Explanation and observability of diffraction in time

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Diffraction in time (DIT) is a fundamental phenomenon in quantum dynamics due to time-dependent obstacles and slits. It is formally analogous to diffraction of light, and is expected to play an increasing role to design coherent matter wave sources, as in the atom laser, to analyze time-of-flight information and emission from ultrashort pulsed excitations, and in applications of coherent matter waves in integrated atom-optical circuits. We demonstrate that DIT emerges robustly in quantum waves emitted by an exponentially decaying source and provide a simple explanation of the phenomenon, as an interference of two characteristic velocities. This allows for its controllability and optimization.

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constructed by a superposition of plane waves. The re-

ψ one particle is emitted, the normalized wave function is

\[ \psi(x,t) = \psi_s(x,t) + \psi_0(x,t) \Theta[\text{Im}(u_0^+)] \]

where \( \psi_s(x,t) = (2t/\pi)^{1/2}e^{-it^2/2} \), and \( \psi_0 = e^{-i\omega_0t}e^{i\tau x} \).

The oscillations are essentially the same as in the stan-
tion for a particle of mass \( 1/2 \) and \( h = 1 \), \( i\hbar \psi(x,t)/\partial t = -\partial^2 \psi(x,t)/\partial x^2 \). The unit of length corresponds to the in-
verse of the real part of the carrier wavenumber and the unit of time to the carrier period divided by 2\( \pi \). The complex dimensionless wavenumber \( k_0 = k_{0R} + ik_{0I} \) and frequency of the carrier \( \omega_0 = \omega_{0R} + i\omega_{0I} \), obey the dis-

tion relation \( \omega_0 = k_0^2 = (1 + ik_{0I})^2 \), so \( \omega_{0R} = 1 - k_{0I}^2 \) and \( \omega_{0I} = 2k_{0I} \), with \( k_{0I} < 0 \) and \( k_{0R} = 1 \). The exact unnormalized solution to the Schrödinger equation for the free particle subjected to the source boundary condition \( \psi(0,t) = e^{-i\omega_0t} \Theta(t) \), \( \omega_{0R} > 0 \), \( \omega_{0I} < 0 \), can be constructed by a superposition of plane waves. The result-
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tions, \( \psi(x,t) = \frac{1}{2\pi e^{i\pi/4}} \left[ w(-u_0^{(+)}(t)) + w(-u_0^{(-)}(t)) \right] \), where \( w(z) := e^{-z^2} \text{erfc}(-iz) \), \( u_0^{(\pm)} = \pm(1 + i) \sqrt{t/2k_0}(1 \mp \tau/t) \), and \( k_0 = x/2t \), \( \tau = x/2k_0 \) are a “saddle point” wave

FIG. 1: (Color online) Unnormalized density versus time at \( x = 1000 \) for a constant or exponentially decaying source.

frequency of the carrier

FIG. 2: (Color online) Normalized probability densities versus time for \( k_0 = 1 - 0.0015i \) at \( x = 1000 \). Exact (red solid line), approximate (Eq. 1, black dashed line), saddle term (blue circles), pole term (orange triangles), and interference term (Eq. 2, green squares).

The oscillations are essentially the same as in the standard MS, modulated by the exponential decay.

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where \( \psi_s(x,t) = (2t/\pi)^{1/2}e^{-it^2/2} \), and \( \psi_0 = e^{-i\omega_0t}e^{i\tau x} \).

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The expression for \( \psi(x,t) \) in terms of the saddle and pole, \( \psi_0 \), and the interference term, \( \psi_s \), can be written as

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The essence of DIT. The wavefunction \( \psi_s \), for times shorter and larger than \( |\tau| \) [18], can be accurately approximated by contributions from the two critical points of its defining integral, saddle and pole,
quency of the DIT oscillation depends on the interference of the saddle and pole frequencies $k_s^2$ and $\omega_{0R}$ and, as $k_s$ depends on time, the DIT oscillation period is not constant. From Eq. (2) we can infer the position of the $n$-th maximum. For $|k_{0f}| \ll 1$, the $\sin \phi$ term of Eq. (2) tends to vanish so the DIT oscillations are essentially due to the $\cos \phi$ term. The maxima correspond to $\phi(x,T_n) = 2n\pi$ at times

$$T_n = \frac{(3 + 8n)\pi + 4x + \sqrt{[(3 + 8n)\pi + 4x]^2 - 16\omega_{0R}x^2}}{8\omega_{0R}},$$

(3)

where $n = 0, 1, 2, \ldots$ ($n = 0$ is for the principal maximum). The interval $T_{n+1,n} = T_{n+1} - T_n$ between two consecutive maxima is in good agreement with the exact, numerically calculated period, see Fig. 3. The small discrepancy at $n = 0$ can be attributed to the dependence on time of the factors multiplying $\cos \phi$ and the proximity of $|\tau|$.

For large times the period of the DIT oscillations tends to the carrier period $\lim_{n \to \infty} T_{n+1,n} = 2\pi/\omega_{0R}$. The amplitude of the oscillations decays relatively slowly compared to the pole term, as $e^{\omega_{0f}t}t^{-3/2}$, see Eq. (2), but exponentially faster than the saddle term.

According to Eq. (3), $T_0$ is not a linear function of $x$. For example, in the limit $k_{0f} \to 0$ the motion of the first maximum is described by $x_0 = 2T_0 - \sqrt{3\omega_{0f}}$. Thus, even though an asymptotic velocity may be defined, $2(1+k_{0f})$ in the general case, see the inset of Fig. 3, there is no oblique asymptote for this function. Therefore a naive linear extrapolation back to the origin at some large distance fails to provide the instant of the source onset. In other words, the times in which the tangents to $x_0(t)$ cut $x_0 = 0$ have no definite limit, in spite of the well defined asymptotic velocity. This is an example of the importance of DIT to correct simple classical-dynamical extrapolation from asymptotic wave features to extract emission characteristics, as practiced e.g. in the analysis of ionization by ultrashort laser pulses [20].

In our dimensionless description two factors affect the visibility of the DIT pattern: the observation position $x$ and the lifetime. Figure 4 shows the moduli of the logarithm of the pole and saddle densities for two different lifetimes. The pole term is a semi-infinite straight line which begins when the pole is crossed by the steepest descent path passing along the saddle in the complex momentum plane, at $t_c$; the saddle term shows a maximum near $|\tau|$ and decays from there slowly. There may be up to two intersections of the two terms, one near the arrival of the main front, and one at a long time that marks the transition to post-exponential decay [13]. When the saddle and pole terms are similar or close enough the interference oscillations appear. The interference region of our interest here is the one following the main front because it relates by continuity to ordinary MS-DIT in the limit $k_{0f} \to 0$; it is also much more easily observable than the oscillations at large times because of the magnitude of the amplitudes.

The oscillations are evidently not present at the source $x = 0$, and will be small at small distances, $x \lesssim 1$, because of the rapid decay and separation from the pole term of the saddle term in these conditions, see Fig. 4.
The saddle term beyond the main front arrival increases with $x$ \[18\]. In the opposite extreme of very large $x$, it eventually dominates entirely and stays above the pole term at all times, suppressing DIT and even exponential decay \[18\]. Between these two extreme scenarios there is an ample range of $x$ for which DIT is prominent. The slope of the pole term also plays a role. For larger values (smaller lifetimes), pole and saddle contributions separate more rapidly leading to fewer visible DIT oscillations which may actually disappear for small enough lifetimes.

To estimate the domain where some oscillations are seen before the decay is too strong we may solve $T_{1,0} < N\tau_0$ for a small $N$, where $\tau_0 = 1/4|k_{0l}|$ is the lifetime. This gives an explicit but lengthy expression. For $N = 5$ and in the $k_{0l} \to 0$ limit, $x \lesssim 30\tau_0^2$.

From the previous discussion it might seem that a very long lifetime is always preferable to attain DIT. Nevertheless long lifetimes also imply a weaker signal because of the normalization. The consequence of opposite tendencies is an optimal lifetime-position point. A good measure of the visibility of DIT is the difference $\Delta$ between the second maximum and the previous minimum of the normalized probability density, see Fig. \[2\]. The optimal parameters are found to be $k_{0l} = -0.03$, $x = 60$.

**Model independence of the results.** We have described the close connection between DIT and resonance decay. DIT will occur when contributions from different resonances are well separated, which generally requires narrow and/or strong confinement. DIT does not depend on the specific properties of the model used so far. We have checked the robustness of DIT from exponential decay explicitly with several additional models. Winter’s decay model \[21\] describes the decay of the ground state of the square well between $-L$ and 0 when the right infinite wall is substituted by a $U\delta(x)$ potential. The wave function outside the trap tends to the source model wavefunction for large $U$ \[22\]. Moreover DIT does not depend dramatically on the strict confinement of the initial wave function on a finite domain. To show this we have calculated the decay of the ground state of a well with a finite right wall once this wall is substituted by the delta. This produces a different fast forerunner at $x$, but the part associated with the dominant, lowest energy resonance remains essentially stable showing DIT as for the infinite wall, see Fig. \[6\]. Moreover we have observed the same stability for finite-width barriers. DIT also survives a smooth source onset \[4\], and again may be observed after the passage of some onset-dependent transients. As for the effect of collisions, in the mean field regime DIT is enhanced for attractive interactions \[8\].

Let us finally point out the possibility to observe DIT in periodic structures \[9\] such as optical lattices, or other physical systems that realize a tight-binding model, for example periodic waveguide arrays that provide a classical, electric field analog of a quantum system with exponential decay \[22\].

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[1] M. Moshinsky, Phys. Rev. **88**, 625 (1952).
[2] C. Brukner and A. Zeilinger, Phys. Rev. A **56**, 3804 (1997).
[3] S. Godoy, Phys. Rev. A **67**, 012102 (2003).
[4] A. del Campo, J. G. Muga, M. Moshinsky, J. Phys. B **40**, 975 (2007).
[5] G. G. Paulus and D. Bauer, Lect. Notes Phys. **789**, 303 (2009).
[6] D. Schneble et al., J. Opt. Soc. Am. B **20**, 648 (2003).
[7] Th. Hils et al., Phys. Rev. A **58**, 4784 (1998).
[8] A. del Campo, G. García-Calderón and J. G. Muga, Phys. Rep. **476**, 1 (2009).
[9] G. Monsivais, M. Moshinsky, and G. Loyola, Phys. Scrip. **54**, 216 (1996).
[10] G. García-Calderón and J. Villavicencio, Phys. Rev. A **64**, 012107 (2001).
[11] M. Kleber, Phys. Rep. **236**, 331 (1994).
[12] P. Szriftgiser et al., Phys. Rev. Lett. **77**, 7 (1996).
[13] Y. Colombe et al., Phys. Rev. A **72**, 061601 (2005).
[14] S. Zamith et al., Phys. Rev. Lett. **87**, 033001 (2001).
[15] S. Godoy, Physica B **404**, 1826 (2009).
[16] V. Manko, M. Moshinsky, and A. Sharma, Phys. Rev. A **59**, 1809 (1999).
[17] S. R. Wilkinson et al., Nature **387**, 575 (1997).
[18] E. Torrontegui et al., Phys. Rev. A **80**, 012703 (2009).
[19] E. Torrontegui et al., Phys. Rev. A **81**, 042714 (2010).
[20] Y. Ban et al., arXiv:1008.3853.
[21] R. G. Winter, Phys. Rev. **123**, 1503 (1961).
[22] E. Torrontegui et al. Adv. Quant. Chem. **60**, 485 (2010).
[23] G. Della Valle et al., Appl. Phys. Lett. **90**, 261118 (2007).