Anomalous quantum reflection as a quasidynamical damping effect

Alexander Jurisch and Jan-Michael Rost
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzerstr. 38, D-01187 Dresden, Germany
(Received 5 January 2010; published 13 April 2010)

We develop a quasianalytical theory for the quantum reflection amplitude of Bose-Einstein condensates. We derive and calculate the decay width of a Bose-Einstein condensate (BEC). A general relation between the time-dependent decay law of the system and its quantum reflection amplitude allows us to explain the quantum reflection anomaly of Bose-Einstein condensates present in BEC-surface systems as a direct consequence of the repulsive particle interaction.

DOI: 10.1103/PhysRevA.81.043610 PACS number(s): 03.75.Hh, 03.65.−w

I. INTRODUCTION

In recent experiments, the quantum reflection of a sodium Bose-Einstein condensate (BEC) from a silicon surface has been investigated [1,2]. Surprisingly the quantum reflection probability fell off to zero at threshold and did not approach unity as expected from corresponding single-atom beam theory, e.g., [3,4], and experiments, e.g., [5–9].

Theoretically so far, two numerical studies were able to qualitatively produce the quantum reflection anomaly. In [1,2], a model was used to motivate the quantum reflection anomaly by introducing an empirical potential which modifies the atom-surface interaction. This led qualitatively to the observed effect. In the second numerical study [10], an *ab initio* numerical simulation of the experimental situation reported in [1] in three dimensions was used to explain the anomalous behavior of the quantum reflection probability with the formation of scattering halos and the building of vortices that destroy the coherence of the condensate while being reflected. The anomalous behavior of the reflection probability emerged when taking into account only regions of the reflected BEC with more than 25% of its initial density.

In the following, we present a quasianalytical approach to describe the anomalous behavior of the quantum reflection probability $|R|^2$. Due to its simplicity, the origin of the anomaly is elucidated. Furthermore, we identify scattering along the axis of normal incidence on the surface as being mainly responsible for the anomalous behavior of the quantum reflection probability. On the base of this, we may use the framework of the well-understood spherical quantum reflection trap model [11,12]. A spherical model has the advantage that there is only the normal direction for s waves. This property strongly reduces the technical complexity of the general three-dimensional system and allows us to focus on the physics behind the quantum reflection of a BEC. Furthermore, our model relies solely on the presence of particle-interaction and mean-field dynamics.

II. QUANTUM REFLECTION

For monochromatic atomic beams or linear wave packets, the universal law of quantum reflection is obtained by the fact that atom-surface potentials behave as step potentials for incident momenta close to threshold, see [3,4,11,13]. The universal threshold law of quantum reflection is given by

$$\lim_{k\to 0}|R(k)| = 1 - 2bk, \tag{1}$$

where the parameter b is called the threshold length and k is the incident momentum. In the case of an atom-surface potential, it has been shown [4,6,14] that close to threshold the retarded Casimir-Polder tail of the potential dominates the process of quantum reflection. The retarded Casimir-Polder tail is given by

$$U(z) = -\frac{\hbar^2}{2m}\frac{\beta_4^2}{|z-L|^4}, \tag{2}$$

where L denotes the location of the surface. For low incident momenta, such potentials behave like

$$U(z) = -\frac{\hbar^2}{2m}b^{-2}\theta(z-L), \quad b = \beta_4. \tag{3}$$

For the quantum reflection of linear wave packets it has been shown in [11] that the quantum reflection amplitude $|R(k)|$ can be extended to the whole k space by

$$|R(k)| = 1 - 2bk \approx \exp[-2bk], \tag{4}$$

with reasonable accuracy. It further has been shown that the decay-law for a linear wave packet is linked to Eq. (4) by

$$P(k,t) = |R(k)|^{\frac{2kt}{2mL}} = \exp\left[-4\frac{bk^2t}{2mL}\right]. \tag{5}$$

III. DERIVATION OF THE CONDENSATE'S DAMPING FUNCTION

To study the influence of particle interaction on the threshold-behaviour of quantum reflection, we turn to the radial system that we have examined in detail from a dynamical point of view [12]. The radial Gross-Pitaevskii equation that describes the time evolution of an initial state $\Psi(x,\tau=0)$ in the atom-surface system in scaled form is given by

$$i\frac{\partial}{\partial\tau}\psi(x,\tau) = -\frac{\partial^2}{\partial x^2}\psi(x,t) - \sigma^2\theta(x-1)\psi(x,\tau) + \gamma\frac{|\psi(x,\tau)|^2}{x^2}\psi(x,\tau). \tag{6}$$

Scaling is carried out by the intrinsic length of the system L,

$$x = \frac{r}{L}, \quad \kappa = kL, \quad \sigma = \frac{L}{\beta_4}, \quad \gamma = \frac{2a_{\rm int}}{L}N, \quad \tau = \frac{t\hbar}{2mL^2}. \tag{7}$$

In [12] we have shown that a repulsive self-interaction provides an additional contribution to the total energy of the system that is responsible for a faster decay of the particle density than found in the linear case. Dynamically, this is explained by a transformation of the self-interaction energy into kinetic energy as the initial state evolves in time. In k space, we interpret the presence of the self-interaction as an additional barrier. The k modes close to threshold lie at the base of this barrier and are thus damped away by driving them over the edge of the potential. The effect of the self-interaction is strongest at the beginning of the time evolution, because its magnitude is directly related to the incident particle density. For larger times, a considerable fraction of particle density has already decayed, such that the influence of the self-interaction becomes more and more negligible.

For small times, we assume that the decay of the system can be described by a product ansatz

$$P(\kappa,\tau;\sigma,\gamma) = P_\sigma(\kappa,\tau)P_\gamma(\kappa,\tau) = |R_\sigma(\kappa)R_\gamma(\kappa)|^{2\kappa\tau} = \exp\left[-4\frac{\kappa^2}{\sigma}\tau\right]|R_\gamma(\kappa)|^{2\kappa\tau}. \tag{8}$$

In Eq. (8), the additional damping induced by the particle interaction is described by $P_\gamma(\kappa,\tau)$. The product ansatz of Eq. (8) reflects our assumption that for early times the effects of the step potential and the particle interaction can be treated independently. By this assumption, we derive the additional damping induced by the particle interaction without taking into account the presence of the atom-surface potential in Eq. (6).

The wave function ψ that solves Eq. (6) without potential can be decomposed into its momentum components by setting

$$\psi(x,\tau) = \int d\kappa\, A(\kappa)\varphi_\kappa(x)\exp[-i\kappa^2\tau]\phi_\gamma(\kappa,\tau), \qquad \phi_\gamma(\kappa,\tau) = \exp\left[-i\int_0^\tau d\tau' E_\gamma(\kappa,\tau')\right]. \tag{9}$$

All effects of particle interaction in Eq. (9) are described by ϕ. The Fourier decomposition in Eq. (9) is defined by

$$A(\kappa) = \int_0^1 dx\,\Psi(x,\tau=0)\varphi_\kappa(x), \tag{10}$$

and the basis of the system is

$$\varphi_\kappa(x) = \sqrt{\frac{2}{\pi}}\sin[\kappa x]. \tag{11}$$

The decay can be calculated from the time-dependent dispersion, which is obtained by inserting the Fourier decomposition (9) into Eq. (6), neglecting the atom-surface potential, multiplying by φ from the left, integrating out x, and separating off the noninteracting parts. We thus obtain the time-dependent dispersion of the self-interacting system:

$$i\frac{\partial_\tau\phi_\gamma(\kappa,\tau)}{\phi_\gamma(\kappa,\tau)} = E_\gamma(\kappa,\tau) = \gamma\int_0^\infty d\kappa_1 d\kappa_2 \times V(\kappa,\kappa_1,\kappa_2)\phi_\gamma^*(\kappa_2,\tau)\phi_\gamma(\kappa_1,\tau) \times \exp\left[-i\left(\kappa_1^2-\kappa_2^2\right)\tau\right]. \tag{12}$$

The function $V(\kappa,\kappa_1,\kappa_2)$ in Eq. (12) is a vertex function, which describes the interaction of the modes of the system in momentum space. The main contribution to the vertex stems from the threshold region. We find

$$V(\kappa,\kappa_1,\kappa_2) = 3\kappa^{-2}A(\kappa_1)A(\kappa_2)\frac{2}{\pi} \times \int_0^1 dx\,\sin^2[\kappa x]\frac{\sin[\kappa_1 x]\sin[\kappa_2 x]}{x^2}. \tag{13}$$

The decay of the system is described by the imaginary part of the dispersion, which can be identified by the linewidth Γ_γ. To calculate Γ_γ, we expand $E_\gamma(\kappa,\tau)$, $\phi_\gamma(\kappa,\tau)$ in frequency space, obtaining

$$E_\gamma(\kappa,\tau) = \int\frac{d\omega}{2\pi}E_\gamma(\kappa,\omega)\exp[-i\omega\tau], \qquad \phi_\gamma(\kappa,\tau) = \int\frac{d\omega}{2\pi}\phi_\gamma(\kappa,\omega)\exp[-i\omega\tau]. \tag{14}$$

By using Eq. (14) we can perform a Laplace transform on Eq. (12). The imaginary part we are interested in can be extracted by using the well-known relation $\frac{1}{\Omega-\omega+i\epsilon} = \mathrm{P}\frac{1}{\Omega-\omega} - i\pi\delta(\Omega-\omega)$. We integrate out the δ function and find

$$-\mathrm{Im}E_\gamma(\kappa,\Omega) = \Gamma_\gamma(\kappa,\Omega) = \gamma\int_0^\infty d\kappa_1 d\kappa_2 V(\kappa,\kappa_1,\kappa_2)\int\frac{d\omega_2}{2\pi}\phi_\gamma^*(\kappa_2,\omega_2) \times \phi_\gamma\left(\kappa_1,\Omega-\kappa_1^2+\kappa_2^2+\omega_2\right). \tag{15}$$

So far, we have only neglected the atom-surface potential. Since we are interested in the damping that is induced by the initial state, we now make a relaxational ansatz that treats Γ_γ independent of ω by setting

$$\phi_\gamma(\kappa,\omega) \approx \frac{i}{\omega+i\Gamma_\gamma(\kappa)}. \tag{16}$$

We insert Eq. (16) into Eq. (15), carry out the remaining integration by the residual theorem, and arrive at

$$\Gamma_\gamma(\kappa) = i\gamma\int_0^\infty d\kappa_1 d\kappa_2\frac{V(\kappa,\kappa_1,\kappa_2)}{\kappa_2^2-\kappa_1^2+i[\Gamma_\gamma(\kappa_1)+\Gamma_\gamma(\kappa_2)]}. \tag{17}$$

Equation (17) is a self-consistent equation for the linewidth of the self-interacting part of the system. From Eqs. (16) and (17) it follows that the self-interacting part of the system initially decays like

$$|\phi_\gamma(\kappa,\tau)|^2 \approx P_\gamma(\kappa,\tau) = \exp[-2\Gamma_\gamma(\kappa)\tau]. \tag{18}$$

Together with Eq. (8), the quantum reflection amplitude readily follows as

$$|R(\kappa;\sigma,\gamma)| = |R_\sigma(\kappa)R_\gamma(\kappa)| = \exp\left[-2\frac{\kappa}{\sigma}\right]\exp\left[-\frac{\Gamma_\gamma(\kappa)}{\kappa}\right]. \tag{19}$$

Following [11], the quantum reflection amplitude in Eq. (19) describes the decay of the initial state in a uniform and

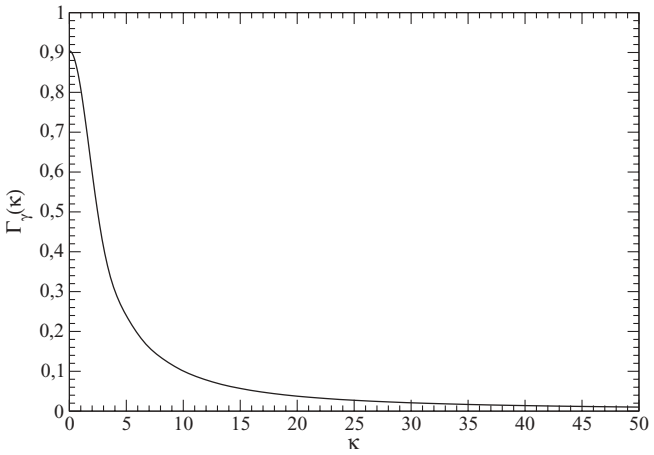

FIG. 1. Damping function $\Gamma_\gamma(\kappa)$ calculated by Eq. (17) for $\gamma = 0.5$.

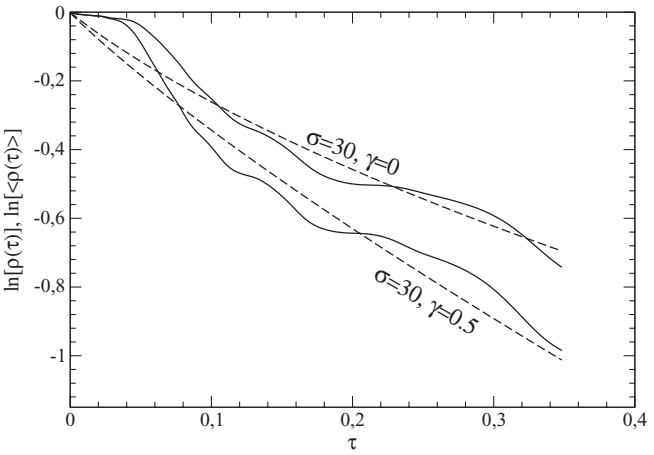

FIG. 2. Comparison between numerically obtained decaying densities $\rho(\tau)$ (full lines) and approximated decaying densities $\langle\rho(\tau)\rangle$ (dashed lines) by Eq. (18) for ($\sigma = 30,\ \gamma = 0$) above and ($\sigma = 30,\ \gamma = 0.5$) below.

quasistationary way by

$$\langle\rho(\tau)\rangle = \int_0^\infty d\kappa\, |A(\kappa)|^2\, |R(\kappa;\sigma,\gamma)|^{2\kappa\tau}, \qquad (20)$$

where $\langle\rho(\tau)\rangle$ stands for the mean value of the time-dependent particle density $\rho(\tau) = \int_0^1 dx |\psi(x,\tau)|^2$, which is obtained from numerics.

IV. DISCUSSION

Now we are going to test the fidelity of our theory by comparing it to numerical results. To make contact with our analysis in [11,12], we use the initial state

$$\Psi(x, \tau = 0) = \mathcal{N} x \exp[-ax]\,\theta[1-x], \qquad (21)$$

where $\mathcal{N}$ is the normalization constant and a is the diffuseness of the wave packet. A diffuseness of $a = 5$, gives an initial kinetic energy $E_{\rm kin} = 1.5 \times 10^{-15}$ a.u. for sodium that corresponds to temperatures of approximately 1 nK, comparable to the experimental setup in [1,2]. As in [11], we chose a length scale $L = 4.47 \times 10^5$ a.u., and together with a potential strength $\beta_4 = 1.494 \times 10^4$ a.u. and mass $m = 4.22 \times 10^5$ a.u. for sodium, we obtain a scaled potential strength $\sigma = 30$. To illustrate the effect of particle interaction, we chose $\gamma = 0.5$.

Figure 1 shows the additional damping that is induced by the particle interaction. It is clearly visible that the low-lying k modes are strongly damped, while higher k modes experience only a moderate to negligible additional damping and thus show a regular decay according to universal quantum reflection [Eqs. (4) and (5)].

Figure 2 shows a comparison between numerically calculated densities as function of the scaled time τ and their mean-value approximation according to Eq. (18) for early times of the decay of the system. We have chosen a logarithmic ordinate for a better resolution. Figure 2 shows clearly that after the *einschwingvorgang* is completed, the mean-value approximation (18) interpolates the numerical curves. Approximation (18) describes the decay in a quasistationary and uniform way and thus does not reflect the oscillations of the numerically obtained data, which originate from the motion of the wave packet on the spatial range of the step. For times $\tau \geqslant 0.35$, our approach is not reliable anymore, because it takes only into account the damping according to the initial state, which naturally must overestimate the decay of the particle density for later times. A scaled time $\tau \sim 0.35$ as a range of fidelity corresponds to times $t \sim 0.144$ s.

Figure 3 shows the quantum reflection probabilities calculated according to Eq. (19). Figure 3 clearly demonstrates how the additional damping that is induced by the particle interaction influences the quantum reflection probability. The depletion of the quantum reflection probability for low-lying k modes corresponds to the results reported in [1,2,10]. The curves shown in Fig. 3 must be interpreted as a quasistationary mean value of the quantum reflection probability that is to be expected for times $\tau \leqslant 0.35$. For later times, as the influence of particle interaction declines along with the decaying density, we expect a reduction of the anomalous behavior that, for very large times, will experience a crossover to the universal law of quantum reflection [Eqs. (1) and (5)].

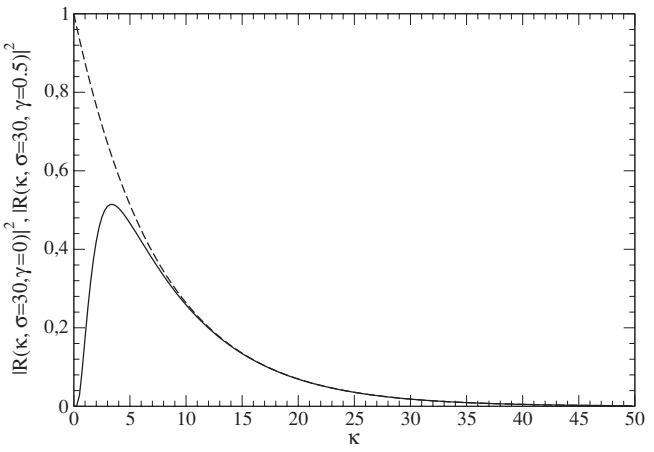

FIG. 3. Quantum reflection probabilities according to Eq. (19) for ($\sigma = 30,\ \gamma = 0.5$) (full line) and ($\sigma = 30,\ \gamma = 0$) (dashed line).

V. SUMMARY AND CONCLUSION

Together with our investigations on the dynamical properties of a BEC-surface system [12], the behavior of Eq. (19) as shown in Fig. 3 proves that quantum reflection has only a limited effect on BECs with repulsive particle interaction. We thus explain the quantum reflection anomaly by the fact that especially the low energetic, collective components of the wave packet moving normal to the surface react extremely sensitively in the presence of an additional positive energetic contribution as a repulsive particle interaction provides. The crucial role of the repulsive particle interaction and its transformation into kinetic energy was already mentioned in [1] and theoretically demonstrated in [12]. The influence of the repulsive interaction on higher energetic components is by far less dramatic, explaining the regular behavior of Eq. (19) for higher momenta. The fact that we can explain the quantum reflection anomaly with the behavior of the linewidth as a function of momentum may give hints for future experiments to measure the linewidth of the condensate instead of the reflection probability, which, as emphasized in [1,2], is quite sensitive to external influences.

The purpose of our present theory is not to exactly recalculate either the experimental data from [1,2] or the numerical results reported in [10], but to elucidate the physical mechanism that is responsible for the anomalous behavior of the quantum reflection probability on the basis of a simple but well-understood model. Our quasianalytical theory focuses exclusively on the direction of normal incidence, which we have assumed and proved that it contributes significantly to the quantum reflection anomaly. Our analysis demonstrates that the anomaly exists and that it may be found in experiments. Furthermore, the experiments reported in [1,2] so far contain enough uncertainties to doubt the relevance of a direct and quantitative comparison between theory and experiment in the present state of the art. However, our analysis may encourage further experimental work in this field.

In the framework of the simple spherical model [12], we have developed a quasianalytical theory for the anomalous behavior of quantum reflection probability. Our theory explains the anomalous behavior of the quantum reflection probability of BECs as a direct consequence of the repulsive particle interaction. The key quantity for understanding the quantum reflection anomaly of BECs was shown to be the linewidth of the condensate as a function of momentum.

[1] T. A. Pasquini, Y. Shin, C. Sanner, M. Saba, A. Schirotzek, D. E. Pritchard, and W. Ketterle, Phys. Rev. Lett. **93**, 223201 (2004).

[2] T. A. Pasquini, M. Saba, G. Jo, Y. Shin, W. Ketterle, D. E. Pritchard, T. A. Savas, and N. Mulders, Phys. Rev. Lett. **97**, 093201 (2006).

[3] R. Côté, H. Friedrich, and J. Trost, Phys. Rev. A **56**, 1781 (1997).

[4] H. Friedrich, G. Jacoby, and C. G. Meister, Phys. Rev. A **65**, 032902 (2002).

[5] F. Shimizu, Phys. Rev. Lett. **86**, 987 (2001).

[6] V. Druzhinina and M. DeKieviet, Phys. Rev. Lett. **91**, 193202 (2003).

[7] H. Oberst, D. Kouznetsov, K. Shimizu, J. I. Fujita, and F. Shimizu, Phys. Rev. Lett. **94**, 013203 (2005).

[8] H. Oberst, Y. Tashiro, K. Shimizu, and F. Shimizu, Phys. Rev. A **71**, 052901 (2005).

[9] D. Kouznetsov and H. Oberst, Phys. Rev. A **72**, 013617 (2005).

[10] R. G. Scott, A. M. Martin, T. M. Fromhold, and F. W. Sheard, Phys. Rev. Lett. **95**, 073201 (2005).

[11] A. Jurisch and H. Friedrich, Phys. Lett. A **349**, 230 (2006).

[12] A. Jurisch and J.-M. Rost, Phys. Rev. A **77**, 043603 (2008).

[13] J. Madronero and H. Friedrich, Phys. Rev. A **75**, 062902 (2007).

[14] A. Jurisch and H. Friedrich, Phys. Rev. A **70**, 032711 (2004).