Particle-wave duality in quantum tunneling of a bright soliton

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Abstract: One of the most fundamental difference between classical and quantum mechanics is observed in the particle tunneling through a localized potential: the former predicts a discontinuous transmission coefficient (T) as a function in incident velocity between one (complete penetration) and zero (complete reflection); while in the latter T always changes smoothly with a wave nature. Here we report a systematic study of the quantum tunneling property for a bright soliton, which behaves as a classical particle (wave) in the limit of small (large) incident velocity. In the intermediate regime, the classical and quantum properties are combined via a finite (but not full) discontinuity in the tunneling transmission coefficient. We demonstrate that the formation of a localized bound state is essential to describe such inelastic collisions, showing a nontrivial nonlinear effect on the quantum transportation of a bright soliton.

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Recently, with the easy realization of some experiments in the optical domain, there is a great deal of attention to unify concepts in physics. For example, the interplay between the interaction effect and disorder potential has long been an interesting subject in condensed matter physics, from Anderson localization in the noninteracting limit [1] to the Bose glass in the strongly interacting region [2]. Similar transport problem can also be investigated in the systems of nonlinear optics and ultracold atoms, where for the latter one Bose-Einstein condensates (BECs) are demonstrated to unify concepts in classical and quantum physics at a macroscopic scale [3]. Fermionic or bosonic particles with a tunable interaction strength can be studied in a well-controlled quasi-disordered potential [4]. In this context, solitons, localized wavepackets undergoing confinement owing to nonlinear effects [5, 6], become an ideal representative for the investigation in a macroscopic scale of the wave-particle duality which is one of the fundamental pillars in modern physics [7]. For example, a bright soliton (BS) resembles a classical particle in their collision properties [8], and should have a complete penetration or reflection predicted by classical mechanics, see Fig. 1(a). On the other hand, due to the underlying wave nature, a soliton should always reveal partial penetration and reflection as predicted in the quantum mechanics, see Fig. 1(b). Therefore, it is of both interest and fundamental importance to study how the nonlinearity (*i.e.*, the interaction effect between bosonic particles) can modify the quantum transportation properties of a BS and related transition between these two regimes [9, 10, 11].

Soliton tunneling [12, 13, 14, 15, 16, 17], *i.e.* scattering of a soliton off finite-size impurities, demonstrates the nonlinear dynamics of a wave packet colliding with a potential, and illustrates the link between classical and quantum mechanics. Apart from the existing literature on solitons moving in a defect [18, 19, 20, 21, 22], in this paper we investigate quantum tunneling

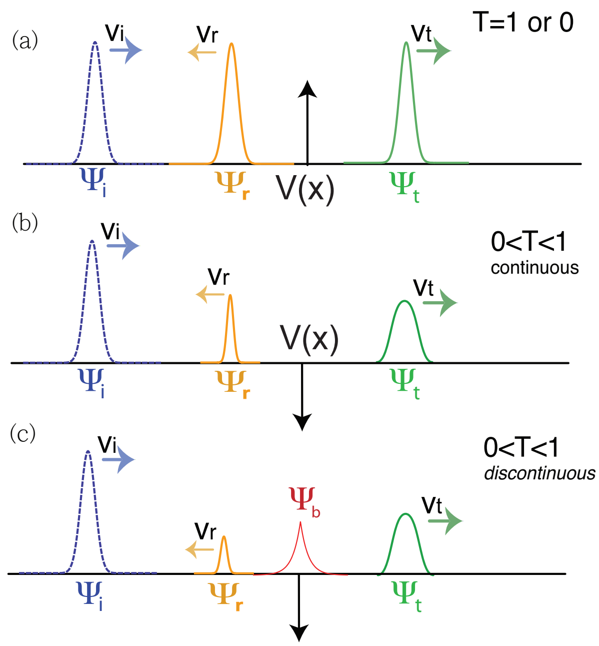

Fig. 1. Schematic plots for different tunneling dynamics through a local potential, $V(x)$. The incident, transmission, and reflection velocities are denoted as v_i, v_t, and v_r, respectively. (a) Classical picture with either a total transmission ($T = 1$) or total reflection ($T = 0$). (b) Quantum mechanical picture with a partial transmission ($0 < T < 1$). The notations, Ψ_i, Ψ_t, and Ψ_r represent the incident, transmitted, and reflected wavefunctions, respectively. (c) Inelastic scattering process of a BS through a potential well, $V(x) < 0$, where a localized bound state, Ψ_b, appears after scattering.

properties for a one-dimension (1D) BS in cases of both potential barrier and well, as a function of the initial soliton velocity. In particular this work demonstrates a full phase diagram of the transmission coefficient, in terms of the potential strength and initial velocity, and gives the analytical formula to explain the role of nonlinear interaction in the soliton tunneling. Through a systematic numerical simulation, we find that a BS is like a classical particle, as illustrated in Fig. 1(a), when the kinetic energy of an incident BS is smaller than the nonlinear interaction energy in a repulsive potential; while it behaves as an ordinary wave in the other limit and is independent of the sign of local potential, as illustrated in Fig. 1(b). In the intermediate regime, the nature of particle-wave dualism from a BS shows a discontinuity in the transmission coefficient (T) as a function of the incident velocity, while the amplitude of the discontinuity is less than one, as required by a true classical particle. We numerically calculate the full phase diagram in such a crossover regime, and observe a qualitative difference in the scattering process between a potential barrier and a potential well: the latter case is an inelastic scattering due to the appearance of a localized bound state, see Fig. 1(c). Semi-analytical curves for such a border are derived both for potential barriers as well as potential wells. The dual nature in quantum tunneling of a BS elucidated in this work should be ready to be observed in the system of ultracold atoms as well as in the dielectric material with electromagnetic waves.

Here, we consider the dynamics of a weakly interacting BEC at zero temperature, which can be well-approximated by the Gross-Pitaevskii equation, referred also as the nonlinear

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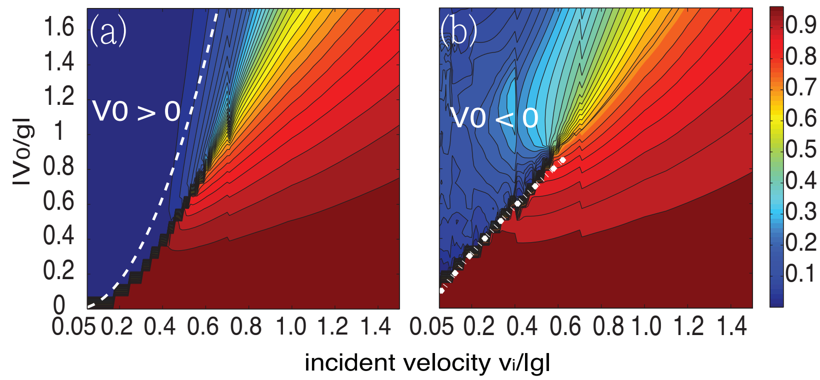

Fig. 2. Contour plot of the transmission coefficient as a function of incident soliton velocity v_i and potential strength $|V_0|$. Cases of potential barrier $V_0 > 0$ and potential well $V_0 < 0$ are separately shown in (a) and (b). White dashed lines are plotted from Eq. (4) and Eq. (9) for the corresponding analytical results (see the text).

Schrödinger equation (NLSE) [23],

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+g|\Psi(x,t)|^2+V(x)\right]\Psi(x,t)=i\frac{\partial}{\partial t}\Psi(x,t), \tag{1}$$

where the particle mass m and $\hbar$ are both set to 1, $\Psi(x,t)$ represents the condensate wavefunction, g measures the inter-particle interaction, and $V(x) = V_0\delta(x)$ indicates a defect potential. When the interaction is attractive, $g < 0$, a stable bright soliton is supported in a uniform system with the solution [5]

$$\Psi_{\rm bs}(x,t)=\frac{\beta}{\sqrt{|g|}}\text{sech}\left[\beta(x-x_c-v_i t)\right]e^{i\theta(x,t)}, \tag{2}$$

where the center of the wavepacket is denoted by x_c, and $\theta(x,t) \equiv v_i x - Et$, with the total energy $E \equiv v_i^2/2+\mu$ and the chemical potential $\mu = -\beta^2/2$, respectively. The velocity for a BS is characterized by v_i. For 1D solitons, the free parameter is β, which can be set to unit with the normalization condition by taking $\beta = |g|/2$, *i.e.*, $\int_{-\infty}^{\infty}|\Psi_{\rm bs}(x,t)|^2\,dx = 2\beta/|g| = 1$. In this case, the only two independent parameters left are the normalized potential strength, $\tilde{V}_0 \equiv V_0/|g|$, and the normalized initial velocity, $\tilde{v}_i \equiv v_i/|g|$, which define our parameter space. In the following, we consider the transportation process when such a BS wavepacket is generated at $t = 0$, centered at $x_c \to -\infty$, and then propagates along the positive x-axis with an initial velocity v_i. This wavepacket then scatters the local defect $V(x)$ at the position $x = 0$, resulting in possible transmitted, reflected, and localized wave functions after a certain time measured.

First of all, the calculated transmission coefficient (T) as a function of v_i and $V_0 > 0$ for a repulsive potential is illustrated in Fig. 2(a) by directly solving Eq. (1) numerically. Here, T is defined as $\equiv \int_a^{\infty}\lim_{t\to\infty}|\Psi(x,t)|^2\,dx$ with a small value $a > 0$ to exclude the contribution from any possible localized bound states. As one can see from Fig. 2(a), in the region with a small value of v_i and $|V_0|$, there exists a line that characterizes the discontinuity in the transmission coefficient. The existence of such a discontinuity certainly reflects the particle nature of a BS, *i.e.*, totally transmitted ($T = 1$) or totally reflected ($T = 0$) as shown in Fig. 1(a). However, this line of border for the particle nature breaks down at a critical point in the parameter space where the incident velocity and corresponding potential strength are denoted by $\tilde{v}_i^* \sim 0.8$ and

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$|\tilde{V}_0^*| \sim 1.2$. Beyond these values, instead of a disrupt change, the contours of transmission coefficient T changes continuously as a regular wave.

On the contrary, in Fig. 2(b), the tunneling properties are different for a BS through an attractive potential ($V_0 < 0$, a potential well). Qualitatively speaking, we have a similar "phase diagram" as the case of a potential barrier, but now the *phase boundary*, the while dashed curve, becomes a nearly linear line. As it would be demonstrated later, at a small value of V_0, such a universal border, independent from any additional parameters, comes from the existence of a localized bound state. The formation of this localized bound state screens the potential well and results in extra interactions on the quantum tunneling of a BS.

In order to give a deeper understanding of these numerical results, we consider the limit of a weak nonlinear interaction for the first step. When the interaction energy is much smaller than the kinetic energy and potential energy, the corresponding transmission coefficient should be similar to that in the standard quantum mechanics textbook [7], *i.e.*,

$$T \approx \frac{(v_i/V_0)^2}{1+(v_i/V_0)^2} + O(\frac{1}{v_i^2}). \tag{3}$$

As expected for a characteristic wave nature, the transmission coefficient T is always continuous and independent of the sign of potential strength, V_0. We note that above results are true both for incident waves in the form of a soliton wavepacket and a plane wave. In such a scenario, the incident BS can be easily distorted by the local potential due to that the nonlinearity is too weak to support the original soliton solution, resulting in a lots of dispersive radiations in the transmitted or reflected waves [24].

On the other hand, in the limit of a weak and repulsive potential along with a small velocity, *i.e.*, the strong interaction limit, we can safely assume that the propagating soliton is not affected by the potential. Hence, one can use the center position of a BS, $x_c(t)$, to describe the whole transportation process if there is no bound state generated during the scattering process. In this limit, one can rigorously show that the dynamics of $x_c(t)$ behaves like a classical particle moving effectively in a conservative potential, $V_{\text{eff}}(x)$, which is just a convolution of the local potential with the soliton wavefunction [25], *i.e.*, $V_{\text{eff}}(x) = \frac{\beta^2}{2|g|} V_0 \,\text{sech}^2(x)$. Therefore, the corresponding "conservation law" for the total energy is found to be,

$$v(t)^2 + \frac{\beta^2}{|g|^2} V_0 \,\text{sech}^2[x_c(t)] = v_i^2 + \frac{\beta^2}{|g|^2} V_0 \,\text{sech}^2(x_i), \tag{4}$$

where $v(t) \equiv \frac{1}{|g|}\frac{dx_c(t)}{dt}$ is the defined particle velocity for a BS. As a result, the border across the regions with $T = 1$ and $T = 0$ can be defined by taking $v(t) = 0$ and $x_c = 0$ as the boundary condition, along with the initial condition $x_i \to -\infty$. Then, we obtain the relation $V_0/|g| = (|g|/\beta)^2(v_i/|g|)^2 = 4(v_i/|g|)^2$, which is depicted as the white dashed line in Fig. 2(a).

However, we know that above semi-classical approach used for Eq. (4) fails when V_0 is larger than a critical value, denoted as V_0^* due to the failure of taking the BS as a classical particle. This critical value can be estimated as following: as the center of a BS reaches the location of a potential, it gains a local potential energy, $V_0|\Psi(0)|^2$, which cannot be larger than the absolute value of the chemical potential, $|\mu| = \beta^2/2 = |g|^2/8$, in order to keep the soliton description valid. From Eq. (2), the critical value for the breakdown is $V_0^*/|g| = 0.5$. In Fig. 2(a), the agreement between the analytical curve defined by Eq. (4) and our direct numerical simulations is good both qualitatively and quantitatively. When V_0 is close to V_0^*, the BS is in the brink of collapsing, then the reflection part as well as the non-soliton radiation become non-negligible. Discrepancies from above analytical results are therefore expected.

Now we come to the potential well, which should have similar results as the potential barrier in the limit of large V_0 and v_i (the wave nature in the weak interaction limit). However,

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in the regime of small V_0 and v_i, the wavepacket description used above fails for the lack in the consideration of possible localized bound states supported in an attractive interaction. The appearance of a localized bound state indicates extra inelastic scatterings. Therefore, the resulting tunneling amplitude changes dramatically, as compared to the case of a potential barrier. The bound state wavefunction for a localized potential has been well-studied in the literature [26, 27, 28, 29], and its analytic form can be written as following:

$$\Psi_b(x) = \frac{\beta_b}{\sqrt{|g|}} \text{sech}(\beta_b |x| + x_b), \tag{5}$$

where β_b measures the slope (the inverse of soliton width) and amplitude of the bound state, and $x_b \equiv \tanh^{-1}(|V_0|/\beta_b)$ is the shift of effective peak position from the potential center. It is easy to see that the bound state wavefunction is composed of two soliton-like solutions, but with different center positions and β. By matching the discontinuity in the wavefunction slopes with the potential strength, for a given renormalization of the bound state, *i.e.*, β_b is fixed, such bound states exist only in a weak potential limit and disappears when $|V_0| > \beta_b$. Such an anti-intuitive result originates from the fact that the maximum slope of a BS is limited by its renormalization due to the nonlinear (interaction) effect. Although the localized bound state also exists in a repulsive potential defect, it cannot be easily produced in the tunneling process due to the mismatch in the boundary conditions. Therefore it does not affect the tunneling property as we discussed above.

Inspired by the numerical simulations of the tunneling process (not shown here), we consider the following simplified picture of tunneling dynamics in the presence of a bound state, *i.e.*, inelastic scattering. To derive an analytical formula for the border when a soliton scatters by a potential well, we assume: (i) the reflected wavefunction is negligible, (ii) the bound state appears after the scattering, and (iii) the transmitted wave also has a soliton profile. Since both the soliton solution and the localized bound state are governed by two parameters, β and v, as shown in Eq. (2), the relevant parameters to describe a soliton tunneling are therefore: (β_i, v_i) for the incident soliton, (β_t, v_t) for the transmitted one, and $(\beta_b, v_b = 0)$ for the localized bound state. Since v_i is given and $\beta_i \equiv |g|/2$ is required for the initial unit normalization, now we only have three parameters to be determined: β_b, β_t, and v_t.

Instead of matching the boundary of wavefunctions during the scattering process, we use the conservation laws to extract these three unknown parameters in a more general method. Based on the above three assumptions, we can write down three equations:

$$\frac{2\beta_i}{|g|} = 1 = \frac{2}{|g|}(\beta_b - |V_0|) + T, \tag{6}$$

$$-\frac{\beta_i^2}{2} + \frac{v_i^2}{2} = \frac{-\beta_b^2}{2}(1-T) + \left(\frac{-\beta_t^2}{2} + \frac{v_t^2}{2}\right) T, \tag{7}$$

$$v_i = \frac{2\beta_t}{|g|} v_t = T v_t \tag{8}$$

where we have expressed the transmission coefficient $2\beta_t/|g|$ as a function of T via the assumption (iii). Equations (6) and (7) represent the conservations of total probability and total energy by including both the localized bound state and the transmitted soliton. Equation (8) can be understood as the conservation of current density due to the change of soliton amplitude. We note that the condition $|V_0| < \beta_b$ is required, in order to have $T > 0$ in Eq. (6). By eliminating the other two variables, one can obtain T as a function of the normalized potential strength

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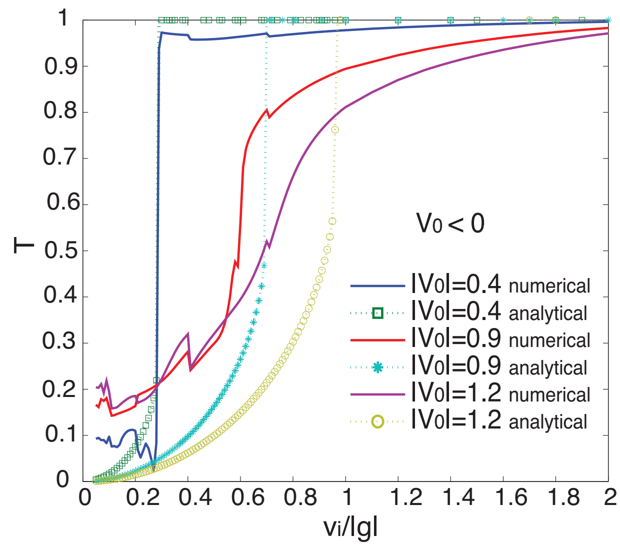

Fig. 3. A comparison of transmission coefficient between numerical simulations (solid lines) and analytical results from Eq. (9) (dashed points). Note that the parameters are the same as those used in Fig. 2(b).

$\tilde{V}_0 \equiv |V_0/g|$ and the normalized initial velocity $\tilde{v}_i \equiv v_i/|g|$,

$$T = \frac{\tilde{V}_0(\tilde{V}_0+1) \mp \sqrt{\tilde{V}_0^2(\tilde{V}_0+1)^2 - (4\tilde{v}_i^2\tilde{V}_0 + 3\tilde{v}_i^2)}}{2\tilde{V}_0 + 3/2}, \tag{9}$$

where the “+” solution is physically invalid. From Eq. (9), we find several interesting properties in the tunneling of a BS through the potential well. First of all, above solution for the transmission coefficient is real only when $|\tilde{V}_0|^2(|\tilde{V}_0|+1)^2 - (4\tilde{v}_i^2|\tilde{V}_0| + 3\tilde{v}_i^2) \geq 0$, or when v_i is smaller than a critical velocity, $v_c(|V_0|)$, *i.e.*,

$$\frac{v_c}{|g|} \equiv \frac{|V_0/g|\,(|V_0/g|+1)}{\sqrt{3+4|V_0/g|}}, \tag{10}$$

where V_0 and v_i has to be bounded by requiring $T < 1$. In Fig. 2(b), the border for the discontinuity in the transmission coefficient is compared with our analytical formula and direct numerical simulations, which results in very good agreement. More importantly, we find that the critical velocity defined in Eq. (10), *i.e.*, the curve for the discontinuous transmission coefficient, shows a rather straight line (although is not exact), instead of a parabolic one for the potential barrier. Now the major contributions come from the existence of a localized bound state in this inelastic scattering process.

The validity of our assumptions used above is totally based on the ”soliton-in” and ”soliton-out” picture, alone with the condition that the formed bound state also has a soliton profile. Although our simplified theory does predict the locations of transition, in Fig. 3 the transmission coefficient T we obtained in Eq. (9) is slightly less than the values obtained by direct numerical simulations. The discrepancy between analytical and numerical data is not surprising because we have neglected the radiation parts (non-soliton waves) in the transmitted waves, which cannot be captured in such a simple theory. It should be remarked that the discontinuity

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in the transmission coefficient, the spikes, comes from our numerical errors due to the choice of different grid sizes in simulations. Last but not least, we restate that the estimations we made here for the tunneling dynamics of a potential well cannot be applied to the potential barrier, because the bound state wavefunction supported by a potential barrier has to be a double-humped one in the profile due to a mismatching boundary condition. On the side of wave nature, the transmission coefficient is identical both for potential well and potential barrier when one considers a regular (noninteracting) wave tunneling, but on the side of particle nature, it turns out to be very different in the classical particle picture. This also reflects the non-trivial effect of interaction (nonlinearity) in the soliton scattering problem.

In conclusion, we have systematically studied the tunneling of a bright soliton subjecting to a localized potential defect. By performing direct numerical simulations, we obtain a full phase diagram of the transmission coefficient in terms of the incident velocity and potential strength. Our results show a fundamentally important transport property, which can be easily observed in ultracold atoms, nonlinear optics, or even soft-matter systems.

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