + \sqrt{(n+1)} \approx 2\sqrt{n} \quad \sqrt{n} - \sqrt{(n+1)} \approx 0. \quad (6.15)$$

For a large enough α (6.9) therefore simplifies to:

$$\begin{aligned} \langle \hat{\sigma}_x \otimes \hat{1} \rangle &\approx \sin(\omega t) \sum_n |A_n|^2 \sin(2\gamma\sqrt{nt}) \\ \langle \hat{\sigma}_y \otimes \hat{1} \rangle &\approx \cos(\omega t) \sum_n |A_n|^2 \sin(2\gamma\sqrt{nt}) \\ \langle \hat{\sigma}_z \otimes \hat{1} \rangle &\approx - \sum_n |A_n|^2 \cos(2\gamma\sqrt{nt}). \end{aligned} \quad (6.16)$$

In this approximation the factors depending on ωt describe the Larmor-precession, while the sum terms give rise to the Rabi-precession.

Expanding the argument of the Rabi-precession around the mean value of the Poisson-distribution yields:

$$\begin{aligned} 2\gamma\sqrt{nt} &\approx \gamma t \left(2\alpha + \frac{1}{\alpha}(n - \alpha^2) \right. \\ &\quad \left. - \frac{1}{2\alpha^3}(n - \alpha^2)^2 + O^3(n - \alpha^2) \right). \end{aligned} \quad (6.17)$$

Since we are only considering contributions from the relevant region, that is contributions with $|n - \alpha^2| \leq \alpha$ in the limit $\alpha \rightarrow \infty$, we can neglect any term beyond second-order and get:

$$2\gamma\sqrt{nt} \approx \gamma t \left(2\alpha + \frac{(n - \alpha^2)}{\alpha} \right). \quad (6.18)$$

Using this approximation and some addition theorems we get on the right hand side of (6.10) fast oscillating terms with a frequency given by the first term in (6.18) and slow oscillating terms with a frequency given by the second term in (6.18). Since the slow oscillating terms from the relevant region oscillate with a frequency of the order of γ regardless of the actual α , we expand those in time to second order, which will be a good approximation as long as γt remains small:

$$P \approx 1 - \gamma^2 t^2. \quad (6.19)$$

This means that in the limit of high intensities of the electromagnetic field, the ‘‘coherence time’’ is independent of the intensity itself and only depends on the strength of the coupling. If that is weak enough, the factorization approximation will be valid for a considerable time.

7 Summary and conclusions

We have shown that bi-partite systems with mutual interactions, that remain unentangled forever, no matter which initial product state was chosen, cannot exist.

One might argue that this is a rather weak statement: in large systems with many degrees of freedom there might be a large number of initial states, starting from which the subsystems would remain entanglement-free, even though there must also be some initial states that lead to entanglement.

But the same could be argued, for example, for a classical Hamilton-system, which has no radial symmetry, say: although angular momentum is not conserved in such a situation in general, there might be special trajectories for which it is conserved. But one probably would not claim that these trajectories are of importance considering the space of all possible trajectories, especially in systems with many degrees of freedom.

The same holds true for the entanglement conservation: there might be special initial states that prevent the systems from getting entangled, but it can be shown that their relative weight decreases with the system size [17].

Thus it is, strictly speaking, unjustified to describe a particle in a box, which is part of an interacting quantum system, by a wave-function.

It is, nevertheless, a potentially very good approximation to describe interacting systems by pure individual wavefunctions, if the entanglement remains small during the time of observation. The underlying equation can then be based on the factorization approximation; this equation has been derived, together with a criterion for its validity.

For a spin interacting with a monochromatic electromagnetic field, we have shown that the criterion is fulfilled for high enough field intensities and for a time that only depends inversely on the coupling strength. Applying the factorization approximation then transforms the full quantum mechanical Jaynes-Cummings-model into a semi-classical one, in which the field acts as an external potential.

We thank C. Granzow, A. Otte, I. Kim, F. Tonner and M. Stollsteimer for fruitful discussions.

References

1. A. Einstein, B. Podolsky, N. Rosen, *Phys. Rev.* **47**, 777 (1935).
2. A. Otte, *Physik und Quanteninformation - Darstellung, Symmetrie und Dynamik* (Diplomarbeit, Stuttgart, 1998).
3. D. Deutsch, *Phys. Lett.* **79**, 325 (1997).
4. P.W. Shor, in *Proc. of the Symp. on the Foundations of Computerscience, Los Alamitos, California* (IEEE Computer Society Press, New York, 1994), pp. 124-134.
5. L. Grover, *Proc. R. Soc. Lond. A* **400**, 97 (1985).
6. I. Chuang, N. Gershenfeld, M. Kubinec, *Phys. Lett.* **80**, 3408 (1998).
7. Q. Turchette *et al.*, *Phys. Lett.* **81**, 3631 (1998).
8. G. Mahler, V. Weberruss, *Quantum Networks* (Springer, Berlin, 1998).
9. V. Vedral, M. Plenio, M. Rippin, P. Knight, *Phys. Lett.* **78**, 2275 (1997).
10. J. Schlienz, G. Mahler, *Phys. Rev. A* **52**, 4396 (1995).
11. B. D'Espagnat, *Found. Phys.* **20**, 1147 (1990).
12. D. Hartree, *Proc. Camb. Phil. Soc.* **24**, 89 (1928).
13. B.W. Shore, P. Knight, *J. Mod. Opt.* **40**, 1195 (1993).
14. L. De la Pena, E. Santos, *Phys. Lett. A* **259**, 83 (1999).
15. E.A. Kane, *Nature* **393**, 133 (1998).
16. Pan Jian-Wei, D. Bouwmeester, A. Zeilinger, *Phys. Lett.* **80**, 3819 (1998).
17. J. Gemmer, A. Otte, G. Mahler, *Phys. Rev. Lett.* **86**, 1927 (2001).