Semiclassical Time Evolution of the Reduced Density Matrix and Dynamically Assisted Generation of Entanglement for Bipartite Quantum Systems

Ph. Jacquod

Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

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Two particles, initially in a product state, become entangled when they come together and start to interact. Using semiclassical methods, we calculate the time evolution of the corresponding reduced density matrix ρ_1, obtained by integrating out the degrees of freedom of one of the particles. We find that entanglement generation sensitively depends (i) on the interaction potential, especially on its strength and range, and (ii) on the nature of the underlying classical dynamics. Under general statistical assumptions, and for short-ranged interaction potentials, we find that $\mathcal{P}(t)$ decays exponentially fast in a chaotic environment, whereas it decays only algebraically in a regular system. In the chaotic case, the decay rate is given by the golden rule spreading of one-particle states due to the two-particle coupling, but cannot exceed the system's Lyapunov exponent.

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"When two systems (...) enter into temporary interaction (...), and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before, viz. by endowing each of them with a representative of its own." This is how entanglement was characterized by Schrödinger almost 70 years ago [1]. Entanglement is arguably the most puzzling property of multipartite quantum systems, and often leads to counterintuitive predictions due to, in Einstein's words, spooky action at a distance. Entanglement has received a renewed, intense interest in recent years in the context of quantum information theory [2].

In the spirit of Schrödinger's above formulation, one is naturally led to ask the following question: "What determines the rate of entanglement production in a dynamical system?" Is this rate mostly determined by the interaction between two, initially unentangled particles, or does it depend on the underlying classical dynamics? This is the question we address in this Letter. Previous attempts to answer this question have mostly focused on numerical investigations [3–8], with claims that entanglement is favored by classical chaos, both in the rate it is generated [3,4,7] and in the maximal amount it can reach [5]. In particular, strong numerical evidences have been given by Miller and Sarkar for an entanglement production rate given by the system's Lyapunov exponents [4]. These findings have, however, been recently challenged by Tanaka *et al.* [6], whose numerical findings show no increase of the entanglement production rate upon increase of the Lyapunov exponents in the strongly chaotic but weakly coupled regime, in agreement with their analytical calculations relating the rate of entanglement production to classical time correlators. Reference [6] is seemingly in a paradoxical disagreement with the almost identical analytical approach of Ref. [7], where entanglement production was found to be faster in chaotic systems than in regular ones [9]. This controversy thus calls for a better analytical understanding of the problem.

We present a semiclassical calculation of the time-evolved density matrix $\rho(t)$ for two interacting, distinguishable particles. In the usual way, entanglement is quantified by the properties of the reduced density matrix $\rho_1(t) \equiv \mathrm{Tr}_2[\rho(t)]$, obtained from the two-particle density matrix by tracing over the degrees of freedom of one (say, the second) particle. At $t = 0$, the two particles are in a product state of two narrow wave packets. We will quantify entanglement by calculating the purity $\mathcal{P}(t) \equiv \mathrm{Tr}[\rho_1(t)^2]$ which varies from 0 for fully entangled to 1 for factorizable two-particle states [10] (the discussion of how this could translate into the violation of a Bell inequality [11] is postponed to later works). Compared to other measures of entanglement such as the von Neumann entropy or the concurrence, the purity presents the advantage of being analytically tractable. For the weak coupling situation we are interested in here, numerical works have moreover shown that von Neumann and linear entropy $S_{\mathrm{lin}} \equiv 1 - \mathcal{P}(t)$ behave very similarly [6]. We thus expect the purity to give a faithful and generic measure of entanglement. We note that our semiclassical approach is straightforwardly extended to the case of undistinguishable particles, provided the nonfactorization of the reduced density matrix due to particle statistics is properly taken care of [12].

Our approach is reminiscent of the semiclassical methods developed by Jalabert and Pastawski [13,14] (see also [15]) in the context of the Loschmidt Echo. We will show how the off-diagonal matrix elements of ρ_1 are related to classical action correlators, in a similar way as in Refs. [6,7]. Under nonrestrictive statistical assumptions, we find that, following an initial transient where ρ_1 relaxes but remains almost exactly pure, entanglement production is exponential in chaotic systems, while it is algebraic in regular systems. The asymptotic rate of entanglement production in chaotic systems depends on the strength of the interaction between the two particles, and is explicitly given by a classical time correlator. We note that, as is the case for the Loschmidt Echo [16,17], this regime is also adequately captured by an approach based on random matrix theory (RMT) [18]—the time correlator is then replaced by the golden rule spreading of one-particle states due to the interaction. For stronger coupling, however, the dominant stationary phase solution becomes interaction independent, and is determined only by the classical dynamics, the system's Lyapunov exponents giving an upper bound for the rate of entanglement production. The crossover between the two regimes occurs once the golden rule width becomes comparable to the system's Lyapunov exponent. Still, one has to keep in mind that long-ranged interaction potentials can lead to significant modifications of this picture, especially at short times, due to an anomalously slow vanishing of off-diagonal matrix elements of ρ_1 within a bandwidth set by the interaction range.

We start with an initial two-particle product state $|\psi_1\rangle \otimes |\psi_2\rangle \equiv |\psi_1, \psi_2\rangle$. The state of each particle is a Gaussian wave packet $\psi_{1,2}(\mathbf{y}) = (\pi\sigma^2)^{-d/4} \exp[i\mathbf{p}_0 \cdot (\mathbf{y} - \mathbf{r}_{1,2}) - |\mathbf{y} - \mathbf{r}_{1,2}|^2/2\sigma^2]$. We write the two-particle Hamiltonian as $\mathcal{H} = H \otimes I + I \otimes H + \mathcal{U}$; i.e., the two particles are subjected to the same Hamiltonian dynamics. At this point, we specify only that the interaction potential $\mathcal{U}$ is smooth, depends only on the distance between the particles, and is characterized by a typical length scale ζ (which can be its range or the scale over which it fluctuates). Setting $\hbar \equiv 1$, the two-particle density matrix evolves according to $\rho(t) = \exp[-i\mathcal{H}t]\rho_0 \times \exp[i\mathcal{H}t]$ starting initially with $\rho_0 = |\psi_1, \psi_2\rangle\langle\psi_1, \psi_2|$. The elements $\rho_1(\mathbf{x}, \mathbf{y}; t) = \int d\mathbf{r}\langle \mathbf{x}, \mathbf{r}|\rho(t)|\mathbf{y}, \mathbf{r}\rangle$ of the reduced density matrix read

$$\rho_1(\mathbf{x}, \mathbf{y}; t) = (\pi\sigma^2)^{-d} \int d\mathbf{r} \int \Pi_{i=1}^4 d\mathbf{y}_i \exp[-\{(\mathbf{y}_1 - \mathbf{r}_1)^2 + (\mathbf{y}_2 - \mathbf{r}_2)^2 + (\mathbf{y}_3 - \mathbf{r}_1)^2 + (\mathbf{y}_4 - \mathbf{r}_2)^2\}/2\sigma^2] \times \exp[i\mathbf{p}_0(\mathbf{y}_1 + \mathbf{y}_2 - \mathbf{y}_3 - \mathbf{y}_4)]\langle \mathbf{x}, \mathbf{r}| \exp[-i\mathcal{H}t]|\mathbf{y}_1, \mathbf{y}_2\rangle\langle \mathbf{y}_3, \mathbf{y}_4| \exp[i\mathcal{H}t]|\mathbf{y}, \mathbf{r}\rangle. \tag{1}$$

We next introduce the semiclassical two-particle propagator

$$\langle \mathbf{x}, \mathbf{r}| \exp[-i\mathcal{H}t]|\mathbf{y}_1, \mathbf{y}_2\rangle = (-i)^d \sum_{s,s'} C_{s,s'}^{1/2} \exp\left[i\left\{S_s(\mathbf{y}_1, \mathbf{x}; t) + S_{s'}(\mathbf{y}_2, \mathbf{r}; t) + S_{s,s'}(\mathbf{y}_1, \mathbf{x}; \mathbf{y}_2, \mathbf{r}; t) - \frac{\pi}{2}(\mu_s + \mu_{s'})\right\}\right],$$

which is expressed as a sum over pairs of classical trajectories, labeled s and s', respectively, connecting $\mathbf{y}_1$ to $\mathbf{x}$ and $\mathbf{y}_2$ to $\mathbf{r}$ in the time t. Each such pair of paths gives a contribution containing one-particle (denoted by S_s and $S_{s'}$) and two-particle {denoted by $S_{s,s'} = \int_0^t dt_1\, \mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]$ [19]} action integrals accumulated along s and s', a pair of Maslov indices μ_s and $\mu_{s'}$, and the determinant $C_{s,s'}$ of the stability matrix corresponding to the two-particle dynamics in the $(2d)$-dimensional space. (With the above definition, $C_{s,s'}$ is real and positive.) We consider sufficiently smooth interaction potentials varying over a distance much larger than σ. We thus set $S_{s,s'}(\mathbf{y}_1, \mathbf{x}; \mathbf{y}_2, \mathbf{r}; t) \simeq S_{s,s'}(\mathbf{r}_1, \mathbf{x}; \mathbf{r}_2, \mathbf{r}; t)$ [still we keep in mind that $\mathbf{r}_1$ and $\mathbf{r}_2$, taken as arguments of the two-particle action integrals, have an uncertainty $O(\sigma)$], and use the narrowness of the initial wave packets to linearize the one-particle actions in $\mathbf{y}_i - \mathbf{r}_j$ ($i = 1, \ldots, 4$; $j = 1, 2$). We consider the weak coupling regime, where the one-particle actions vary faster than their two-particle counterpart. We thus perform a stationary phase approximation on S's to get the semiclassical reduced density matrix as

$$\rho_1(\mathbf{x}, \mathbf{y}; t) = (-4\pi\sigma^2)^d \sum_{s,l} \exp[i\{S_s(\mathbf{r}_1, \mathbf{x}; t) - S_l(\mathbf{r}_1, \mathbf{y}; t)\}] \times \int d\mathbf{r} \sum_{s'} \mathcal{M}_{s,s'} \mathcal{M}_{l,s'}^\dagger \exp[i\{S_{s,s'}(\mathbf{r}_1, \mathbf{x}; \mathbf{r}_2, \mathbf{r}; t) - S_{l,s'}(\mathbf{r}_1, \mathbf{y}; \mathbf{r}_2, \mathbf{r}; t)\}],$$
$$\mathcal{M}_{s,s'} = C_{s,s'}^{1/2} \exp\left[-i\frac{\pi}{2}(\mu_s - \mu_{s'})\right] \exp\left[-\frac{\sigma^2}{2}\{(\mathbf{p}_s - \mathbf{p}_0)^2 + (\mathbf{p}_{s'} - \mathbf{p}_0)^2\}\right]. \tag{2}$$

It is straightforward to see that $\mathrm{Tr}[\rho_1(t)] = 1$ and $\rho_1(\mathbf{x}, \mathbf{y}; t) = [\rho_1(\mathbf{y}, \mathbf{x}; t)]^*$, as required. Enforcing a further stationary phase condition on Eq. (2) amounts to performing an average over different initial conditions $\mathbf{r}_{1,2}$. It results in $s = s'$, $\mathbf{x} = \mathbf{y}$, and thus $\langle \rho_1(\mathbf{x}, \mathbf{y}; t)\rangle = \delta_{\mathbf{x},\mathbf{y}}/\Omega$ (Ω is the system's volume), i.e., only diagonal elements of the reduced density matrix have a nonvanishing average [the ergodicity of $\langle \rho_1(\mathbf{x}, \mathbf{x}; t)\rangle$ is due to the average over initial conditions]. For each initial condition, ρ_1 has, however, nonvanishing off-diagonal matrix elements, with a zero-centered distribution whose variance is given by $\langle \rho_1(\mathbf{x}, \mathbf{y}; t)\rho_1(\mathbf{y}, \mathbf{x}; t)\rangle$. Squaring Eq. (2), averaging over $\mathbf{r}_{1,2}$, and enforcing a stationary phase approximation on S's, one gets

$$\langle \rho_1(\mathbf{x}, \mathbf{y}; t)\rho_1(\mathbf{y}, \mathbf{x}; t)\rangle = (4\pi\sigma^2)^{2d} \int d\mathbf{r}\, d\mathbf{r}' \sum_{s,s'} \sum_{l,m} \mathcal{M}_{s,s'} \mathcal{M}_{l,m} \mathcal{M}_{l,s'}^\dagger \mathcal{M}_{s,m}^\dagger \langle \mathcal{F}\rangle, \tag{3}$$

$$\mathcal{F} = \exp[i\{S_{s,s'}(\mathbf{r}_1, \mathbf{x}; \mathbf{r}_2, \mathbf{r}; t) - S_{l,s'}(\mathbf{r}_1, \mathbf{y}; \mathbf{r}_2, \mathbf{r}; t)\}] \exp[i\{S_{l,m}(\mathbf{r}_1, \mathbf{y}; \mathbf{r}_2, \mathbf{r}'; t) - S_{s,m}(\mathbf{r}_1, \mathbf{x}; \mathbf{r}_2, \mathbf{r}'; t)\}]. \quad (4)$$

Our analysis of Eqs. (3) and (4) starts by noting that $\langle|\rho_1|^2\rangle$ is given by the sum of two positive contributions. First, those particular paths for which $\mathbf{r} = \mathbf{r}'$ and $s' = m$ accumulate no phase ($\mathcal{F} = 1$) and thus have to be considered separately. On average, their contribution does not depend on $\mathbf{x}$ nor $\mathbf{y}$, and decays in time only because of their decreasing measure with respect to all the paths with $\mathbf{r} \neq \mathbf{r}'$. Their average contribution is given by

$$\Sigma_0^2(t) = (4\pi\sigma^2)^{2d}\Omega^{-2} \int d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r} \sum_{s,l,m} |\mathcal{M}_{s,m}|^2 |\mathcal{M}_{l,m}|^2 \propto \begin{cases} \Omega^{-2}\exp[-(\lambda_1 + \lambda_2)t]; & \text{chaotic} \\ \Omega^{-2}\left(\frac{t_0}{t}\right)^2; & \text{regular.} \end{cases} \quad (5)$$

This is obtained by taking half of the C's in the $\mathcal{M}$'s as Jacobians for the coordinate transformation from $\mathbf{r}$'s to $\mathbf{p}$'s, and replacing the other half by the large time limit [20] $C_{s,m} \equiv C_s^{(1)} C_m^{(2)} \propto (t_0/t)^2$ for regular, and $\approx \exp[-(\lambda_1 + \lambda_2)t]$, for chaotic systems [in Eq. (5), we explicitly wrote particle indices; in our case, where the two particles are subjected to the same Hamiltonian, the Lyapunov exponents are equal, $\lambda_1 = \lambda_2$]. Two facts are noticeable here: These contributions do not depend on the interaction strength; moreover, Eq. (5) gives a lower bound for the decay of $\langle|\rho_1|^2\rangle$.

The second, generic contributions to $\langle|\rho_1|^2\rangle$ decay in time with $\langle\mathcal{F}\rangle$. From Eq. (4), it is natural to expect that $\langle\mathcal{F}\rangle$ is a decreasing function of $|\mathbf{x} - \mathbf{y}|$ and t only. Summations and integrations in Eq. (3) can then be performed separately to get $\langle\rho_1(\mathbf{x}, \mathbf{y}; t)\rho_1(\mathbf{y}, \mathbf{x}; t)\rangle = \Sigma_0^2(t) + \langle\mathcal{F}(\mathbf{x}, \mathbf{y}; t)\rangle/\Omega^2$, with

$$\langle\mathcal{F}(\mathbf{x}, \mathbf{y}; t)\rangle = \exp\left[-2\int_0^t dt_1\, dt_2 \langle\mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]\mathcal{U}[\mathbf{q}_s(t_2), \mathbf{q}_{s'}(t_2)]\rangle\right] \times \exp\left[+2\int_0^t dt_1\, dt_2 \langle\mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]\mathcal{U}[\mathbf{q}_l(t_2), \mathbf{q}_{s'}(t_2)]\rangle\right]. \quad (6)$$

The behavior of $\langle\mathcal{F}(\mathbf{x}, \mathbf{y}; t)\rangle$ sensitively depends on the distance $|\mathbf{x} - \mathbf{y}|$ between the end points of the classical trajectories $\mathbf{q}_s(t)$ and $\mathbf{q}_l(t)$ connecting $\mathbf{r}_1$ to $\mathbf{x}$ and $\mathbf{y}$, respectively. For small $|\mathbf{x} - \mathbf{y}|$, the second line on the right-hand side of Eq. (6) almost compensates the first one [21], and a Taylor expansion of the difference of the two-particle action integrals in Eq. (4) gives in lowest order

$$\langle\mathcal{F}(|\mathbf{x} - \mathbf{y}| \leq \zeta; t)\rangle = \exp\left[-2\sum_{\alpha,\beta=1}^{d} (\mathbf{x} - \mathbf{y})_\alpha (\mathbf{x} - \mathbf{y})_\beta \int_0^t dt_1\, dt_2 \langle\partial_\alpha^{(s)}\mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]\partial_\beta^{(s)}\mathcal{U}[\mathbf{q}_s(t_2), \mathbf{q}_{s'}(t_2)]\rangle\right]. \quad (7)$$

The reduced density matrix has a Gaussian decay away from the diagonal, which we expect to hold for $|\mathbf{x} - \mathbf{y}| \ll \zeta$ (the distance over which the two terms in Eq. (6) almost cancel each other], and for short enough times $t < \tau$ (after which very different, uncorrelated classical paths l and s may still reach two neighboring end points). An estimate for τ is given by the time it takes for two initial conditions within a distance σ (this is the uncertainty in $\mathbf{r}_1$) to move away a distance $\propto \zeta$ from each other. In a chaotic system, this is the Ehrenfest time $\tau = \lambda_1^{-1}\ln(\zeta/\sigma)$, while in a regular system τ is much longer, $\tau = O([\zeta/\sigma]^\beta)$ [23]. At larger distances, $|\mathbf{x} - \mathbf{y}| \gg \zeta$, $\langle\mathcal{F}\rangle$ is given by the first term on the right-hand side of Eq. (6). Note that, because the four classical paths in that term come in two pairs, the dependence on $|\mathbf{x} - \mathbf{y}|$ vanishes.

This concludes our semiclassical calculation of the reduced density matrix for interacting two-particle systems. We have learned that the variance of off-diagonal matrix elements of ρ_1 is determined by classical correlators, with the important caveat that they are bound downward by the expressions given in Eq. (5). For the rest of the discussion, we note that, provided the correlators in Eqs. (6) and (7) decay faster than $\propto|t_1 - t_2|^{-1}$, the off-diagonal matrix elements exhibit a dominant exponential decay in time. This condition is rather nonrestrictive and is surely satisfied in a chaotic system. We therefore assume from now on a fast decay of the correlations,

$$\langle\mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]\mathcal{U}[\mathbf{q}_s(t_2), \mathbf{q}_{s'}(t_2)]\rangle = \Gamma\delta(t_1 - t_2), \quad (8)$$

$$\langle\partial_\alpha^{(s)}\mathcal{U}[\mathbf{q}_s(t_1), \mathbf{q}_{s'}(t_1)]\partial_\beta^{(s)}\mathcal{U}[\mathbf{q}_s(t_2), \mathbf{q}_{s'}(t_2)]\rangle = \gamma\delta_{\alpha,\beta}\delta(t_1 - t_2). \quad (9)$$

Entanglement is quantified by the purity $\mathcal{P}(t) = \int d\mathbf{x}\, d\mathbf{y} \langle\rho_1(\mathbf{x}, \mathbf{y}; t)\rho_1(\mathbf{y}, \mathbf{x}; t)\rangle$, which is straightforward to compute from Eqs. (3)–(9). We get three distinct regimes of decay: (i) an initial regime of classical relaxation for $t < \tau$. During that time, ρ_1 evolves from a pure, but localized $\rho_1(0) = |\mathbf{r}_1\rangle\langle\mathbf{r}_1|$ to a less localized, but still almost pure $\rho_1(t)$, with an algebraic purity decay obtained from Eqs. (7) and (9) as $\mathcal{P}(t < \tau) \simeq \Omega^{-1}(\pi/2\gamma t)^{d/2}(1 - \exp[-2\gamma L^2 t])$ [$L \sim \Omega^{1/d}$ is the linear system size; even in the case of a correlator (9) saturating at a finite value for $|t_1 - t_2| \to \infty$, which may occur in regular systems, this initial decay will still be algebraic $\propto t^{-d}$]; (ii) a regime where quantum coherence develops between the two particles so that ρ_1 becomes a mixture. From Eq. (5) and the first line of Eq. (6) with

Eq. (8), one gets $\mathcal{P}(t) \simeq \exp[-\min(2\Gamma; \lambda_1 + \lambda_2)t]$ in a chaotic system; in a regular system one has $\mathcal{P}(t) \propto (t_0/t)^{-2}$, since $\Sigma_0^2(t)$ dominates the decay of $\mathcal{P}(t)$ independently of the correlators in Eqs. (8) and (9); (iii) a saturation regime where the purity reaches its minimal value. In the chaotic limit, this saturation value can be estimated using a RMT approach as $\mathcal{P}(\infty) = 2(\sigma^d/\Omega) + O(\Omega^{-2})$ [18], which is in qualitative agreement with the results obtained in Ref. [5] for the von Neumann entropy. There is no reason to expect a universal saturation value in the regular regime.

Analyzing these results, we note that Eqs. (6) and (7) are reminiscent of the results obtained for $\mathcal{P}(t)$ by perturbative treatments in Refs. [6,7], but they apply well beyond the linear response regime. Our weak coupling condition that the one-particle actions S vary faster than the two-particle actions S roughly gives an upper bound $U \leq E$ for the typical interaction strength U (E is the one-particle energy). The linear response regime is, however, restricted by a much more stringent condition $U \leq \Delta \ll E$ (Δ is the mean level spacing) [16]. The decay regime (ii) of $\mathcal{P}(t)$ reconciles the *a priori* contradicting claims of Refs. [3,4,7] and Ref. [6]. For weak coupling, the decay of $\mathcal{P}(t)$ is given by classical correlators, and thus depends on the interaction strength, in agreement with Ref. [6]. However, $\mathcal{P}(t)$ cannot decay faster than the bound given in Eq. (5), so that at stronger coupling, and in the chaotic regime, one recovers the results of Ref. [4]. Simultaneously, regime (ii) also explains the data in Figs. 2 and 4 of Ref. [7], showing an exponential decay of $\mathcal{P}(t)$ in the chaotic regime, and a power-law decay with an exponent close to 2 in the regular regime (this power-law decay was left unexplained by the authors of Ref. [7]). Our semiclassical treatment thus presents a unified picture of the problem.

Three more remarks are in order here. First, the stationary phase solutions leading to the above results still hold in the case when the two particles are subjected to different one-particle Hamiltonians. Second, the power-law decay of $\mathcal{P}(t)$ predicted above for regular systems is to be taken as an average over initial conditions $\mathbf{r}_{1,2}$ (in that respect, see Refs. [14,24]), but may also hold for individual initial conditions, as, e.g., in [7]. Finally, there are cases when the correlators (8) and (9) decay exponentially in time with a rate related to the spectrum of Lyapunov exponents. This also may induce a dependence of $\mathcal{P}(t)$ on the Lyapunov exponents, which can be captured by the linear response approach of Ref. [6]. We note, however, that this is not a generic situation, as most fully chaotic but nonhyperbolic systems have power-law decaying correlations.

As a concluding line, and noting similarities between the problem treated here and that of decoherence by an environment [10], we anticipate that a semiclassical approach as the one presented here (see also Ref. [25]) could clarify how decoherence relates to the intrinsic dynamics of the system [10,26].

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