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Resonant reflection of a Bose–Einstein condensate by a double barrier within the Gross–Pitaevskii equation

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Abstract
Resonant reflection of a Bose–Einstein condensate by a double delta-function barrier has been considered analytically using the Gross–Pitaevskii approximation for nonlinearity. The reflecting coefficient has been derived taking into account a weak nonlinearity of the Schrödinger equation produced by the interaction between cold alkali atoms. A nonlinear term is given in the Hartree approximation for short-range interaction between atoms. The one-dimensional potential is approximated by two repulsive delta-function barriers. The analytical solution was obtained for the reflecting coefficient by a multiple-scale method in order to remove secular terms. The most interesting case corresponds to the condensate energies for which reflection is absent without a nonlinear term. Thus, reflection is determined only by the nonlinearity. The reflecting coefficient is derived in the first order on the nonlinearity parameter.

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1. Introduction

Only in a few cases with the simplest one-dimensional potentials, like a rectangular barrier, or the Rosen–Morse potential, the Schrödinger equation can be solved exactly. In most cases, exact solutions are difficult to obtain not only because of the presence of an external field, but also due to the interaction between particles. The most direct generalization of the single-particle case is a tunneling of the mean field through a barrier in the Gross–Pitaevskii or nonlinear Schrödinger equation [1]. We emphasize that this is a nonlinear tunneling problem in the mean-field approximation. From the theoretical point of view, the main complication in the description of a quasi-stationary scattering process of particles obviously comes from the presence of atom–atom interaction. In leading order, the effect of this interaction is included in a nonlinear term in the Schrödinger-like Gross–Pitaevskii equation for wave function, using the Hartree self-consistent approximation with zero range interaction between atoms. The dynamics of solutions of this equation is very complex and rich. In [2] we considered the above barrier reflection of cold atoms by resonant laser light within the Gross–Pitaevskii approximation. In [3] resonance reflection by the one-dimensional Rosen–Morse potential well in the Gross–Pitaevskii problem was considered by us using the multiple-scale analysis [4].

In [5] the double delta-shell potential was investigated numerically:

$$V(x) = \begin{cases} \infty, & x < 0, \\ \kappa_1\delta(x-a) + \kappa_2\delta(x-b), & x > 0. \end{cases}$$

This potential consists of an infinitely high wall and two repulsive delta barriers. The resonance states and the decay dynamics of the nonlinear Schrödinger equation for a double delta-shell potential were analyzed. The stability of the first excited state of one-dimensional Bose–Einstein condensates in a double well potential was studied by Ichihara [6]. From the excitation spectrum, they determined the critical barrier height, above which the excited state is dynamically unstable. They also found that the critical barrier height decreases monotonically as the number of condensate atoms increases. Their simulation results show that the condensate density notch in the dynamically unstable region develops a large-amplitude oscillation; this behavior is significantly different from that in the dynamically stable region.

The nonlinear transport of Bose–Einstein condensates in a double barrier potential was considered numerically also in [7]. It was shown that the transport of Bose–Einstein condensed atoms in this system is a stable nonlinear transport. The analytical perturbation solution of the BEC system was obtained by using the direct perturbation technique.

2. A multiple-scale analysis

Our theoretical approach is based on a multiple-scale method for a one-dimensional stationary Gross–Pitaevskii equation:

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

with the potential

$$V(x)=\kappa\delta(x)+\kappa\delta(x-a).$$

The system of units $\hbar=m=\kappa=1$ is used here and hereafter for the sake of simplicity. The chemical potential can be presented as $\mu=p^2/2$, where p is a momentum. The potential $V(x)$ allows us to obtain an analytic solution when $g=0$. We consider the most interesting case when in the corresponding linear problem ($g=0$) total transmission occurs. It should be noted that this effect does not take place in the case of one delta barrier potential. Then the momentum p is determined from a transcendent equation

$$\tan pa=-p. \tag{2}$$

Let us consider now the nonlinear equation (1). Its solution at $x>a$ can be chosen as only a transmitting wave. In the first approximation with respect to the small dimensionless nonlinear parameter

$$\alpha=\frac{g}{\mu}\ll 1,$$

one obtains that the wave function can be written in the form

$$\psi(x)=-(1+\alpha d)\exp[-2\mathrm{i}pa+\mathrm{i}px(1-\alpha/2)]. \tag{3}$$

The quantity d should be determined using the boundary conditions for wave functions and their first derivatives. When the nonlinearity is absent, the simple solution of the corresponding linear problem follows from (3).

Let us introduce a new independent variable $y=px$. In the region $0<x<a$, the Gross–Pitaevskii equation (1) is of the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}y^2}+\psi=\alpha|\psi|^2\psi. \tag{4}$$

The multiple-scale analysis is one of the versions of perturbation theory [4]. Let us introduce further new independent variables

$$y_1=y,\quad y_2=\alpha y,\quad y_3=\alpha^2 y\ldots.$$

Then

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}y^2}=\frac{\partial^2\psi}{\partial y_1^2}+2\frac{\partial^2\psi}{\partial y_1\partial y_2}+\cdots.$$

In the first approximation one obtains

$$\psi_1(y_1,y_2)=B(y_2)\exp(\mathrm{i}y_1)+C(y_2)\exp(-\mathrm{i}y_1).$$

In the second approximation we find the equation

$$\frac{\partial^2\psi_2}{\partial y_1^2}+\psi_2=|\psi_1|^2\psi_1-2\frac{\partial^2\psi_1}{\partial y_1\partial y_2}.$$

According to the multi-scale analysis, secular terms on the right part of this equation, which are proportional to $\exp(\pm y_1)$, should be neglected. Then the wave function in the region $0<x<a$ takes the form (taking into account terms of zero and first approximation on the nonlinear parameter)

$$\psi(x)=(1-\mathrm{i}/p+\alpha b)\exp(\mathrm{i}k_1x)+(\mathrm{i}/p+\alpha c)\exp(-\mathrm{i}k_2x)$$
$$+\frac{\mathrm{i}\alpha}{8p}\left(1-\frac{\mathrm{i}}{p}\right)^2\exp(3\mathrm{i}px)+\frac{\alpha}{8p^2}\left(1+\frac{\mathrm{i}}{p}\right)\exp(-3\mathrm{i}px). \tag{5}$$

Here the following notations are introduced:

$$k_1=p\left[1-\frac{\alpha}{2}\left(1+\frac{3}{p^2}\right)\right],$$
$$k_2=p\left[1-\alpha\left(1+\frac{3}{2p^2}\right)\right].$$

The quantities b and c should be determined from the boundary conditions for wave functions and their first derivatives. Third harmonics in (5) follows from nonlinearity of the Gross–Pitaevskii equation. When the nonlinearity is absent, the well-known solution of the linear problem follows from (5).

Analogously we consider the region $x<0$. The wave function in this region contains both incident and reflecting waves:

$$\psi(x)=\exp(\mathrm{i}k_3x)+\alpha f\exp(-\mathrm{i}px). \tag{6}$$

Here $k_3=p(1-\alpha/2)$.

The quantity f should also be determined from the boundary conditions for wave functions and their first derivatives. Then the small reflecting coefficient R is determined only by the nonlinearity:

$$R=\alpha^2|f|^2\ll 1.$$

The matching conditions for wave functions (3), (5) and (6) are of the form

$$\psi(+0)=\psi(-0),$$
$$\psi(a+0)=\psi(a-0).$$

Substituting the wave functions (3), (5) and (6), one obtains (for the sake of simplicity we consider further only the case $a=1$)

$$f-b-c=\frac{\mathrm{i}}{p}+\frac{3}{8p^2},$$
$$b\exp(\mathrm{i}p)+c\exp(-\mathrm{i}p)+d\exp(-\mathrm{i}p)=a_1,$$
$$a_1=3\left(1+\frac{1}{p^2}\right)\left(1+\mathrm{i}\frac{p}{2}\right)\cos p$$
$$-\frac{3+\mathrm{i}p}{8p^2}\cos 3p+\frac{1}{8p^2}\left(p-\frac{2}{p}-\mathrm{i}\right)\sin 3p. \tag{7}$$

The matching conditions for the first derivatives of wave functions are of the form

$$-\tfrac{1}{2}[\psi'(+0)-\psi'(-0)]+\psi(0)=0,$$
$$-\tfrac{1}{2}[\psi'(a+0)-\psi'(a-0)]+\psi(a)=0.$$

Substituting the wave functions (3), (5) and (6), one obtains (for the sake of simplicity we again consider only the case $a=1$)

$$b-c+\left(1+\frac{2\mathrm{i}}{p}\right)f=\frac{9}{8p^2}-\frac{9\mathrm{i}}{4p^3}-\frac{15\mathrm{i}}{8p},$$
$$b\exp(\mathrm{i}p)-c\exp(-\mathrm{i}p)+\left(1+\frac{2\mathrm{i}}{p}\right)d\exp(-\mathrm{i}p)=a_2,$$
$$a_2=-\left(\frac{\mathrm{i}}{2p}+\frac{\mathrm{i}p}{2}+p^2+\frac{3}{2}+\frac{3}{2p^2}\right)\cos p$$
$$+\left(\frac{3\mathrm{i}}{4p^3}-\frac{3\mathrm{i}}{8p}-\frac{3}{8p^2}\right)\cos 3p+\left(\frac{3}{8p}-\frac{9\mathrm{i}}{8p^2}\right)\sin 3p. \tag{8}$$

The solution of four algebraic equations (7) and (8) for the four quantities f, b, c and d is elementary though sufficiently cumbersome. According to (2) one obtains, for example, the first root $p=2.0287$ when $a=1$. Then the reflecting coefficient is

$$R=\alpha^2|f|^2=11.6\alpha^2. \tag{9}$$

Thus, because of the large numerical factor in (9) even a small nonlinearity can produce significant reflection under the condition that the total transmission takes place without nonlinearity.

3. Conclusion

In conclusion, some comments can be made with respect to the definition of the reflecting coefficient in nonlinear problems. The coherent flow of a Bose–Einstein condensate through a quantum dot in a magnetic waveguide was studied in [8]. By numerical integration of the time-dependent Gross–Pitaevskii equation in the presence of a source term, Paul *et al* simulated the propagation process of the Bose–Einstein condensate through a double barrier potential in the waveguide. They found that resonant transport is suppressed in interaction-induced regimes of bistability, where multiple scattering states exist at the same chemical potential and the same incident current. They demonstrated, however, that a temporal control of the external potential can be used to circumvent this limitation and to obtain enhanced transmission near the resonance on experimentally realistic time scales. Our multi-scale analysis allows us to consider these effects analytically.

It should be noted that our simple approach is valid only when the nonlinearity parameter is small. When this parameter is large, terms of the form

$$e_3\exp(3\mathrm{i}px),\quad f_3\exp(-3\mathrm{i}px),$$
$$e_5\exp(5\mathrm{i}px),\quad f_5\exp(-5\mathrm{i}px)\ldots$$

should be added to (6). Therefore, the averaged reflecting current will be of the form

$$j=\alpha^2p|f|^2+3p|f_3|^2+5p|f_5|^2+\cdots,$$

i.e. we should take into account terms of higher orders in the nonlinearity parameter. The incident current J is also modified by analogy. Then the reflecting coefficient can be determined as

$$R=\frac{j}{J}.$$

We postulate the ansatz that when we expand an arbitrary function into Fourier series, then exponents with positive wave numbers $p, 3p, 5p, \ldots$ correspond to the incident wave function, while exponents with negative wave numbers $-p, -3p, -5p, \ldots$ correspond to the reflecting wave function. Indeed, in contrast to the case of the linear Schrödinger equation the transmission coefficient cannot be computed by simply decomposing the wave function into an incident and a reflecting part because the superposition principle of quantum mechanics is not valid in the presence of the nonlinear term. However, such a decomposition is possible in the limit of a small nonlinearity, or small back reflections. Another definition of the transmission coefficient was suggested in [8]: the transmission coefficient is evaluated by the ratio of the current in the presence of the potential $V(x)$ (i.e. the transmitting current) to the current obtained in the absence of $V(x)$ (the incident current that is emitted by the source). Leboeuf *et al* [9] follow an ansatz closely related to usual experimental setups, and choose to work with an incident and a reflecting beam that can be approximated by plane waves. This corresponds to a regime where a semi-classical Schrödinger-like equation for the amplitude of the wave function can be linearized in the far upstream region. They numerically solve the exact nonlinear equation and use the linearization procedure only to define the transmission coefficient. In particular, they consider an abrupt step-like constriction. The conclusion can be made that the definition of the transmission coefficient in nonlinear quantum problems requires some additional assumptions.

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