HIGHER ORDER TRANSMISSION RESONANCES IN ABOVE-BARRIER REFLECTION OF COLD ATOMS IN THE MEAN-FIELD GROSS-PITAEVSKII APPROXIMATION

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Abstract. The quantum above-barrier reflection of ultra-cold atoms by finite-width potentials created, e.g., by laser fields is analytically considered within the mean field Gross-Pitaevskii approximation. It is shown that the approximate solution of the problem is constructed through a limit solution for the probability written as a root of a polynomial equation of the third order. This zero-order approximation allows one to linearize the problem for the next approximation term. Using this approach, the correction for the specific depth of the squared hyperbolic-secant Rosen-Morse potential that provides (as a result of the common action of the potential barrier and the nonlinearity) total transmission of the incident wave caused by a weak nonlinearity of the Schrödinger equation is derived for higher order transmission resonances. The obtained results are compared with those for the rectangular potential.

The realization of Bose-Einstein condensation [1] in dilute gases of neutral atoms has stimulated a renewed interest to the effect of above-barrier reflection of particles [2] since the condensates provide a different test of fundamental principles of quantum mechanics due to the essentially nonlinear nature of the many-body dynamics of Bose-condensates. Several physical situations for which the linear analogue is known have recently been discussed [3-8]. The above-barrier reflection of cold atoms by the Rosen-Morse potential has been addressed in [6-8]. In the present paper, we consider the *higher order* transmission resonances for this potential viewed in terms of incoming and outgoing waves. We show that in the nonlinear case, in contrast to the linear case, the total transmission is possible for positive potential heights, i.e., for potential barriers. Furthermore, we show that in the nonlinear case the spectrum of the nonlinear resonances becomes a function of the chemical potential. Finally, we compare the results for the Rosen-Morse potential with those for the rectangular barrier which suggests an essentially different behavior.

The dynamics of Bose- condensates in the mean-field approximation is described by the Gross-Pitaevskii equation [1]

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

where $V(x)$ is the reflecting potential and the nonlinearity parameter g determines the mean-field self-interaction. Applying the ansatz $\Psi(x,t)=\exp(-i\,\mu\,t/\hbar)\psi(x)$, where μ is the chemical potential, this equation is reduced to the following stationary version

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

The reflecting potential we consider is the finite-height Rosen-Morse potential

$$V(x)=V_0\,\mathrm{sech}^2 x\,. \qquad (3)$$

In the linear case $g=0$ the total transmission is known to occur for a discrete spectrum of *negative* values of the potential height defined as [2]

$$V_{Ln}=-\frac{1}{2}n(n+1)\,,\quad n=1,2,3,... \qquad (4)$$

The corresponding solution of the Schrödinger equation for these transmission resonances is written in terms of the Gauss hypergeometric function:

$$\psi_{Ln} = e^{ikx}\, {}_2F_1(-n, 1+n, 1+ik_0, z)\,, \quad k_0 = \sqrt{2\mu}\,, \quad z = (1+\text{th}x)/2\,. \tag{5}$$

Our treatment of the nonlinear problem is based on the following *exact* third order differential equation for the probability $p = |\psi(x)|^2$

$$\frac{d}{dx}\left[-\frac{p''}{4} + (-\mu + V + g\,p)\,p\right] + (-\mu + V + g\,p)\,p' = 0\,. \tag{6}$$

The boundary conditions applied for reflectionless transmission to occur are $p(-\infty) = p(+\infty) = 1$. These boundary conditions define a nonlinear eigenvalue problem for Eq. (6). Note that since we look for a solution with asymptotic behavior $\psi(-\infty) \sim e^{ikx}$ the function $p(x)$ should additionally obey the conditions $p'(-\infty) = 0$, $p''(-\infty) = 0$.

We first consider the *exact* solution of Eq. (6) describing the first nonlinear transmission resonance. This solution is readily obtained when searching of a particular solution of the form

$$p = 1 + a\,\text{sech}^2 x\,. \tag{7}$$

After straightforward calculations one obtains

$$a = \frac{-1}{1+2(\mu - g)}\,, \quad V_0 = -1 + \frac{g}{1+2(\mu - g)}\,. \tag{8}$$

Since when passing to the linear limit by tending $g \to 0$ the potential depth defined by the last equation becomes equal to -1 it is clear that this solution describes the nonlinear transmission resonance V_{NL1} corresponding to the first linear resonance $V_{L1} = -1$. Analyzing now the obtained formula we note that the shift from the value of the linear resonance's potential depth is negative for attractive interaction ($g < 0$) and is positive for repulsive interaction ($g > 0$). We note that if the nonlinearity is repulsive and strong enough, the positive shift in the dept of the potential may prevail the first term in the second equation (8) and thus produce a positive value of $V_0 = V_{NL1}$. Hence, in contrast to the linear case, in the nonlinear case reflectionless transmission may occur not only for potential wells but also for potential barriers. This happens when $g > (1+2\mu)/3$.

To discuss the higher order resonances, we recall that we have previously shown that the position of these resonances is given as [9]

$$V_{NLn} = V_{Ln} + g\,F_n / C_n\,, \tag{9}$$

where

$$F_n = \int_0^1 z^{ik}(1-z)^{-ik} F(u_{Ln})\,u_{Ln}\,dz\,, \quad F(u) = \frac{|u|^2 - 1}{4z(z-1)}\,u \tag{10}$$

and

$$C_n = \int_0^1 z^{ik}(1-z)^{-ik} u_{Lm} u_{Ln}\,dz\,, \tag{11}$$

where $u_{Ln}(z)$ is the solution of the linear problem for the nth-order linear resonance given by Eq. (5). It has been numerically proven that these formulas provide a highly accurate description of the nonlinear shift of the position of the reflectionless transmission resonances for all the resonance orders n and all the variation range of the chemical potential μ if the self-interaction parameter g is relatively small, more precisely, the formulas provide a relative error of the order of 10^{-3} if $g/\mu < 0.25$. Notably, the result for the first resonance turns out to be exact, i.e., for $n = 1$ Eqs. (9)-(11) produce the exact result (7)-(8).

Now, we consider the *limit* solution $p_0(x)$ of Eq. (6) that is obtained when neglecting the second derivative term in square brackets. This solution is written as a root of the cubic polynomial equation

$$C_0 + (-\mu + V + g\,p_0)\,p_0^2 = 0\,, \tag{12}$$

where C_0 is the integration constant. The boundary condition $p(-\infty) = 1$ gives $C_0 = \mu - g$.

Further, we use the limit solution to estimate the integrals (10) and (11) for higher order resonances $n > 1$. To do this, we construct an approximate solution of Eq. (12) by means of successive iterations taking $p_0 = 1$ for the zero-order initial approximation. The result for the first order approximation reads

$$p_0(z) = \sqrt{\frac{\mu - g}{\mu - g - V(z)}}\,, \quad V(z) = -V_0\,4z(z-1)\,. \tag{13}$$

Numerical testing shows that this is a good enough approximation. Notably it corresponds to the limit solution of a linear problem for the effective chemical potential $\mu - g$. For this function, the integrals (10) and (11) are calculated analytically:

$$F_n = \frac{-V_{Ln}}{\mu - g - V_{Ln}}\,, \tag{14}$$

$$C_n = \frac{1}{2}\sqrt{\frac{\mu - g}{-V_{Ln}}}\ln\left(\frac{V_{Ln} + \sqrt{V_{Ln}(\mu - g)}}{-V_{Ln} + \sqrt{V_{Ln}(\mu - g)}}\right). \tag{15}$$

For fixed wave vector $k = \sqrt{2(\mu - g)}$, the asymptotes of F_n and C_n for large $n >> 1$ are $F_n \sim 1$ and $C_n \sim 1/\sqrt{-V_{Ln}} \sim 1/n$, hence, we conclude that

$$V_{NLn} - V_{Ln} \sim g\,n\,. \tag{16}$$

Thus, the nonlinear shift of the resonance position is approximately a linear function of the resonance order n. This conclusion is further supported by numerical simulations (Fig. 1a). Recalling now the formula for the first transmission resonance, we finally obtain

$$V_{NLn} \approx V_{Ln} + \frac{g\,n}{1 + 2(\mu - g)}\,. \tag{17}$$

This formula provides a quick estimate of the nonlinear transmission resonance position and hence may be especially useful for qualitative discussions.

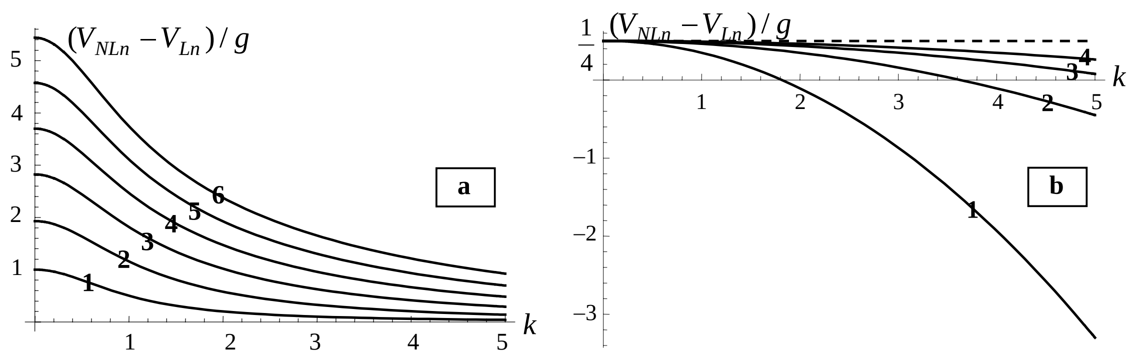

Fig. 1. The nonlinear shift of the resonance position $(V_{NLn} - V_{Ln})/g$ as a function of k:
a) Rosen-Morse potential and b) rectangular barrier.
The resonance orders are indicated by bold-face numbers.

It is interesting to compare the obtained result with the one for the rectangular barrier. Applying essentially the same technique as above, in this case we derive

$$V_{NLn} = V_{Ln} + \frac{g}{4}\left(1 - \frac{3k^2}{\pi^2 n^2}\right). \tag{18}$$

This is a fairly good approximation. The numerical simulations show that the derived formula defines the position of the resonances with accuracy of the order of 10^{-4} (or less) for all the resonance orders and for all the variation range of the parameters μ and g. The dependence of the resonance position on the wave vector k of the incoming matter-wave is demonstrated in Fig. 1b. It is clearly seen that the situation is radically changed compared with the case of the Rosen-Morse potential (Fig. 1a). An immediate observation indicated by Eq. (18) is that for the rectangular barrier the nonlinear shift of the resonance position is approximately constant for higher order resonances $n >> 1$:

$$V_{NLn} - V_{Ln} \approx \frac{g}{4}. \tag{19}$$

We see that the Rosen-Morse potential suggests an essentially different behavior [Eq. (17)] not indicated by the rectangular barrier [see Eq. (19)]. It is supposed that this is because of the smooth variation of the Rosen-Morse potential's shape. A conjecture following from this observation is that the case of asymmetric potentials involving two different scales for the variation of the potential in different space intervals is potent to suggest further effects.

Thus, we have discussed the transmission resonances in the above-barrier reflection of Bose-condensates by the Rosen-Morse potential. Applying an exact third order nonlinear differential equation obeyed by the condensate density, we have derived the exact solution of the problem for the first-order resonance. We have shown that in the nonlinear case the total transmission is also possible for potential barriers, not only for the potential wells as it is the case in the linear case. We have constructed a simple approximation for the shift of the nonlinear resonance potential's depth from the corresponding linear resonance's position for higher order resonances. We have shown that the nonlinear shift of the resonance position is an approximately linear function of the resonance order. This behavior essentially differs from the result for the rectangular barrier for which the nonlinear shift is approximately constant. By noting that this radical difference is probably caused by the smooth variation of the Rosen-Morse potential's shape in contrast to the sharp variation in the case of the rectangular barrier, it is supposed that the case of asymmetric potentials involving two different scales for the variation of the potential in different space intervals is potent to suggest further effects.

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