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Quantum simulation of classically chaotic systems

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Abstract. The evolution of a classically chaotic Hamiltonian system is characterised by a computational complexity that increases exponentially with the time elapsed. Quantum systems do not exhibit such behaviour. It is therefore tempting to solve a classical problem by quantising it and following the motion of a small wavepacket. This paper shows that nothing can be gained by this subterfuge: an adequate quantum simulation requires a Hilbert space whose dimension increases exponentially with the planned duration of the simulation.

1. Formulation of the paradox

Classical Hamiltonian systems have two qualitatively different kinds of orbits [1, 2]. The 'regular' orbits of integrable systems are multiply periodic in time and are constrained to lie on n-dimensional tori in the $2n$-dimensional phase space. On the other hand, the orbits of a non-integrable system explore part or all of the energy surface, which is $(2n-1)$ dimensional. Intermediate cases also exist.

For a non-integrable system, the Hamilton equations of motion

$$\mathrm{d}q/\mathrm{d}t = \partial H/\partial p \qquad \mathrm{d}p/\mathrm{d}t = -\partial H/\partial q \tag{1}$$

cannot be integrated analytically, but numerical methods are available. For the resulting 'chaotic' orbits a small deviation from the initial data grows exponentially with time [3, 4]. Even when the initial data are perfectly known, the motion is unpredictable for long times if we use a finite computer [5]. The hallmark of classical chaos is a *computational complexity* (see appendix 1) that increases exponentially with the duration of the evolution for a given demand in precision. Then, if the complexity of that computation is beyond our means, we cannot predict the final state, except statistically [5]. Thus chaos is *ineffectiveness*—specifically, ineffectiveness in the compression of information [6].

Is there a similar situation in quantum dynamics? It has long been known empirically that quantum mechanics tends to suppress the appearance of chaos [7]. Quantum wavepackets may remain localised even though classical orbits are strongly chaotic, because cantori, associated with the breakup of invariant KAM surfaces, may effectively act as barriers to quantum wavepacket evolution while permitting extensive classical flow. A similar phenomenon appears in models where the Hamiltonian includes a time-dependent external force [8-11]. In these models, which usually have a single degree of freedom, the system is prepared in a state involving one, or at most a few, energy levels of the unperturbed Hamiltonian. Such a quantum system is found to

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spread to only a few more neighbouring energy levels, so that the energy remains localised in a narrow domain. (In the corresponding classical evolution the energy would increase diffusively without bounds.) As a consequence, the quantum motion is almost periodic and the initial state recurs [12]. The same is true for any time-independent Hamiltonian with a discrete spectrum [13]. The problem here is not the recurrence itself, which has the same character as a Poincaré cycle [14] and is completed after an extremely long time [15], but the fact that the quantum state, after an arbitrarily long time t, can be computed accurately with a limited amount of work: the solution of the equations of motion has *null* complexity [5].

This suggests a curious paradox [16]. Rather than computing classically chaotic evolution by integrating (1), we could quantise the classical system in the standard canonical way (with a fixed positive $\hbar$) and then integrate the Schrödinger equation in order to follow the motion of a small wavepacket. For example, we could integrate the evolution of the Solar System for trillions of years, assuming that the Sun, planets, moons and asteroids are point particles with known masses. Replacing these classical points by Gaussian wavepackets of optimum size, would the quantum claculation be a less complex task (for $t \to \infty$) than the direct integration of the Hamilton equations (1)?

Let us examine what has to be done in this quantum calculation. The standard procedure for integrating the time-dependent Schrödinger equation is to compute the eigenvalues and eigenfunctions of the Hamiltonian by solving

$$Hu_n(q) = \hbar\omega_n u_n(q) \tag{2}$$

where for simplicity it is assumed that the Hamiltonian has a discrete spectrum. With normalised $u_n(q)$ we expand the initial state as

$$\psi_0(q) = \sum c_n u_n(q) \tag{3}$$

where

$$c_n = \int u_n^*(q)\psi_0(q)\,\mathrm{d}q. \tag{4}$$

The time-evolved wavefunction is

$$\psi(q, t) = \sum c_n u_n(q) \exp(-\mathrm{i}\omega_n t). \tag{5}$$

This result is essentially different from the classical one, because the computational complexity does *not* increase exponentially with time. It does have some increase because in order to have meaningful phases in (5) the error in $\omega_n t$ must be small modulo 2π. Actually, from (5) alone one cannot reach conclusions about complexity. The sum in (5) is infinite, so that its evaluation represents an infinite amount of numerical work. What is done is to truncate the sums (3) and (5). By convergence, this involves an arbitrarily small error. We thus replace $\psi_0(q)$ by

$$\psi_0'(q) = \sum{}' c_n u_n(q) \tag{6}$$

where Σ' denotes the summation of a finite number of terms. Likewise we define

$$\psi'(q, t) = \sum{}' c_n u_n(q) \exp(-\mathrm{i}\omega_n t). \tag{7}$$

If $\psi_0'(q)$ is close to $\psi_0(q)$, then $\psi'(q, t)$ is close to $\psi(q, t)$, by unitarity.

We appear to have reached the following conclusion: if we ask what are the initial conditions for a classical orbit so that, after a time t, it will land with 99% probability in a small region of phase space, the computational complexity increases exponentially

with t. On the other hand, if we want to specify a *quantum state* such that, at a time t later, it will become a wavepacket localised in the *same* small region of phase space, then the computational complexity will increase at most as a polynomial in t.

The purpose of this paper is to show that nothing can be gained by this subterfuge because a reliable quantum simulation requires a value of $\hbar$ that decreases exponentially with t. Specifically, in the last paragraph we tacitly implied that the quantum calculation would yield a localised wavepacket. That statement, which may or may not be true, is not what our earlier discussion established. What we in fact showed is that the wavefunction will be known with high accuracy with little computational effort. However, in a chaotic situation that wavepacket will, even in its exact form, be widely spread. Its form will therefore not yield the classical position and the subterfuge fails. What it takes to reduce wavepacket spreading is a smaller value of $\hbar$ (which in turn allows a smaller initial optimal packet). We will show that the value of $\hbar$ giving the required accuracy has exponential shrinking. It then follows that the effective dimensionality of the Hilbert space—the number of terms that must be summed in (7)—increases exponentially with t. Moreover, its increase is related to the same Lyapunov exponent that appears in the classical case.

2. Semiclassical evolution of wavepackets

Consider the evolution of a cluster of points which fill, at time $t = 0$, a small volume in the classical phase space, as shown in figure 1. In that figure, each component p_k and q_k has been rescaled by a factor

$$a_k = (\Delta p_k / \Delta q_k)^{1/2} \tag{8}$$

where Δp_k and Δq_k arise from the finite resolving power of the instruments that prepare the initial sate. In this way, the small initial domain has pairs of principal axes of equal lengths

$$r_k \sim \Delta p_k / a_k = a_k \Delta q_k = (\Delta p_k \Delta q_k)^{1/2}. \tag{9}$$

In the following application, we shall be interested in a domain which is a Gaussian wavepacket with all r_k equal, so that the initial domain is a small sphere.

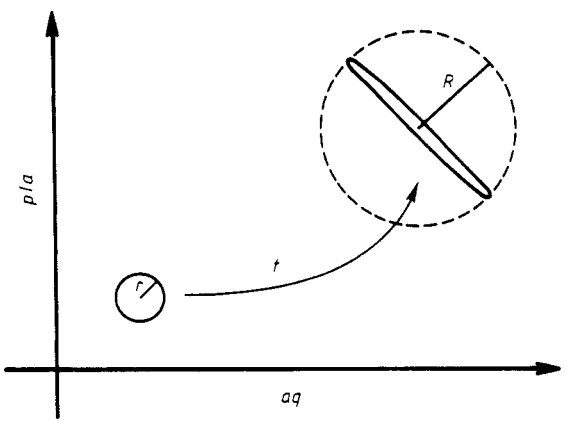

Figure 1. A small spherical ball in phase space evolves into an ellipsoid whose longest axis grows exponentially with time.

As time passes the sphere becomes an ellipsoid that rotates and vibrates erratically, while its centre moves along the classical trajectory that starts at the centre of the initial sphere [4]. The volume of this ellipsoid is constant, by Liouville's theorem. Asymptotically, for large t, its longest axis grows exponentially:

$$R \sim e^{\lambda t} r \tag{10}$$

where λ is the Lyapunov exponent of the cluster of orbits. This exponential growth proceeds as long as the sphere of radius R remains small enough so that non-linear effects within its volume can be ignored. Ultimately, the sphere will span an appreciable domain of phase space, the ellipsoid will be distorted in a bizarre way, growing protuberances known as 'whorls and tendrils', which may be close to any point of the energy surface. In this paper, we consider only the case where the initial radius r is so small that these non-linear effects can be ignored within the ball of radius R.

The practical problem of long-range forecasting is to determine whether the end-point of the evolution will lie within a given ball of radius R. Conversely, one could specify the location and size of the target area and calculate the location and size of the launch area. The radius of the latter is then $r \sim R\, e^{-\lambda t}$, by virtue of (10).

The same problem can be formulated in quantum mechanics, the initial and final states being Gaussian wavepackets. The latter have Wigner distributions [17, 18]

$$W(p, q) = (\pi\hbar)^{-n} \int d^n y\, \psi^*(q+y)\psi(q-y) \exp(2ip\cdot y/\hbar) \tag{11}$$

(p, q, etc, are n vectors) which are nowhere negative, so that a semiclassical interpretation presents no difficulty. Moreover, it can be shown [19] that the Wigner distributions evolve as classical Liouville distributions so long as it is legitimate to ignore non-linear effects within the size of the wavepackets.

Since a Gaussian wavepacket has minimal uncertainty, we have

$$r^2 \sim \Delta p \Delta q \sim \hbar \tag{12}$$

whence

$$\hbar \sim \exp(-2\lambda t) R^2. \tag{13}$$

In appendix 2 we provide a more explicit derivation of this result.

We next show that the smaller $\hbar$, the larger the number of energy levels appreciably involved in the wavepacket. By 'appreciably involved' we mean that a truncation of the sort contemplated in (6) would lead to small errors. The number N of these energy levels can be written as

$$N = \rho(E)\Delta E \tag{14}$$

where $\rho(E)$ is the density of states and ΔE the energy spread of our packet. Let $\nu(E)$ be the number of states of energy equal to or less than E so that $\rho(E) = d\nu/dE$. In the semiclassical limit

$$\nu(E) = (2\pi\hbar)^{-n} \int_{\Omega_E} d^n p\, d^n q$$

where Ω_E is the volume enclosed by the surface $H(p, q) = E$. We can therefore write

$$\rho(E) = A'\hbar^{-n}\rho_c(E) \tag{15}$$

where $A' = (2\pi)^{-n}$ and $\rho_c(E)$ is the classical density of states, namely $(\mathrm{d}/\mathrm{d}E)\int_{\Omega_E} \mathrm{d}^n p\, \mathrm{d}^n q$. We next calculate ΔE, the energy spread of the wavepacket (or of the corresponding classical Liouville distribution). If the energy of the classical motion we wish to simulate is large, we can use the classical relation

$$\Delta E \sim \frac{\partial H}{\partial p}\Delta p + \frac{\partial H}{\partial q}\Delta q = v\Delta p - F\Delta q. \tag{16}$$

To find the energy spread, we orient Δp and Δq along directions that maximise ΔE. Since $|\Delta p| \sim a\sqrt{\hbar}$ and $|\Delta q| \sim \sqrt{\hbar}/a$, we get

$$\Delta E \sim \sqrt{\hbar}\,[(F/a)^2 + (va)^2]^{1/2} \tag{17}$$

where indices have been omitted for brevity. The right-hand side of (17) does not, in general, vanish.

Combining these results, we find that the number of energy levels behaves as

$$N \sim A\hbar^{(1-2n)/2} \tag{18}$$

where A is a purely classical quantity, independent of $\hbar$, so that

$$N \sim B\exp[(2n-1)\lambda t] \tag{19}$$

where B is independent of t. This is the minimum dimension of the Hilbert space needed for a reliable quantum mechanical simulation of the classical motion, over a time t, when the final precision is specified. For smaller N, or longer times, the classical-quantum analogy does not achieve the required accuracy.

We close with a comment on the limitations inherent in our demonstration. We have shown that a particular implementation of a subterfuge for bypassing classical complexity does not work. There are two caveats in any such demonstration. First, you can never be sure some clever new idea will not bypass your implicit assumptions and manage to accomplish what you said was impossible. Second, we do not claim that we have presented the best estimates even within the context we have defined. For example, by adjusting the time intervals in the Runge-Kutta algorithm one can improve the coefficient given in appendix 1, but not change the fact of exponential growth. Similarly if, for our initial quantum states, we took ellipsoids narrow along the most explosive directions (as a referee suggested) we might gain a factor of 2 in T. Notwithstanding these possible improvements, we believe we have provided evidence that the apparent computational ease within the quantum framework does not help one escape the essential complexity of the problem.

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Appendix 1

One would like to have an objective measure for the amount of computation needed to accomplish a given task [20, 21]. This is the quantity we call 'computational

complexity.' It is essentially equivalent to the notion of 'logical depth,' as defined by Bennett [21], which is, roughly speaking, the number of elementary logical steps required to compute a message from its minimal algorithmic description. Unfortunately, neither algorithmic information nor logical depth are effectively computable properties. This limitation follows from the unsolvability of the halting problem [22, 23]. Moreover, the length of computation can decrease if the minimal program that generates it is replaced by a longer, but more efficient, one. Nevertheless, if we postulate a rate of exchange between run time and program size, the resulting logical depth—or computational complexity—can be shown to be reasonably machine independent.

There are other definitions of complexity. In particular, within the context of classical mechanics, Brudno [24, 25] has shown a relation between complexity and metric entropy which, together with the work of Pesin [26, 27] relating entropy to Lyapunov exponents, connects complexity to the Lyapunov exponents.

We next substantiate the claim made following (1), namely that for integrating chaotic classical equations of motion the computational effort increases exponentially in time. Consider, for example, a Runge-Kutta integration [28] of the equations of motion. At the end of the calculation we wish an error less than a given R. We use time steps of size $\varepsilon = T/N$ and an order-k Runge-Kutta algorithm. What we wish to determine is the smallness of ε, or the growth of N, to ensure the required accuracy at time T.

The error after the first step is $c\varepsilon^k$ for some c of order unity. After the second step the error will be be $e^{\varepsilon\lambda}c\varepsilon^k + c\varepsilon^k$, where λ is the Lyapunov exponent and 'c' refers to a generic order unity quantity. Calling E_n the error after n steps we have $E_{n+1} = e^{\varepsilon\lambda}E_n + c\varepsilon^k$. With $E_0 = 0$, the solution to this recursion is $E_N = c\varepsilon^k(e^{\lambda T} - 1)(e^{\lambda\varepsilon} - 1)^{-1}$. Requiring $E_N < R$ implies $\varepsilon < \exp[-\lambda T/(k-1)]^{-1}$. Thus

$$N \sim \exp[\lambda T/(k-1)].$$

Allowing for independent errors ('c') of varying sign leads to $N \sim \exp[\lambda T/(k-\frac{1}{2})]$.

Appendix 2

We provide a direct quantum calculation for the evolution of a wavepacket in the semiclassical approximation so as to estimate the smallness of $\hbar$ required to guarantee accurate positional information. This calculation shows the features anticipated by our more general considerations. Let the initial wavefunction be given by

$$\psi_0(x) = C\exp\left(-\sum_{i=1}^{N}\frac{(x_i - x_{0i})^2}{4\Delta_i^2} + \frac{\mathrm{i}}{\hbar}\sum p_{0i}(x_i - x_{0i})\right). \tag{A2.1}$$

For convenience we rewrite this in matrix notation:

$$\psi_0(x) = C\exp[-x^{\mathrm{T}}Kx + (i/\hbar)p_0^{\mathrm{T}}(x - x_0)] \tag{A2.2}$$

where x, etc, are n vectors ($n = 3N$), T denotes transpose and K is the matrix describing the time-zero spread. At a later time t the wavefunction is given by

$$\psi(x, t) = \int \mathrm{d}y\, G(x, t; y)\psi_0(y) \tag{A2.3}$$

with G the propagator. In the semiclassical approximation [29]

$$G(x, t; y) = \exp[(\mathrm{i}/\hbar)S(x, t; y)] \tag{A2.4}$$

where $S(x, t; y)$ is the classical action for the classical path from y at time zero to x at time t. Notice that (A2.4) has been stripped of complications. We ignore the van Vleck determinant, ie. the prefactor given roughly by $[\det \partial^2 S/\partial x \partial y]^{1/2}$. This is because we are only going to look at the way in which the dominant Gaussian dependence evolves (in effect, the development of the matrix K). It is also implicit in formula (A2.4) that there is one and only one path connecting the endpoints. In general this is not the case. However, we use G to evolve a specific ψ_0, so that classical paths that contribute to G are unimportant unless they also have initial momenta close to the given p_0. (See the exercise in ch 3 of [29].)

To use (A2.4) we expand S about its endpoints; expansion about y is justified by keeping Δ_i small, that about x by the smallness of $\hbar$. First perform the y expansion and define

$$p_j = -\frac{\partial S(x, t; y)}{\partial y_j}\bigg|_{y=x_0} \qquad A_{jk} = \frac{\partial^2 S(x, t; y)}{\partial y_j \partial y_k}\bigg|_{y=x_0}. \tag{A2.5}$$

Classically p is the momentum of the path starting at x_0 and arriving at x. Combine (A2.2)-(A2.5), define $w = y - x_0$ and drop $O(w^3)$ terms to get

$$\psi(x, t) = C \int d^n w \exp\{-w^T K w + (i/\hbar) p_0^T w + (i/\hbar)[S(x, t; x_0) - p^T w + \tfrac{1}{2} w^T A w]\}. \tag{A2.6}$$

The phase factor involving $S(x, t; x_0)$ does not interest us here and we absorb it into C. The integrand in (A2.6) is a Gaussian and we use the general (matrix) formula

$$\int d^n w \exp(-w^T M w + \mu^T w) = \left(\frac{\pi^n}{\det M}\right)^{1/2} \exp(\tfrac{1}{4}\mu^T M^{-1} \mu) \tag{A2.7}$$

with

$$M = K - (i/2\hbar)A \qquad \mu = (1/\hbar)(p_0 - p) \tag{A2.8}$$

to yield

$$\psi(x, t) = C \exp\left(-\frac{1}{4\hbar^2}(p - p_0)^T \frac{1}{K - (i/2\hbar)A}(p - p_0)\right). \tag{A2.9}$$

By (A2.5), p is a function of x; the point x_t where $p = p_0$ is the position of a particle at time t that had initial conditions (x_0, p_0) at time zero. This is where ψ will be maximal and we now compute the spread about that point x_t. We assume the spread continues to be small. In the ordinary sort of quantum calculation this assumption need not be justified because the finiteness of $\hbar$ restricts the ability to minimise the spread at multiple times [30]. However, in our calculation $\hbar$ is not physically determined and we ask how small it must be so that spreading will be less than a certain preassigned quantity. The expansion is

$$p_k \equiv -\frac{\partial S(x, t; y)}{\partial y_k} = p_{0k} - \sum_l F_{kl} u_l + O(u^2) \tag{A2.10}$$

where $u_l = x_l - x_{tl}$ and

$$p_{0k} = -\frac{\partial S(x_t, t; y)}{\partial y_k}\bigg|_{y=x_0} \tag{A2.11a}$$

$$F_{kl} = \frac{\partial^2 S(x, t; y)}{\partial x_k \partial y_l}\bigg|_{y=x_0, x=x_t}. \tag{A2.11b}$$

Using (A2.10) in (A2.9) gives

$$\psi(x, t) = C \exp\left(-\frac{1}{4\hbar^2} (Fu)^{\mathrm{T}} \frac{1}{K - (\mathrm{i}/2\hbar)A} (Fu) \right). \tag{A2.12}$$

Notice that for $O(u^2)$ accuracy in (A2.12) only $O(u)$ terms were retained in (A2.10).

The properties of ψ in (A2.12) are governed by the second derivatives of S. These are of two sorts: $\partial^2 S/\partial x\, \partial y$ (F) and $\partial^2 S/\partial y^2$ (A). It is in $\partial^2 S/\partial x\, \partial y$ that the interesting features of the problem reside. Essentially, this quantity is the inverse of $\partial(x_{\mathrm{final}})/\partial(p_{\mathrm{initial}})$, as one can see by comparing (A2.5) and (A2.11). The time-dependent change in final position with fixed change in initial momentum is a quantity that grows with the Lyapunov exponent. In our multidimensional context the logarithms of the eigenvalues of the matrix $\partial(x_{\mathrm{final}})/\partial(p_{\mathrm{initial}})$ $(=F^{-1})$ are exponents reflecting divergence or convergence of trajectories, the largest of these being the Lyapunov exponent. On the other hand, the second derivatives $\partial^2 S/\partial y^2$ do not generally behave in any dramatic way because they relate quantities at the same time. Thus $\partial^2 S/\partial y^2 = -\partial(p_{\mathrm{initial}})/\partial(y_{\mathrm{initial}})$. This is of order unity, as can be seen by reversing the time direction: two paths start from the same point with extremely close values of momentum $(O(\mathrm{d}y\, \mathrm{e}^{-\lambda T}))$ and end a distance $\mathrm{d}y$ from one another. The fact that the dynamics are chaotic imposes no growth on the difference in their final momenta. For example, in one dimension one gets divergent paths from the inverted simple harmonic oscillator, i.e. the equation $\ddot{x} - \Omega^2 x = 0$ with solution

$$x(s) = y[\sinh \Omega(t-s)/\sinh \Omega t] + x[\sinh \Omega s/\sinh \Omega t].$$

The classical action is

$$S(x, t; y) = (m\Omega/2 \sinh \Omega t)[(x^2 + y^2) \cosh \Omega t - 2xy].$$

In this case $\partial^2 S/\partial x\, \partial y (= -m\Omega/\sinh \Omega t \sim \mathrm{e}^{-\Omega t})$ has the expected exponential shrinking. The other second derivative $\partial^2 S/\partial y^2 (= m\Omega/\tanh \Omega t \sim m\Omega)$, however, tends to a constant.

The essential features of (A2.12) are therefore governed by F and we simplify our calculation by taking A to be diagonal and of order unity. We also take all eigenvalues of A and K to be equal. Thus

$$K - (\mathrm{i}/2\hbar)A = \mathrm{diag}[(1/4\Delta^2) - (\mathrm{i}/2\hbar)a]. \tag{A2.13}$$

Inserting this in (A2.12) we find

$$\psi(x, t) = C \exp\left(\frac{-1}{\hbar^2/\Delta^2 + 4a^2\Delta^2} (Fu)^{\mathrm{T}} (Fu) + \mathrm{i}(\mathrm{real}) \right). \tag{A2.14}$$

Notice that the phase of ψ has been ignored since we are aiming to estimate the spread in its norm. Our attention is therefore focused on the quadratic form

$$Q = \frac{1}{\hbar^2/\Delta^2 + 4a^2\Delta^2} (Fu)^{\mathrm{T}} (Fu). \tag{A2.15}$$

If F is diagonalised and Q written

$$Q = \sum (1/4\Delta_l^2(t))\tilde{u}_l^2 \tag{A2.16}$$

it is clear that the spread of the wavefunction will be determined by the largest eigenvalue of F^{-1}. As discussed above, F^{-1} is $\partial x/\partial p$ with x the final position and p the initial momentum. The largest eigenvalue of this matrix therefore has its growth

determined by the Lyapunov exponent. Denoting this largest eigenvalue by f_t we have $f_t \sim f_0 e^{\lambda t}$. It follows that

$$\Delta^2_{\max}(t) = f_0^2 \exp(2\lambda t)[\hbar^2/\Delta^2 + 4a^2\Delta^2)]. \tag{A2.17}$$

The last step is the determination of Δ, the initial spread. There is the usual trade-off of momentum and position uncertainty; in our formal development this takes the form of requiring minimisation of the function

$$g(\Delta^2) \equiv \hbar^2/\Delta^2 + 4a^2\Delta^2. \tag{A2.18}$$

The minimum is achieved with $\Delta = (\hbar/2a)^{1/2}$ and we have finally

$$\Delta^2_{\max}(t) = (4af_0^2)\hbar \exp(2\lambda t). \tag{A2.19}$$

Recall that our goal is to set $\hbar$ sufficiently small so that at the end of the evolution the maximum spread is less than some preassigned number R. From (A2.19) this is seen to imply

$$\hbar \sim (R/4af_0^2) \exp(-2\lambda t) \tag{A2.20}$$

in agreement with (13).

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