BOUNDS ON DECOHERENCE AND ERROR

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ABSTRACT

When a confined system interacts with its walls (treated quantum mechanically), there is an intertwining of degrees of freedom. We show that this need not lead to entanglement, hence decoherence. It will generally lead to error. The wave function optimization required to avoid decoherence is also examined.

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Introduction

Physical implementation of quantum computing algorithms,\(^1\) experimental tests of certain theories,\(^2\) as well as other contemporary problems, require that for fairly large systems the time evolution be fully described by \(\psi \to \exp(-iHt/\hbar)\psi\), with no “measurement,” or to be more precise, no decoherence or interaction with the environment. Such interaction can cause entanglement with environmental degrees of freedom and prevent interference with portions of the wave function that have not experienced the identical interaction. Moreover, those same interactions can induce errors, that is, system wave function different from that providing the desired output, computational or otherwise.

For any laboratory system one can expect a degree of entanglement with the environment, simply due to the fact that the system is pinned to the table. In particular, when part of the system rebounds from the walls confining it (even electromagnetic walls) conservation of momentum demands an intertwining of the degrees of freedom.

Taking the approach in [3], I here begin from this inevitable intertwining and establish the extent to which it leads to entanglement. The measure of entanglement is that given in [4]. There is a surprise in the calculation: for appropriately tailored wave functions, there need be no decoherence! This leads us to explore the
significance of the tailoring. However, although decoherence is avoidable, we will show that error is not.\textsuperscript{5}

Whether the decoherence is large or small (for nearly matching wave functions it is of order system/container mass ratio) the resulting amplitude defect must be subtracted from the wave function for each collision, allowing for physically significant effects.

**Interacting with a wall**

A confined system will, from time to time, interact with its container. Dissipative walls, in the sense that the interaction is an inelastic collision, immediately lead to significant entanglement; for our bounds we therefore assume that the collision is elastic and involves no degree of freedom beyond that required to contain the system. Our model is therefore the scattering of two point particles, one small (mass $m$) representing a piece of the quantum computer, and one large (mass $M$), representing the container.\textsuperscript{6}

Before the collision we assume the wave function to be unentangled, that is, $\Psi_I = \Gamma(X)\Phi(x)$, with position variables $X$ and $x$ corresponding to the large and small masses, respectively. We make several simplifying assumptions: 1.) Restriction to one dimension, reasonable if the large “particle” is in fact a wall. 2.) Rapid completion of the scattering. 3) Short range, infinite repulsion. 4.) Gaussian wave packets. Assumptions #2 and #3 would not be true in detail, but I expect that departures from them will only make things worse (with respect to decoherence and error). We further comment below on these assumptions.

If the interaction with the wall could be treated as a pure potential-interaction with a fixed object, the wave function after the collision would be\textsuperscript{7} $\Gamma(X)\Phi(-x)$. On the other hand, the correct form of the final wave function can be seen by going to center of mass coordinates, $R = (MX + mx)/M$, $u = x - X$, with $M = M + m$. In these coordinates $\Psi_I = \Gamma(R - \delta u)\Phi(R + \gamma u)$, where $\delta = m/M$ and $\gamma = M/M$. With the above assumptions, the wave function after the collision is $\Psi_F = \Gamma(R + \delta u)\Phi(R - \gamma u)$, i.e., $u \rightarrow -u$. To show this, recall that the exact propagator for this problem is $G(R'', u''; R', u') = g_0^M (R'' - R', t) [g_0^m (u'' - u', t) - g_0^m (u'' + u', t)]$, with $g_0^\mu (y, t) \equiv (\mu/2\pi i\hbar)^{1/2} \exp(i\mu y^2/2\hbar)$, the free propagator. To a good approxi-
mation, before the collision the wave function is given by the integral involving $g_0^m(u'' - u', t)$, after the collision by that involving $g_0^m(u'' + u', t)$. Thus to get the final wave function, one reverses "u".

When re-expressed in terms of $x$ and $X$, $\Psi_F = \Gamma(X(1 - 2\delta) + 2x\delta)\Phi(-x(1 - 2\delta) + 2X\gamma)$, suggesting that the final wave function has become entangled. For interactions more general than the hard wall there will be more complicated changes in the functions, but since the separate evolution of $u$ and $R$ follows from momentum conservation and the general nature of the two-particle interaction, there is no getting away from the intertwining.

The form we take for the wave function is

$$\Psi_I = \sqrt{N} \exp \left(-\frac{X^2}{4\Sigma^2}\right) \exp \left(-\frac{x^2}{4\sigma^2} + ikx\right)$$

with both $x$ and $X$ taking values on the entire real line. ($N = 1/2\pi\sigma\Sigma$, and the position spreads are $\Delta X = \Sigma$ and $\Delta x = \sigma$, both assumed real.) In principle we should use a wave function with "$x - x_0$" in place of "$x$" above and restrict the relative coordinate to (say) negative values (because of the hard wall). However, the form of the propagator given above allows us to use the simpler form, Eq. (1). That propagator says that one can look upon this scattering as taking place on the entire line but with a second source at a reflected position (this is the method of images applied to the path integral). The wave emanating from the image is the wave function for large positive times, and this is the portion we wish to study. In particular we look at its inner product with a test wave function (what you would have taken to be the wave function had you not treated the wall as a quantum dynamical object) and study its entanglement properties using the measure of [4]. However, the answer to neither of these questions will change with time so that we can study the reflected wave at whatever time is most convenient and, as in Eq. (1), that time is the time for which there is symmetry in $x$. However, since this is now to be thought of as the reflected wave moved back to an earlier time, the entire reflected wave must be used, i.e., variables range over the entire line. Although this trick is available only when the method of images can be applied, the general tenor of our results does not depend on it. You can (also in this case) start the wave packet at some (say, negative) $x_0$ and propagate it through the impact. The
only thing to be careful of (which also applies to our argument above) is that the incoming and outgoing waves separate on a time scale less than that for wave packet spreading.

There are now two things to check: error and decoherence. To compute “error,” we compare the outgoing wave to what would have been expected had the wall not been treated dynamically. To compute decoherence we measure the degree of entanglement as defined in [4].

Error

We examine the overlap integral of the actual $\Psi_F$ with the wave function that would have resulted from the idealization, $x \rightarrow -x$, namely $\Psi_{\text{test}} \equiv \Gamma(X)\Phi(-x) = \Gamma(R - \delta u)\Phi(-R - \gamma u)$. Using Eq. (1)

$$A \equiv \int \Psi_{\text{test}}^* \Psi_F \propto \int dRdu \Gamma^*(R - \delta u)\Phi^*(-R - \gamma u)\Gamma(R + \delta u)\Phi(R - \gamma u)$$

$$= \mathcal{N} \int dRdu \exp \left( -\frac{(R - \delta u)^2}{4\Sigma^2} \right) \exp \left( -\frac{(-R - \gamma u)^2}{4\sigma^2} - ik(-R - \gamma u) \right)$$

$$\times \exp \left( -\frac{(R + \delta u)^2}{4\Sigma^2} \right) \exp \left( -\frac{(R - \gamma u)^2}{4\sigma^2} + ik(R - \gamma u) \right)$$

We find

$$A^{-2} = \left[ \gamma^2 + \delta^2 + \gamma^2\lambda + \frac{\delta^2}{\lambda} \right] \exp \left( \frac{4k^2\lambda\sigma^2}{1 + \lambda} \right) \quad \text{with} \quad \lambda \equiv \frac{\Sigma^2}{\sigma^2}$$ \hspace{1cm} (2)

Particular experiments have their own particular wave functions; hence $A$’s deviation from 1 varies. Here we seek the minimum deviation in the face of the interaction with the wall. To this end, we vary $\sigma$ and $\Sigma$ so as to maximize $A$. First we study $k = 0$. $A$ now depends only on $\lambda$ (not the sigmas separately), and varying $\lambda$, we find the optimum to be given by

$$\lambda_{\text{max}} = \frac{\delta}{\gamma} \approx \frac{m}{M}$$

Substituting yields $A = 1$. There is no error! (N.B., . . . only for $\lambda = \lambda_{\text{max}}$.) When $k \neq 0$ we maximize $A$ by optimizing $\lambda$ for given $k\sigma$. We will see that the optimum
A always falls below unity, by an amount of order $\delta$. For small and large $k\sigma$ analytic forms are

\begin{align*}
\text{Small } k\sigma & \quad \lambda_{\text{max}} \approx \delta/\gamma \text{ (as before)} \quad 1 - A \approx 2\delta k^2 \sigma^2 \\
\text{Large } k\sigma & \quad \lambda_{\text{max}} \approx \delta/2k\sigma \quad 1 - A \approx 2\delta k\sigma
\end{align*}

These behaviors smoothly mesh at $k\sigma \sim 1$. Eq. (3) represents a lower bound on error. The factor $\delta \approx m/M$ keeps this effect small and is reminiscent of similar factors in measurement theory. It may be appropriate to think of the confinement process as one in which the system’s components are constantly bumping up against their container, so that the small $\delta$ could pick up a large factor related to an effective frequency of such interactions.

How bad is the error without optimization? Writing $\Sigma^2/\sigma^2 \equiv \delta e^y$ and still assuming the error to be relatively small, one finds $(1 - A)/\delta \approx \cosh y + 2k^2 \sigma^2 e^y$.

**Decoherence**

This is potentially the more damaging effect. A basis independent measure of the degree of entanglement of the particle and wall is given in [4]. The degree of entanglement is 1 minus the largest eigenvalue of $\psi^\dagger \psi$ (or $\psi \psi^\dagger$) considered as a matrix operator with matrix indices the arguments of $\psi$.

Because we wish to use the variable $x$ (for the system) as if it were unentangled, the wave function variables should be $x$ and $X$. In terms of these

$$
\Psi_F(x, X) = \sqrt{N} \exp \left\{ -\Omega [X(1 - 2\delta) + 2\delta x]^2 - \omega [x(1 - 2\gamma) + 2\gamma X]^2 \\
+ ik (x(1 - 2\gamma) + 2\gamma X) \right\}
$$

\begin{equation}
\tag{4}
\end{equation}

with $N = (2/\pi)^{1/2} \Omega \omega$, $\Omega \equiv 1/4\Sigma^2$, and $\omega \equiv 1/4\sigma^2$. We can form an operator (following [4]) in two ways, by integrating over either $X$ or $x$. We choose

$$
F(x', x) \equiv \int dX \Psi_F^\dagger(X, x') \Psi_F(X, x)
$$

$$
= \sqrt{\frac{2\omega \Omega}{\pi D}} \exp \left\{ -(x^2 + x'^2) \frac{\omega \Omega}{D} - (x - x')^2 \frac{E^2}{D} + ik(1 - 2\gamma)(x - x') \right\}
$$

\begin{equation}
\tag{5}
\end{equation}
with \[ D \equiv \Omega (\gamma - \delta)^2 + 4\omega \gamma^2, \quad \text{and} \quad \rho \equiv |(\gamma - \delta)(\Omega \delta - \omega \gamma)| \]

Following [4], we want the largest eigenvalue of \( F \) (now thought of as the integral kernel of an operator). First note that the factor \( \exp[ik(1 - 2\gamma)(x - x')] \) can be dropped because it does not affect the eigenvalue. Next observe that \( F \) is almost the same as the kernel of the propagator for the simple harmonic oscillator. Using a standard form for this operator, we note the following fact. The operator

\[
G(x, y) \equiv \sqrt{\frac{\beta}{\pi \sinh u}} \exp \left[ -\frac{\beta}{\sinh u} [(x^2 + y^2) \cosh u - 2xy] \right]
\]

has the spectrum \( G_n = \exp(-u(n + 1/2)), n = 0, 1, 2, \ldots, \) irrespective of \( \beta \). (The connection with the harmonic oscillator is \( \beta = m\omega/2\hbar \) and \( \omega t = -iu \).) It is now straightforward to deduce that the spectrum of \( F \) is \( F_n = (1 - e^{-u}) e^{-nu}, \) with \( n = 0, 1, \ldots \) and \( \sinh u/2 = \sqrt{\omega \Omega / 2\rho} \). From this it follows that the largest eigenvalue of \( F \) is

\[
F_0 = 1 - z^2, \quad \text{with} \quad z = \sqrt{\frac{w^2}{4} + 1 - \frac{w}{2}}, \quad \text{and} \quad w \equiv \frac{\sqrt{\omega \Omega}}{\rho}
\]

For small \( w \), \( F_0 \sim w \), and for large \( w \), \( F_0 \sim 1 - 1/w^2 \).

The first issue is minimizing entanglement, that is maximizing \( F_0 \). Clearly \( F_0 \) reaches its theoretical maximum for \( w = \infty \), which requires in turn \( \Omega \delta = \omega \gamma \). Recalling the definitions of \( \omega \) and \( \Omega \) this brings us to the same relation, \( \Sigma^2/\sigma^2 = \delta/\gamma \), that we found when minimizing error. It is interesting that here the entanglement is strictly zero even when the momentum, \( k \), is non-zero—if there is the special matching of wave function spreads. In the absence of matching, the entanglement, hence the decoherence, can be considerable, as indicated by \( F_0 \sim w \) for small \( w \).

It should be emphasized that this decoherence cuts down on the amplitude of the wave function that can ultimately yield an accurate computational result. From [4] we know that the maximum amplitude available in a putative unentangled wave function \( \psi(x) \) is \( \sqrt{F_0} \) and that for two such successive independent collisions it will be the product of two such terms. If \( F_0 \) is not extremely close to 1, the effect can build rapidly. Such behavior is to be contrasted with say, decay, where the initial
small deviation is in a phase, so that the effect of many independent such deviations is only quadratic in each of them.

**Optimal coherence**

The minimization of both error and entanglement have brought to light a matching condition on the spreads of the system and apparatus, $\Sigma^2/\sigma^2 = m/M$. This may be surprising. Based on the usual idealization of macroscopic objects, one might have thought that there should be no restriction on the *smallness* of “$\Delta X$”.\textsuperscript{11} Aside from considerations of the sort in [2] (and for which $F_0 = 1$ provides an example of a “special state”), there is no reason to think that Nature would evolve into minimally decohering states. Of course the constructor of a quantum computer may have a strong interest in such minimizing. In any case it is of interest to consider the possibility that the optimizing condition hold generally. In [3] it was observed that _all_ pairs of objects could satisfy the relation above if for each object, its mass, $\mu$, and its position uncertainty, $\sigma_\mu$, were related by $\sigma_\mu^2 \sim 1/\mu$. Possible justifications (kinds of environmental decohering) were considered in [3], but we here take the relation as a hypothesis and extend it using dimensional analysis. Taking $\hbar = 1$ and $c = 1$, it is clear that another length is needed, alternatively an energy or mass. For a confined system the quantities that come to mind are an overall distance scale for the system and the temperature. The former seems to me ill defined, and in particular an attractive feature of the relation proposed is that it is not vital to distinguish between “system” and walls. Using then the temperature ($T$) and restoring $\hbar$, we find

$$\sigma_\mu^2 \sim \frac{\hbar^2}{\mu k_B T}$$  \hspace{1cm} (9)

with $k_B$ the Boltzmann constant. Eq. (9) gives a mass-$\mu$ object a packet size that is the geometric mean of its Compton wavelength and $\sim 0.2 \text{ cm } / T \text{ kelvins}$. This does not seem inconsistent with experience. Lower temperature allows larger coherent wave packets, distinguishing this effect from others\textsuperscript{12} where position fluctuations decrease with decreasing temperature. If the effective momentum, $k$, of the small mass is the result of thermal fluctuations, then equipartition relates this to temperature
as well. We then have $k^2\sigma^2 \sim (2\hbar^2 k^2/2\mu)/k_B T \sim 1$, independent of temperature. (For $k\sigma = 1$, $1 - A \approx 1.2\delta$.) This suggests that in a heat bath, $\Delta p \sim \hbar/\Delta x$, since $\langle p \rangle = 0$.

**Limitations and extensions**

We have shown that confinement need not force entanglement, but if the confined objects strike the walls at finite velocity, there must be some “error.” It must be emphasized that the no-entanglement result depends not only on a particular ratio of spreads for small and large system, but also on the Gaussian form of the wave packet and on the form of the interaction with the wall. In this article we have not explored the effect of relaxing these assumptions. The minimizing of error relies on the same framework, so that one could entertain the idea of reducing error through tailoring of the wave packet or the walls. Based on preliminary exploration, I would say that more complicated wave packets or walls only increase both entanglement and error.

For application of the bounds presented here it is desirable to identify the wall mass, “$M$”. Even for a steel vacuum chamber one would not look to the mass of the entire chamber, but only the region affected by the particle’s collision, perhaps defined by the wavelength of the appropriate phonon. For “chambers” that are magnetic fields (etc.) one can ultimately look to the laboratory equipment that produces these fields.

Finally, there is our decoherence-minimizing relation, $\sigma^2_\mu \sim 1/\mu$, or more ambitiously, $\sigma^2_\mu \sim \hbar^2/\mu k_B T$. Do particles settle into wave packets of this size? Are two-time boundary condition considerations (as in [2]) at work? Yet another question is the form such a relation might take for massless particles. Here too one could ask for decoherence-minimizing scattering.

In conclusion, we have shown that pinning a system to the table does not in itself force entanglement with the degrees of freedom of the container—treating the latter as a fully quantum object. Nevertheless, subject to reasonable assumptions, that pinning will introduce “error,” in the sense of changed outgoing wave function. Minimizing both decoherence and error are best accomplished when a particular relation exists between the wave function spreads of system and container. We
have also computed the degree of entanglement in situations where the minimum spread condition does not hold.

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**References**

[1] Among many references, see for example, I. L. Chuang, R. Laflamme, P. W. Shor and W. H. Zurek, Science 270, 1633 (1995).

[2] L. S. Schulman, *Time’s Arrows and Quantum Measurement*, Cambridge Univ. Press, Cambridge (1997).

[3] L. S. Schulman, Phys. Lett. A 211, 75 (1996). Note a misprint: “ε” there should be $2m/M$ (not $m/M$).

[4] L. S. Schulman and D. Mozyrsky, Measure of decoherence, preprint.

[5] By “decoherence” I mean loss of the primary wave function through entanglement with other degrees of freedom, hence the inability to interfere with portions of the wave function not so entangled. By “error” I mean non-entangled wave function whose value is changed from that in the absence of the scattering.

[6] For electromagnetic or other confinement this picture will need extension. However, the primitive underpinning of the derivation, momentum conservation, suggests that such extension is possible.

[7] A treatment neglecting the dynamical nature of the wall would generally omit the function $\Gamma$.

[8] M. M. Yanase, Phys. Rev. 123, 666 (1961).

[9] L. S. Schulman, *Techniques and Applications of Path Integration*, Wiley, New York (1981).

[10] Disentanglement with spread matching could have been noted directly from $\Psi_F$, so that the surprise in being able to disentangle despite collisions did not
require [4]. However, measure of the amplitude defect without matching does
require those results.

[11] There is of course Feynman’s variation on the two slit experiment (in R. P.
Feynman, R. B. Leighton and M. Sands, *The Feynman Lectures on Physics*,
Addison-Wesley, Reading, MA (1965)), which relates uncertainties in a macro-
scopic object to putative measurements of a microscopic one. The correspond-
ing restriction here would be that $\Delta X (= \Sigma)$ not be so small that the associated
$\Delta P$ destroy the small-system interference patterns that we seek. Our optimal
$\Sigma$ is far from such values. We estimate this kinematic effect as follows. Momentum
uncertainty $\Delta P$ in the big system means uncertainty $\Delta P/M$ in the (velocity)
transformation going into the center of mass frame. For the small system
this velocity uncertainty gives a momentum uncertainty $(\Delta p)' \sim m(\Delta P/M)$
(the prime on $(\Delta p)'$ distinguishes it from the momentum uncertainty in the
original wave function, namely $(\Delta p)_{\text{usual}} \sim \hbar/\sigma$). Taking $\Delta P \sim \hbar/\Sigma$, we find
$(\Delta p)' \sim m\hbar/M\Sigma$. Using $\Sigma^2/\sigma^2 \approx m/M$ yields $(\Delta p)'/(\Delta p)_{\text{usual}} \sim \sqrt{m/M}$.

[12] H. Grabert, P. Schramm and G. Ingold, Phys. Rep. 168, 115 (1988). See in
particular Table 2, p. 159.