Strong and weak single particle nonlocality induced by time-dependent boundary conditions

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We investigate the issue of single particle nonlocality in a quantum system subjected to time-dependent boundary conditions. We first prove that contrary to earlier claims, there is no strong nonlocality: a quantum state localized at the center of a well with infinitely high moving walls is not modified by the wall’s motion. We then show the existence of a weak form of nonlocality: when a quantum state is extended over the well, the wall’s motion induces a current density all over the box instantaneously. We indicate how this current density can in principle be measured by performing weak measurements of the particle’s momentum.

Introduction. Quantum systems with time-dependent boundary conditions are delicate to handle. Even the simplest system – a particle in a box with infinitely high but moving walls – remains the object of ongoing investigations. From a mathematical standpoint, a consistent and rigorous framework hinges on unifying an infinite number of Hilbert spaces (one for each time $t$), each endowed with its own domain of self-adjointness. The particle in a box with moving walls has also been taken as a paradigm of quantum chaos, particularly regarding the existence of Fermi acceleration, ie the unbounded energy gain of a particle subjected to a time dependent potential. More recently this system has been employed as a tool to investigate expanding boxes and quantum pistons, particularly in the context of mimicking adiabatic dynamics without genuine adiabaticity, a technique that is of interest for the experimental quantum control of different systems, such as atomic transitions or Bose-Einstein condensates.

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The Hamiltonian for a particle of mass $m$ in an infinite well of width $L(t)$ with moving boundaries is given by

$$H = \frac{p^2}{2m} + V$$

$$V(x) = \begin{cases} 0 & \text{for } -\frac{L(t)}{2} \leq x \leq \frac{L(t)}{2} \\ +\infty & \text{otherwise} \end{cases}$$

The solutions of the Schrödinger equation $i\hbar \partial_t \psi(x,t) = H \psi(x,t)$ must obey the boundary conditions $\psi(\pm L(t)/2) = 0$. The instantaneous eigenstates of $H$,

$$\phi_n(x,t) = \sqrt{2/L(t)} \cos[(2n+1)\pi x/L(t)]$$

verify $H |\phi_n\rangle = E_n(t) |\phi_n\rangle$ where $E_n(t) = (2n+1)^2 \hbar^2 \pi^2 / 2mL^2(t)$ are the instantaneous eigenvalues, but the $\phi_n$ are not solutions of the Schrödinger equation. Indeed, due to the time-varying boundary conditions, the problem is ill defined, eg the time derivative $\partial_t \psi(x,t)$ involves the difference of two vectors with different boundary conditions belonging to different Hilbert spaces. To tackle this problem, different approaches, like introducing a covariant time derivative or implementing an ad-hoc change of variables yielding differential equations involving non-Hermitian
operators have been used. The most general approach to solve the problem is to use a time-dependent quantum canonical transformation mapping the Hamiltonian $H$ of the time-dependent boundary conditions to a new Hamiltonian $\tilde{H}$ of a fixed boundary problem. Let

$$\mathcal{M}(t) = \exp \left( \frac{i\xi(t)}{2\hbar} (XP + PX) \right)$$

be a unitary operator with a time-dependent real function $\xi(t)$ defining the canonical transformation

$$|\tilde{\psi}\rangle = \mathcal{M}(t) |\psi\rangle$$

$$\tilde{H}(t) = \mathcal{M}(t) H(t) \mathcal{M}^\dagger(t) + i\hbar \mathcal{M}(t) \partial_t \mathcal{M}^\dagger(t)$$

the latter holding for time-independent observables $A$ such as $X$ or $P$. Note that $\mathcal{M}(t)$ represents a dilation, i.e. any arbitrary function $f(x)$ transforms as $\mathcal{M}(t)f(x) = e^{\xi(t)/2}f(e^{\xi(t)/2}x)$. It is therefore natural to choose $\xi(t) = \log (L(t)/L_0)$ where $L_0 \equiv L(t = 0)$ so as to map the original problem to the initial interval $[-L_0/2, L_0/2]$, with

$$\psi(x, t) = \langle x | \mathcal{M}^\dagger(t) |\tilde{\psi}\rangle = \sqrt{\frac{L_0}{L(t)}} \tilde{\psi} \left( \frac{L_0}{L(t)} x, t \right).$$

$|\tilde{\psi}\rangle$ is the solution of the fixed boundary Hamiltonian whose explicit form is

$$\tilde{H}(t) = \frac{\tilde{p}^2}{2m} + V(\tilde{x}) - \frac{\partial_x L(t)}{L(t)} (XP + PX).$$

**Strong nonlocality.** Let us now consider linearly expanding walls, $L(t) = L_0 + qt$ with $q > 0$. This has been indeed the main case studied in the context of nonlocality induced by boundary conditions, due to the existence of exact solutions of the canonically transformed Schrödinger equation $i\hbar \partial_t \tilde{\psi}_n = \tilde{H} \tilde{\psi}_n$. By an educated guess (from the known solutions, originally obtained by inspection), of differential equations similar to the Schrödinger equation for $\tilde{H}$ these are found to be given by

$$\tilde{\psi}_n(x, t) = \sqrt{\frac{2}{L_0}} e^{i m \pi^2 L(t) L_0^{2n+1}} \cos \left( \pi(2n+1)x/L_0 \right)$$

where $n = 0, 1, 2, \ldots$ The $\tilde{\psi}_n$ are not eigenfunctions of $\tilde{H}$, but they can be employed as a fundamental set of solutions in order to obtain the time-evolved state $|\tilde{\psi}(t)\rangle$ from an arbitrary initial state $|\tilde{\psi}(t = 0)\rangle$ expressed as

$$|\tilde{\psi}(t)\rangle = \sum_n \langle \tilde{\psi}_n(t = 0) |\tilde{\psi}(t = 0)\rangle |\tilde{\psi}_n(t)\rangle.$$
In general $\psi$ as well as $z$ and $\kappa$ depend on $q$, the velocity of the walls motion. We will explicitly denote this functional dependence, i.e. $\vartheta(q), \kappa(q)$. The particular case $q = 0$ corresponds to static walls with fixed boundary conditions.

In order to compare the time evolved wavefunction in the static and moving problems, let us compute $\psi(x,t; q = 0)/\psi(x,t; q)$ which after some simple manipulations takes the form [27]

$$
\frac{\psi(x,t; q = 0)}{\psi(x,t; q)} = e^{i\frac{z^2}{4\kappa^2} - \frac{z^2}{\kappa^2}} \left(\frac{\kappa(0)}{\kappa(q)}\right)^{1/2} \frac{\vartheta_2(z(0), \kappa(0))}{\vartheta_2(z(q), \kappa(q))}.
$$

We now prove that this expression is unity. The first step is to use the Jacobi transformation [26]

$$
\vartheta_2(z, \kappa) = \frac{e^{-iz^2/\kappa \pi}}{(-i\kappa)^{1/2}} \vartheta_4\left(\frac{z}{\kappa} - \frac{1}{\kappa}\right)
$$

for both $\vartheta_2$ functions of Eq. [17]. $\vartheta_4$ is the Jacobi Theta function defined by $\vartheta_4(z, \kappa) = \sum_{n=-\infty}^{\infty} (-1)^n e^{i\kappa n^2} e^{2inz}$. Eq. [17] then becomes

$$
\frac{\psi(x,t; q = 0)}{\psi(x,t; q)} = \frac{\vartheta_4\left(\frac{z(0)}{\kappa(0)} - 1/\kappa(0)\right)}{\vartheta_4\left(\frac{z(q)}{\kappa(q)} - 1/\kappa(q)\right)}.
$$

We then note that $\text{Im} -1/\kappa(q) = d^2m^2L(t)^2/\pi (4d^4m^2 + h^2t^2)$, and this quantity needs to be much less than the spatial extension of the wall since by assumption the particle remains localized at the center of the box, far from the box boundaries. Hence we have $(\Delta x)^2 \ll L_0^2$ from which it follows that $\text{Im} -1/\kappa(q) \gg 1$. Now from the definition of $\vartheta_4$, it is straightforward to see that under these conditions only the $n = 0$ term contributes to the sum, leading to $\vartheta_4(z(q)/\kappa(q), -1/\kappa(q)) = 1$ for any value of $q$ (including $q = 0$). Hence provided the quantum state remains localized throughout the evolution, we have

$$
\psi(x,t; q) = \psi(x,t; q = 0)
$$

meaning that the dynamics of the wavefunction initially localized at the center of the box does not depend on the expanding motion of the walls at the boundaries of the box. In particular the adiabatic condition does not play any particular role, as Eq. [20] holds for any value of $q$. While each individual state $\psi_n(x,t)$ does stretch out as time increases, the sum for $\psi(x,t)$ ensures that the interferences cancel the stretching for the localized state. From a physical standpoint there is no strong nonlocality. The same results holds for walls contracting linearly, as well as in the periodic case (wall expansion followed by a contraction). In the latter case it should be noted that the analytic solutions [19] and [12] do not verify the Schrödinger equation during the reversal, and as a consequence an expanding basis state $\psi_n(x,t)$, does not evolve into the “reversed” state $\psi_n(x,t)$ after the walls motion reversal [27].

**Weak nonlocality.** We have seen that the dynamics of an initially localized state is not modified by moving boundary conditions. However a state extended all over the box and thus in contact with the walls will naturally be modified as the boundary conditions change. This process creates a current density at any arbitrarily chosen point inside the box. For example for linearly expanding walls, the current density in a basis state $\psi_n$ [Eq. [12]] is

$$
j_n(x,t) = \frac{2q x \cos^2 \left(\frac{(2n+1)x}{L_0 + qt}\right)}{(L_0 + qt)^2}.
$$

Note that this current density is modified instantaneously, i.e $\Delta j_n(x) = j_n(x, \epsilon) - j_n(x, 0)$ is non-vanishing at $x$ for a small time interval $\epsilon$ even if a signal emitted at the wall reaches $x$ in a time $t_c > \epsilon$ with $t_c = (L_0/2 - |x|)/c$ ($c$ is the light velocity). This is a weak form of nonlocality, in that the modification of the quantum state is due to a local interaction with the wall but
takes place globally and instantaneously in most of the spatial regions in which the wavefunction amplitude does not vanish. This weak nonlocality takes a particularly acute form in the de Broglie-Bohm interpretation [21] (or Bohmian model, BM): according to BM a quantum system comprises a point-like particle having an exact but unknown position, whose motion is guided by the wavefunction. The velocity $v(x, t)$ of the Bohmian particle is directly linked to the current density

$$v(x, t) = \frac{j(x, t)}{|\psi(x, t)|^2} \tag{22}$$

so that in the BM there is a clear nonlocal action of the boundary motion on the particle dynamics.

The Bohmian velocity field can be measured by performing weak measurements. A weak measurement [28] of an observable $A$ involves a weak coupling between the system and a pointer followed by a distinct projective measurement of the system. In the limit of asymptotically weak couplings, the system state is essentially undisturbed and the pointer is shifted by $\text{Re} A_w$ where $A_w$ is known as the weak value [28] of $A$. It can be shown [29, 31] that for a system in state $|\psi\rangle$ the real part of the weak value $P_w$ of the momentum operator $P$ conditioned on a projective measurement at point $x$ is given by

$$\text{Re} P_w = \text{Re} \frac{\langle x | P | \psi \rangle}{\langle x | \psi \rangle} = m v(x, t) \frac{j(x, t)}{|\psi(x, t)|^2}. \tag{23}$$

Weak momentum values have already been experimentally determined for photons [32] and specific proposals to perform such measurements with single electron sources have been put forward very recently [33].

Fig. 1 displays $\text{Re} P_w(t)$ when the system is initially in the quantum state $(\phi_1(x, 0) - \phi_1(x, 0))/\sqrt{2}$ where $\phi_1(x, 0)$ given by Eq. [3] is an eigenstate of the fixed walls box, with $j(x, 0) = 0$. We allow for a continuous transition from the fixed walls to the linear regime by setting $L(t) = L_0 + \alpha (1 - e^{-\beta t})$ with $\beta \gg 1$. The light cone boundary is indicated by the green-grided plane. It can be seen that the current density reacts to the walls motion before a signal can reach the point where the weak measurement takes place. This is the signature of weak nonlocality. Whether such an effect can be experimentally observed in practice (under the present configuration, an experiment would require to carry out a weak measurement in a sub-femtosecond timescale) as well as its status relative to the no signaling principle remains to be investigated. Note that the nature of single particle nonlocality here is different than in the case of entangled particles, for which weak momentum measurements have been recently performed [10, 20] by establishing correlations between the polarization of one photon and the current density of the other.

**Conclusion.** To sum up we have shown that contrary to widespread claims, time-dependent boundary conditions do not induce a strong form of nonlocality that would modify the dynamics of a quantum state entirely localized at the center of a box. However when the state of the system is extended over the box a weaker form of nonlocality is induced by the varying boundary conditions: a current density appears instantaneously at any point of the box, however far from the moving walls. This effect can in principle be tested experimentally by performing weak measurements.

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These solutions are symmetric in $x$, the odd solutions are obtained similarly but we will not need them here.