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Transmission resonances in reflection of Bose-condensates by a symmetric rectangular double-barrier potential

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Abstract. Within the framework of the mean-field Gross-Pitaevskii approximation, we investigate the transmission resonances in quantum above-barrier reflection of Bose-Einstein condensates by a symmetric rectangular double-barrier (double-well). We present a rigorous analysis of the problem based on an exact third order nonlinear differential equation written for the probability density. We show that in general the set of transmission resonances is split into two series of distinct nature. One subset of resonances occurs in the case when the single barrier itself supports a resonance. In this case, the separation distance between the two barriers does not play a role: the transmission is always resonant for any distance between the two involved barriers. Another subset corresponds to the case when the single barrier itself does not support resonance transmission. We show that in this case there exists an infinite set of periodically located separation distances between the two barriers that support complete transmission of the condensate across the double-barrier potential.

Keywords: Gross-Pitaevskii equation, above-barrier reflection, resonance transmission, quantum tunneling

1. Introduction

In 2005 the quasi-continuous flow [1-2] of Bose-condensed atoms [3-5] was realized experimentally. In the mean-field regime, the dynamics of Bose-condensates is described by the Gross-Pitaevskii equation, which in the one-dimensional case is written as [6-8]

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+(V(x)+g\left|\Psi\right|^2)\Psi=0\,. \tag{1}$$

Here, the nonlinearity parameter g determining the mean-field self-interaction is given through the s-wave scattering length a_s for binary elastic collisions of two interacting bosons of mass m as $g=4\pi\hbar^2a_s/m$, and $V(x)$ is the external field's potential. The nonlinearity parameter may be negative or positive, corresponding to attractive or repulsive atomic interactions respectively.

In the present paper, we consider the quantum transmission of Bose-condensates above a symmetric double-barrier potential. Though the repulsive interactions are more common in experimental condensates, our treatment is applicable to both repulsive and attractive cases. The reflecting potential we consider consists of two identical finite-height/depth rectangular barriers/wells of width a which are separated by distance b, that is, we assume that $V(x)=V_0$, where V_0 is a positive or negative constant, if $x\in[0,a]\cup[a+b,a+b+a]$ and $V(x)=0$ elsewhere (Fig.1):

$$V(x)=\begin{cases}V_0 \text{ if } x\in[0,a] \text{ or } x\in[a+b,a+b+a]\\ 0 \text{ elsewhere}\end{cases} \tag{2}$$

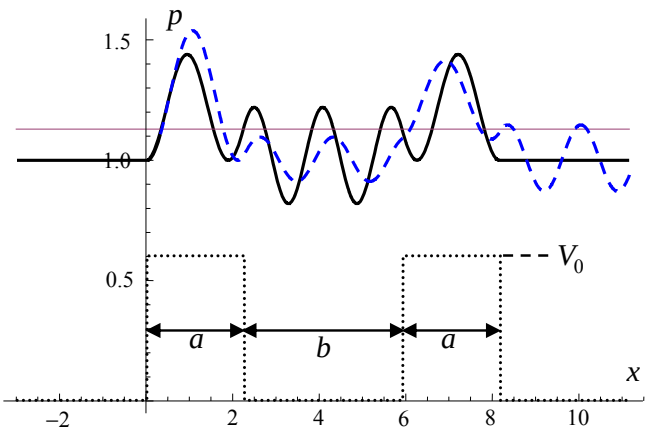

Fig.1. Transport of a Bose-Einstein condensate across two rectangular barriers of width $a = 2.25$ and height $V_0 = 0.6$ (dotted line) separated by distance $b = 3.66432$ at $g = 0.02$ under resonance ($\mu = 2$, solid line) and non-resonance ($\mu = 1.75$, dashed line) conditions.

2. Single barrier case

Applying the ansatz $\Psi(x,t) = \exp(-i\mu t/\hbar)\psi(x)$, where μ is the chemical potential for a conserved number of particles, equation (1) is reduced to the following stationary version

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + (-\mu + V(x) + g|\psi|^2)\psi = 0 \tag{3}$$

(we use the units $\hbar = m = 1$). Applying further the transformation $\psi(x) \sim \sqrt{p}e^{i\theta(x)}$, one can show that the probability density $p = |\psi(x)|^2$ obeys the following exact third order nonlinear differential equation [9]

$$\frac{d}{dx}\left[-\frac{p''}{4} + (-\mu + V + g\,p)p\right] + (-\mu + V + g\,p)p' = 0, \tag{4}$$

where the prime denotes differentiation with respect to x. Since we look for a solution with traveling-wave-like asymptotic behavior $\psi(-\infty) \sim \sqrt{\rho_0}e^{ikx}$, $k = \sqrt{2(\mu - g\rho_0)}$, the function $p(x)$ obeys the initial conditions

$$p(-\infty) = \rho_0, \quad p'(-\infty) = 0, \quad p''(-\infty) = 0. \tag{5}$$

Since it follows from the Gross-Pitaevskii equation that the normalization of the wave

function can always be incorporated into the definition of the nonlinearity coefficient g, without loss of generality we choose the normalization $\rho_0 = 1$ so that we assume $p(-\infty) = 1$. The boundary condition for reflectionless transmission through the barrier then reads

$$p(+\infty) = 1. \tag{6}$$

Note that this condition defines a nonlinear eigenvalue problem for equation (4).

Consider the solution of equation (4) in the region $x \in [0, a]$. For a constant V_0, the equation is twice integrated to produce the following first order equation

$$\frac{1}{8}\left(\frac{dp}{dx}\right)^2 = \left((-\mu + V_0)p^2 + \frac{g}{2}p^3\right) + C_1 p + C_0. \tag{7}$$

Examination of the initial conditions at $x = 0$ shows that $p(0) = 1$, $p'(0) = 0$, $p''(0) = 4V_0$. Then, in order to match the solution of equation (7) with $\psi = e^{ikx}$ which is valid for $x \le 0$, one should choose

$$C_{0a} = g - \mu \quad \text{and} \quad C_{1a} = -\frac{3g}{2} - V_0 + 2\mu. \tag{8}$$

Equation (7) is then rewritten as

$$\left(\frac{dp}{dx}\right)^2 = 4(1-p)\left(-k^2 + [k_a^2 + g(1-p)]p\right), \tag{9}$$

where $k_a = \sqrt{2(\mu - g - V_0)}$. Applying now the transformation $p = 1 + e_{1a}u(bx)^2$ with $b = \sqrt{g e_{2a}}$ for $g > 0$ (repulsive interaction), this equation is straightforwardly reduced to the equation obeyed by the Jacobi elliptic sn function [10]:

$$u'^2 = (1-u^2)(1-mu^2) \tag{10}$$

with $$m_a = \frac{e_{1a}}{e_{2a}}, \quad e_{1a,2a} = \frac{k_a^2 - g \mp \sqrt{(k_a^2+g)^2 - 4gk^2}}{2g}. \tag{11}$$

Accordingly, the solution of the problem in the region $x \in [0, a]$ is written as

$$p_a = 1 + e_{1a}\left(sn\left[\sqrt{g e_{2a}}\,x, \frac{e_{1a}}{e_{2a}}\right]\right)^2. \tag{12}$$

This is a periodic function with the period given in terms of the Gauss ordinary hypergeometric function ${}_2F_1$ as

$$T_a = \frac{\pi}{\sqrt{ge_{2a}}}\,{}_2F_1(1/2,1/2;1;m_a)\,. \tag{13}$$

Reflectionless transmission occurs if $p(a) = p(+\infty) = 1$. The derived solution (12) shows that this condition is fulfilled if

$$a = nT_a\,, \quad n = 1,2,3,... \tag{14}$$

In the linear limit $g = 0$ the period of the solution becomes $T_{a0} = \pi / k_a = \pi / \sqrt{2(\mu - V_0)}$ so that for the linear resonances we have the known result [11]

$$V_{Ln}(g=0) = \mu - \frac{\pi^2 n^2}{2a^2}\,. \tag{15}$$

In the nonlinear case $g \neq 0$, equation (14) is a complicated transcendental equation with no known exact solution. However, one may try to construct a simple approximation applying a power series expansion [12,13] for relatively small nonlinearity parameter g. In this way, one obtains the following approximation for the nonlinear shift of the resonance position

$$V_{NLn} - V_{Ln}(g=0) = -\frac{3g}{4}\left(1 + \frac{k^2a^2}{\pi^2 n^2}\right). \tag{16}$$

This formula confirms our previous result derived by applying a different approach [14].

In the region $x > a$ applies the same equation (7), where now one should replace V_0 by 0 and apply the initial conditions $p(a) = p_a(a)$, $p'(a) = p'_a(a)$ and $p''(a) = p''_a(a)$. Using equations (7) and (12), after some straightforward algebra, one obtains that the integration constants C_0 and C_1 in this case read

$$C_{0b} = C_{0a} \quad \text{and} \quad C_{1b} = C_{1a} + V_0 p_a\,, \tag{17}$$

where C_{0a} and C_{1a} are defined by equations (8). This leads to the following equation for the dynamics in the region $x > a$:

$$\left(\frac{dp}{dx}\right)^2 = 4(1-p)^2\left(-k^2 + gp\right) - 8V_0(1-p_a)p\,. \tag{18}$$

The general solution to this equation is again written in terms of the Jacobi elliptic sn function. Let $p_{0,1,2}$ are the three roots of the cubic polynomial equation defined by the right-hand side of equation (18) so that the equation is rewritten as

$$\left(\frac{dp}{dx}\right)^2 = 4g(p-p_0)(p-p_1)(p-p_2)\,. \tag{19}$$

Let p_0 is the smallest positive root and $|p_1|<|p_2|$. Then for positive $g>0$ the solution $p_b(x)$ of the equation for $x>a$ is written as

$$p_b = p_0 + e_{1b}\left(sn\left[\sqrt{g e_{2b}}(x-x0), m_b\right]\right)^2 \tag{20}$$

with

$$m_b = \frac{e_{1b}}{e_{2b}}, \quad e_{1b} = p_1 - p_0, \quad e_{2b} = p_2 - p_0\,. \tag{21}$$

equation (20) defines an oscillatory, periodic function with the period given as

$$T_b = \frac{\pi}{\sqrt{g e_{2b}}}\,{}_2F_1(1/2,1/2;1;m_b)\,. \tag{22}$$

Since the amplitude of oscillations is given by e_{1b}, it is understood that transmission resonances occur if $e_{1b}=0$. Since, additionally, should be $p_0=1$, we see that resonances occur when $p_0=p_1=1$, that is when the cubic polynomial equation defined by the right-hand side of equation (18) has a multiple root equal to 1. Because then the solution for the whole region $x>a$ is $p(x>a)\equiv 1$, it is seen from equation (18) that should be $p_a=1$ and this is a necessary condition.

3. Double-barrier case

Now, let us add a *second barrier*. If a single barrier itself supports a resonance, then, obviously, double barrier will do so (irrespective of the distance between the barriers). This is the first subset of resonances, since one barrier can support a resonance for different heights (approximately given by equation (16)).

However there exists another subset, corresponding to the case when a single barrier itself reflects the incident matter-wave but with a right choice of the distance between them one arrives to the complete transparency of the double barrier. Since the barrier is symmetric, a solution for the probability density, corresponding to the total transmission resonance should be symmetric too, and this means that at the points $x=a$ and $x=a+b$ the probability density of the condensate should have the same value. Thus,

$$b = T_a(n+1/2), \quad n=1,2,3,... \tag{23}$$

For a fixed set of parameters of the problem (barrier width a, nonlinearity parameter g, chemical potential μ and barrier height V_0) T_a is a constant which means that there exists an infinite set of periodically located separation distances between the two barriers that support total transmission of the condensate across the double-barrier potential.

Extending this result to the case of multiple identical rectangular barriers, we note that if a single barrier supports a total transmission resonance, then the composite potential will do the same. However, if a single barrier is not of the resonant height, the composite barrier will support a resonance only if it consists of even number of barriers (of course, provided the distance between them is chosen according to equation (23)). In the case of odd number of barriers, if the distance is well chosen, the whole construct will scatter the incident matter-wave (atomic laser) as an effective single barrier.

4. Conclusion

Thus, we have presented the exact solution of the Gross-Pitaevskii equation for matter-wave propagation above a symmetric double-rectangular barrier written in terms of the Jacobi elliptic functions. We have shown that there exist two distinct series of above-barrier transmission resonances. First, if a single barrier itself produces zero reflection, the set of two such barriers will also provide a transmission resonance. However, even if one rectangular barrier itself is not of resonant height, the addition of a second one, put on a certain distance, may result in a total transmission. This may be used, in particular, to recover the information distorted by the action of a scattering barrier, via adding a second barrier of the same form.

The presented observations may concern to other situations of the dynamics of a quantum many-body system in a double-barrier potential, for instance, π-electron transport in a single-wall carbon nanotube with two point impurities (say, non-carbon atoms). Indeed, the self-interaction of such electrons is described by the Gross-Pitaevskii-type mean-field approximation and point impurities in a single-wall carbon nanotube serve as scattering centers for the electrons. Charge carriers in 1D are confined to a single trajectory and cannot avoid the scattering centers nor scatter into nearby momentum states. The interest in properties of such non-ideal nanotubes is due to their applications, e.g., as one-electron transistors that work at room temperature or as chemical sensors [15]. For other possible applications, one may further discuss the above-barrier reflection with a periodic potential as a generalization of the symmetric double rectangular barrier discussed in the present paper.

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