Quantum particle displacement by a moving localized potential trap

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Abstract – We describe the dynamics of a bound state of an attractive $\delta$-well under displacement of the potential. Exact analytical results are presented for the suddenly moved potential. Since this is a quantum system, only a fraction of the initially confined wave function remains confined to the moving potential. However, it is shown that besides the probability to remain confined to the moving barrier and the probability to remain in the initial position, there is also a certain probability for the particle to move at double speed. A quasi-classical interpretation for this effect is suggested. The temporal and spectral dynamics of each one of the scenarios is investigated.

Introduction. – Recent developments in nanotechnology allow displacing miniscule particles, which can be as small as an atom. These particles’ relocation can be achieved either by optical tweezers [1] or by Scanning Tunneling Microscopy (STM) [2]. The STM moves an atom by creating a potential well at its vicinity. The atom is then trapped in the tip of the STM’s needle and can easily be relocated along with the tip’s position (see fig. 1). Beautiful structures with incredible (sub-Ångström) accuracy were achieved [3].

Since the atom is a quantum particle, localization at finite space is always partial. The sudden activation of the trapping well could cause an atom loss as in an equivalent decay process [4–6]. Moreover, in this paper we show that the sudden movement itself (not only the abrupt capturing) can be responsible for the atom escape. It is also shown that not only do some of the atoms remain (on the average) at their initial state, but some will move beyond the tip’s influence at double velocity.

Bound states subjected to sudden perturbations have been studied in relation to the so-called deuteron problem [7]. The tunneling dynamics of a bound state has been reported in a time-dependent well [4] and after suddenly weakening the strength of the potential [6]. Here, we describe the transport of particles initially trapped in a well which is shifted at constant velocity along a waveguide. Under strong transverse confinement, the dynamics becomes effectively one-dimensional (1D) whenever all relevant energies are much smaller than the excitation quantum in the radial direction.

The model. – To simplify the system, the well is modeled by a 1D delta function potential well. It should be stressed that a 1D negative (positive) delta potential

Fig. 1: System schematic. A single atom displacement by an STM tip.

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is, in fact, an exponentially shallow potential well, and it can model with great accuracy any well (barrier) whose physical dimensions are smaller than the de Broglie wavelength of the particle [8].

Prior to \( t = 0 \), the well is localized at \( x = 0 \); however, for \( t > 0 \) the well moves at constant velocity \( v \). The potential well can then be formalized

\[
V(x, t) = \begin{cases} -\gamma \delta(x) & \text{for } t \leq 0, \\ -\gamma \delta(x - vt) & \text{for } t > 0. \end{cases}
\]

(1)

Thus, the system dynamics is fully characterized by the Schrödinger equation:

\[
i\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x, t)\psi,
\]

(2)

where we adopted the units \( \hbar = 2m = 1 \).

The dynamics begins with the bound state of \( |\psi(x, t = 0)\rangle \), and it can be obtained using the superposition principle

\[
\psi(x, t = 0) = \sqrt{\frac{\gamma}{2}} e^{-\gamma |x|^2/2}.
\]

(3)

**Free evolution of the bound state.** – If it had not been for the potential well, the particle’s probability density would spread out freely. If it is assumed that for \( t > 0 \) the well is absent, and the Hamiltonian becomes purely kinetic, then for \( t > 0 \) the dynamics is free, and it can be obtained using the Schrödinger equation:

\[
\psi(x, t > 0) = \frac{1}{\sqrt{4\pi t}} e^{i(x-k\gamma t)^2/2t}.
\]

(4)

The time evolution of the initial bound state can be then simply written in terms of the Moshinsky function as

\[
|\psi_{\text{b}}(x, t)\rangle = e^{-i\gamma x^2/2} [M(x, -i\gamma/2, 2t) + M(-x, -i\gamma/2, 2t)],
\]

(5)

where the Moshinsky function reads [9–11]

\[
M(x, k, t) := \frac{e^{i\pi x^2/2}}{2} w(-z), \quad z = \frac{1 + i}{2} \sqrt{t} \left( k - \frac{x}{t} \right)
\]

(6)

in terms of the Faddeyeva function \( w(z) \), which is defined as \( w(z) := e^{-z^2} \text{erfc}(-i z) \). On physical grounds, it is clear that each of the \( M \) functions corresponds to a freely time-evolved cut-off plane wave. Such solution entails the well-known diffraction in time phenomenon, which consists of a set of oscillations in the density profile [9,10,12]. However, the imaginary wave vector \(-i\gamma/2\) makes such transients evanescent [13], leading to a uniform expansion.

**Uniformly moving well.** – For \( t > 0 \), the propagator should be extended to the \( v \neq 0 \) case, for which the corresponding propagator can be obtained using Duru’s method [14] and as well as by means of the path integral perturbation series [15]. It can be conveniently written in terms of the free propagator and a perturbation term, represented by a Moshinsky function

\[
K_{\text{b}}^{\text{h}}(x, t|x', t') = K_0(x, t|x', t') + \frac{\gamma}{2} \times e^{i\gamma(x-vt')^2/2} \times M(|x - vt| + |x' - vt'|, +i\gamma/2, t).
\]

(8)

The time evolution of the state in eq. (3) can be also obtained in close-form, using the integral [16]

\[
\int_{-\infty}^{0} dx' e^{i(kx' - \gamma x'^2)/2} M(|x'|, -i\gamma/2, 2t) - M(|x' - vt|, -i\gamma/2, 2t)
\]

(9)

Taking \( t' = 0 \) and using eqs. (3), (8), and (9), one can readily find

\[
|\psi_{\text{b}}^{(v)}(x, t)\rangle = \psi_0(x, t) - e^{i\gamma x^2/2} \left[ \frac{\gamma}{2} \right]^{\frac{1}{2}} \times [M(|x - vt|, -i\gamma/2, 2t) - M(|x - vt|, -i\gamma/2, 2t)]
\]

(10)

as the sum of a free term plus a perturbation.

The adiabatic Massey parameter [16], which distinguishes the distinct dynamical regimes is therefore

\[
\theta = \frac{v}{\gamma},
\]

(11)

so that for \( \theta \ll 1 \) the adiabatic dynamics is recovered while \( \theta \gg 1 \) corresponds to the infinitely fast displacement of the well (free evolution).

Indeed, the Galilean transformation [17] on the time-dependent eigenstate of a moving delta well yields [14]

\[
|\psi_{\text{b}}^{(v)}(x, t)\rangle = \sqrt{\gamma/2} \frac{e^{-i\gamma x^2/2} e^{i\gamma x^2/2} e^{-i\gamma x v t}}{\gamma + iv^2/2} \times [M(|x - vt|, i\gamma/2, 2t) - M(|x - vt|, i\gamma/2, 2t)]
\]

(12)

which becomes \( e^{i\gamma x^2/2} \psi(x, 0) \) for \( t = 0 \). The fraction that remains bounded for \( t \rightarrow \infty \) is

\[
|\langle \psi_{\text{b}}^{(v)}(0)|\psi(0)\rangle|^2 = \frac{\gamma^4}{\gamma^2 + \gamma^2} = \frac{16}{4 + \theta^2 x}
\]

(13)

for \( v \gamma \ll 1 \), the exponential becomes \( e^{i\gamma x^2/2} \sim 1 \) in the spatial range of the initial bound state, and the overlap becomes unity.
It is instructive in this point to see a physical realization of this model. If we pick, for example, a rubidium atom from an atom trap at $T \approx 10^{-7}$ K, the atom de Broglie wavelength is approximately $\lambda \approx 1 \mu$m, which is about three orders of magnitude larger than the tip of the STM needle. Moreover, for this scenario, this wavelength corresponds to a critical velocity of approximately $v \approx 0.4$ m/s.

**Three scenarios.** — When $t \to \infty$ the three domains that were discussed at the introduction (the particles that remain at the vicinity of $x = 0$, the ones that are localized to the well at uniform velocity and the ones that propagate at double velocity) eventually appear (see fig. 2). The wave function can be written as a superposition of three terms:

$$\psi \sim \psi_{\text{free}} + \psi_{\text{well}} + \psi_{2v},$$

where

$$\psi_{\text{free}}(x, t) \approx \frac{2}{\sqrt{i \pi \gamma t}} e^{i \pi x^2 + i2\pi x vt} \frac{1}{1 + (x/\gamma t)^2},$$

$$\psi_{\text{well}}(x, t) \approx \frac{\sqrt{i/4 \pi}}{1 + (v/2\gamma)^2} e^{i \pi x \theta + i2\pi x^2 \theta} - \frac{1}{2} (\gamma t)^{-1} |x - vt|,$$

$$\psi_{2v}(x, t) \approx \frac{1}{4} e^{i \pi x \theta - i2\pi x^2 \theta} - \frac{1}{2} (\gamma t)^{-1} (x - 2vt),$$

The first term $\psi_{\text{free}}$ describes the free evolution of the initial state in the absence of the well, as can be appreciated from the structure of the propagator. The second contribution remains localized in the moving trap and follows its classical trajectory $x = vt$, while the last term is responsible for the appearance of a peak in the density profile at $x = 2vt$. This contribution results from the partial reflection from the attractive well of the initial state probability density located at $x > vt$.

Since in the initial state, the particle was localized in a region as small as $\Delta x \sim \gamma^{-1}$ the uncertainty in the particle's velocity behaves as $\Delta v \sim \gamma$ and therefore, as can be seen in eq. (14), the spatial width of the two peaks 0 and $2v$ gets wider approximately as $\Delta x \sim \gamma t$ (unlike the width of the localized part, which remains $\sim \gamma^{-1}$). Therefore, the distinction between the three parts can appear only when $v > \gamma$ (or $\theta > 1$). Moreover, due to their initial width, the peaks shape appears only when $t \gg (\gamma t)^{-1}$.

The probability density of the exact solution with a comparison to the approximation, which focuses on the three terms is illustrated in fig. 3.

**Asymptotics.** — The transition from the initial stationary bound state to the final moving one involves the two natural frequencies of the system: The frequency (energy) of the initial state $f_1 = \gamma^2/8\pi$ and the kinetic energy of the moving particle $f_2 = v^2/8\pi$. The $x = 0$ and the $x = 2vt$ peaks are affected only by the frequency $f_2$, however, the $x = vt$ one oscillates with three harmonics $f_1, f_2 - f_1, \text{ and } 2f_2 - f_1$. In fig. 4, the temporal dynamics of the three peaks is shown. The $x = 0$ and the $x = 2vt$ decay as $\sim t^{-1/2}$, while the $x = vt$ one converges to its final constant value

$$|\psi(x = vt, t \to \infty)|^2 \approx \frac{\gamma^2}{(1 + (v/2\gamma)^2)^2}. \quad (16)$$

In fig. 5, a numerical spectral distribution $\Psi(f) \equiv \text{FFT}[|\psi|^2]$ (FFT stands for the Fast Fourier Transform) of each one of the peaks is presented. The four different frequencies are clearly shown.

The “A” peak corresponds to the frequency $f_1 = \gamma^2/8\pi$. The “D” and “E” peaks correspond to the frequency
Fig. 4: The temporal dynamics of the three peaks ($x = 0$, $x = vt$ and $x = 2vt$). The system’s parameters are: $\gamma = 10$, $v = 20$.

$f_2 = v^2/8\pi$, the “B” peak stands for $f_3 = |f_2 - f_1| = |v^2 - \gamma^2|/8\pi$ and finally the “C” peak stands for $f_4 = f_3 + f_2 = |2v^2 - \gamma^2|/8\pi$.

Semiclassical realization. – Clearly, the double-velocity effect cannot be classical, since a localized state will remain localized in the classical world. However, the origin of this effect has partially a classical interpretation. Quantum mechanically, the particle in the initial state is not completely localized inside the well. In fact, when the well is very narrow most of the chance is to find the localized particle outside the well.

It is also instructive to investigate the system in a moving frame of reference, in which the well is at rest (originally, at the laboratory reference the well moves to the right). It should be noted that in the moving frame of reference the transmission through the (now) stationary well is trivial (see, for example, refs. [18,19]).

At $t = 0$, the particle (at the well’s reference frame) begins to move to the left with respect to the well. We can regard it as three different scenarios: particle at the right of the well (gray), at the well (black), and at its left (white).

At $t = 0$, all three types begin to move simultaneously to the left at velocity $v$ (fig. 6A).

The white is free — so it remains at velocity $v$ to the left. The black is trapped — so its average velocity is zero. But the gray hits the barrier and turns back with velocity $-v$, i.e., the final scenario is shown in fig. 6B.

When we return to the laboratory frame of reference (where the well moves to the right), we see that the white one did not move, the black moved with the well at velocity $v$, and the gray moved with velocity $2v$ (fig. 6C).

Obviously, this semiclassical interpretation is possible only due to the partial localization, which is a manifestation of quantum mechanics.

Conclusion and discussion. – We have presented a 1D quantum model for an atom displacement with an STM tip. The model consists of a delta function well, which models the STM’s potential at the vicinity of its tip end, which moves uniformly. It was shown that the probability to remain trapped in the moving tip is $\gamma^2/(\gamma^2 + v^2)^2 = 16/(4 + \theta^2)^2$. Moreover, it was shown that besides the trapped particles, and the particles that remain close to their initial state, there is also a third group of particles, which propagate at double velocity ($2v$) away from their initial position. We show that the probability for each one of the three groups has a different temporal dynamics.

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