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# Interaction of a propagating guided matter wave with a localized potential

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**Abstract.** We provide a theoretical framework to describe the interaction of a propagating guided matter wave with a localized potential in terms of a quantum scattering approach in a confined environment. This interaction generates entangled states for which the longitudinal and transverse degrees of freedom are correlated. The number of terms of the entangled state is dictated by the incident energy. We analyze this scattering analytically under the Born approximation using a Gaussian localized potential. In this limit, it is possible to engineer the potential and achieve the coherent control of the output channels. The robustness of this approximation is studied by comparing the stationary scattering theory to numerical simulations involving incident wave packets. It remains valid in a domain of weak localized potential achievable experimentally. We infer a possible method to determine the longitudinal coherence length of a guided atom laser. Then, we detail the non-perturbative regime of the interaction of the guided matter wave with the localized potential using a coupled channel approach. This approach is worked out explicitly with a square potential. It yields new non-perturbative effects such as the occurrence of confinement-induced resonances. The perspectives opened by this work are, finally, discussed.

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The recent realization of guided atom lasers with a macroscopic fraction of the atoms in the ground state of the transverse confinement is a crucial step for the development of guided atom optics [1, 2, 3, 4]. The description of the propagation in the presence of a single extra, localized, potential is an important issue in the context of the exploration of more complex propagating structures. This extra potential, also called defect in the following, can be generated by a local modification of the transverse confinement such as a constriction [5, 6, 7], or a local curvature [8, 9]. Alternatively, one can use a far-off resonance light beam<sup>‡</sup> superimposed on the guide to produce a large variety of shapes and strengths. This potential acts as an obstacle and enables one to revisit superfluidity for quantum degenerate guided beams [11].

The interaction between a guided matter wave and a localized potential belongs to the more general topic of elastic scattering in a multimode quantum waveguide. This topic has already been the subject of experimental and theoretical investigations in condensed matter [12, 13, 14, 15, 16, 17, 18, 19, 20]. The motivation therein was to study the effect of disorder on the electron transmission and, in particular, on conductance quantization in narrow constrictions.

Confinement can dramatically modify the scattering properties, and thus the properties of interacting quantum gases as exemplified by the observation of the Tonks gas regime in one dimension [21, 22], or the Kosterlitz Thouless transition in two dimensions [23]. Recent theoretical studies on atom-atom interaction where the true interacting potential is replaced by the standard Huang-Fermi pseudo-potential have shown the occurrence of resonances in the two-body scattering length for atoms that are strongly transversally confined by a waveguide or more generally confined to quasi 1D geometry. These confinement-induced resonances have been predicted by Olshanii [24, 25], and experimental evidence of such resonances have been recently reported for bosons [21, 22] and fermions [26].

In this article, we study the interaction of a guided atom laser with extra localized optical potentials. The atom laser is modelled as a propagating matter wave without any atom-atom interaction because of the diluteness of the experimentally realized guided atom lasers [1, 2, 3]. In contrast with scattering length studies, we take into account the details of the interaction potential and envision their tailoring to control the output channels after the interaction. In Sec. 1, we derive the theoretical framework to describe the interaction between a dilute guided atom laser and a localized potential using the Green's function formalism taking into account the transverse harmonic confinement [27, 28, 29, 30]. This approach yields an expression of the solution as a series expansion in the powers of the strength of the localized potential. In Sec. 2, we derive analytical results for a weak localized potential using the Born approximation. We also investigate the validity domain of the scattering results in the perturbative limit for a propagating wave packet, and emphasize the role played by the longitudinal size of the wave packet. For a sufficiently strong localized potential the calculation of higher-order contributions

<sup>‡</sup> A theoretical study with an on-resonance laser beam has also been carried out in Ref. [10].

is cumbersome. To circumvent this limitation, we develop, in Sec. 4, a non-perturbative formalism inspired by the theory of vibrational energy transfer in non reactive collisions investigated in the context of quantum chemistry [31]. Using a model potential, we show how the coupling between external degrees of freedom that occurs in the localized potential region generates controlled entangled states that correlate the longitudinal wave vector to the transverse state, and yields resurgences of quantum reflection.

Without loss of generality, the theoretical description made in the following is done for a two dimensional problem; the matter wave propagates along the  $x$  axis and the transverse confinement, assumed to be harmonic with an angular frequency  $\omega_\perp$ , is provided along an orthogonal direction,  $y$ . In the absence of extra potential, the Hamiltonian is therefore given by

$$H_0(x, y) = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{1}{2}m\omega_\perp^2 y^2. \quad (1)$$

The defect is taken into account as an extra potential term  $U(x, y)$ , so that the total Hamiltonian reads  $H(x, y) = H_0(x, y) + U(x, y)$ .

## 1. Green's function formalism

To study the interaction of the guided atom laser with the defect, we determine the scattering states by solving the stationary Schrödinger equation:

$$[H_0 + U] |\varphi\rangle = E|\varphi\rangle. \quad (2)$$

The formal solution of this equation is given by the implicit Lippmann-Schwinger form as [32]

$$|\varphi\rangle = |\varphi_0\rangle + G^+ U |\varphi\rangle, \text{ where } G^+ = \lim_{\epsilon \rightarrow 0} \frac{\mathbb{1}}{E - H_0 + i\epsilon} \quad (3)$$

is the retarded propagator,  $\mathbb{1}$  is the identity matrix, and  $|\varphi_0\rangle$  a solution in the absence of extra potential  $H_0|\varphi_0\rangle = E|\varphi_0\rangle$ . This formulation is well suited for a formal perturbative expansion in powers of the localized potential  $U$ :

$$|\varphi\rangle = |\varphi_0\rangle + G^+ U |\varphi_0\rangle + G^+ U G^+ U |\varphi_0\rangle + \dots \quad (4)$$

A natural basis of the Hilbert space for this scattering problem is provided by the vectors  $\{|k, n\rangle = |k\rangle \otimes |n\rangle\}$ , tensor products of the longitudinal plane wave eigenvectors along the  $x$  direction by the eigenvectors of the harmonic potential associated to the transverse degree of freedom. By definition, one has  $H_0|k, n\rangle = E_{k,n}|k, n\rangle$ , with  $E_{k,n} = \hbar^2 k^2 / 2m + E_n$ , where  $E_n = (n + 1/2)\hbar\omega_\perp$  is the energy of the  $n^{\text{th}}$  level of the transverse harmonic confinement. In space representation,  $\langle \vec{r} | k, n \rangle = (2\pi)^{-1/2} e^{ikx} \psi_n(y)$ , where  $\psi_n(y)$  is the eigenvector wavefunction of eigenenergy,  $E_n$ . The space representation of the retarded resolvent is by definition the Green's function, and its expansion on the  $\{|k, n\rangle\}$  basis gives [33]:

$$G^+(\vec{r}, \vec{r}'; E) = \sum_{n=0}^{\infty} \psi_n(y) \psi_n^*(y') g^+(x, x'; E, n), \quad (5)$$

where  $g^+(x, x'; E, n)$  is the Green function of an effective one-dimensional scattering problem. Using the residue theorem, one finds

$$g^+(x, x'; E, n) = -\frac{mi}{\hbar^2} \frac{e^{ik_n(E)|x-x'|}}{k_n(E)}, \quad (6)$$

with  $\hbar k_n(E) = [2m(E - E_n)]^{1/2}$ . We obtain two kinds of modes: propagating ones, for which  $k_n(z)$  is real, and evanescent ones, for which  $k_n(z)$  is imaginary.

In the following we consider an incident wave function of the form  $|k_0, 0\rangle$ . Such a monomode incident beam is experimentally achievable as recently reported in Ref. [3] where 85 % of the atoms of the guided atom laser occupy the transverse ground state of the confinement. The interaction of the atom laser with the localized potential produces the contamination of the modes  $|k_n, n\rangle$  in the forward direction and  $|-k_n, n\rangle$  in the backward direction:

$$\varphi(x \rightarrow \infty, y) = \sum_n t_n \langle \vec{r} | k_n, n \rangle, \quad (7)$$

$$\varphi(x \rightarrow -\infty, y) = \langle \vec{r} | k_0, 0 \rangle + \sum_n r_n \langle \vec{r} | -k_n, n \rangle, \quad (8)$$

where  $t_n$  and  $r_n$  are respectively the transmission and reflection amplitude coefficients in the  $n^{\text{th}}$  transverse mode. The physical meaning of Eqs. (7) and (8) is clear. The incoming plane wave propagates from the left to the right, the outgoing plane waves resulting from the interaction move in both directions; to the right as transmitted waves and to the left as reflected waves.

Therefore, the output wave resulting from the interaction of the incident wave with the scattering potential  $U(x, y)$  is an entangled state that is a linear superposition of correlated bipartite states involving both a transverse state of quantum number  $n$  and a specific longitudinal state  $\pm k_n$ . By controlling the incident energy, one can choose the number of propagating modes, and thus the number of bipartite states that participate in the output state.

Let us consider an incident wave packet characterized by a linear superposition of longitudinal wave vectors and transversally in the ground state of the confinement. In the following, the mean value of the wave vectors of the initial packet is denoted  $k_0$ . After its interaction with the defect, the transmitted wave packet will undergo a kind of distillation in the course of its propagation. Indeed, as a result of energy conservation, for each incident wave vector component,  $k$ , the components with a non zero transverse quantum number  $n$  have a reduced wave vector  $k_n < k$ :

$$\frac{\hbar^2 k^2}{2m} + 0 = \frac{\hbar^2 k_n^2}{2m} + n\hbar\omega_{\perp}. \quad (9)$$

For a sufficient long propagation time, one therefore expects the packet to split into a sum of packets if the initial dispersion  $\delta k$  in  $k$  is small enough, and the front wave packet will be made of the components correlated to the ground state i.e. whose state has not changed after the interaction with the localized potential.

## 2. Born approximation

Determination of the coefficients  $r_n$  and  $t_n$  is straightforward for a weak localized potential. In this limit, one applies the Born approximation which consists in keeping only the first two terms of the expansion of Eq. (4). From the space representation of Eq. (4) combined with Eqs. (5) and (6), one obtains the expression for the transmission and reflection coefficients in the Born limit for  $n > 0$ :

$$t_n = -\frac{2\pi mi}{\hbar^2 |k_n|} \langle k_n, n | U | k_0, 0 \rangle \quad \text{and} \quad r_n = -\frac{2\pi mi}{\hbar^2 |k_n|} \langle -k_n, n | U | k_0, 0 \rangle. \quad (10)$$

These expressions are valid in the perturbative regime,  $|t_n| \ll 1$  and  $|r_n| \ll 1$ .

### 2.1. The Gaussian potential

Let us apply the previous formalism to a model potential that is of practical interest, a dipole potential generated by a Gaussian beam:

$$U_g(x, y) = U_0 u_g(x/w_x) u_g(y/w_y), \quad (11)$$

where  $u_g(x) = e^{-2x^2}$  is a Gaussian function of waist unity. This potential explicitly couples the longitudinal and transverse degrees of freedom. By combining Eqs. (10) and (11), one finds:

$$\begin{aligned} t_{2p}(k_{2p}) &= -i \frac{U_0}{\hbar \omega_\perp} \sqrt{\frac{\pi}{2}} \frac{e^{-(k_{2p}-k_0)^2 \frac{w_x^2}{8}}}{|k_{2p}| a_{\text{ho}}^2} w_x g_{2p}(\eta), \\ r_{2p}(k_{2p}) &= t_{2p}(-k_{2p}), \end{aligned} \quad (12)$$

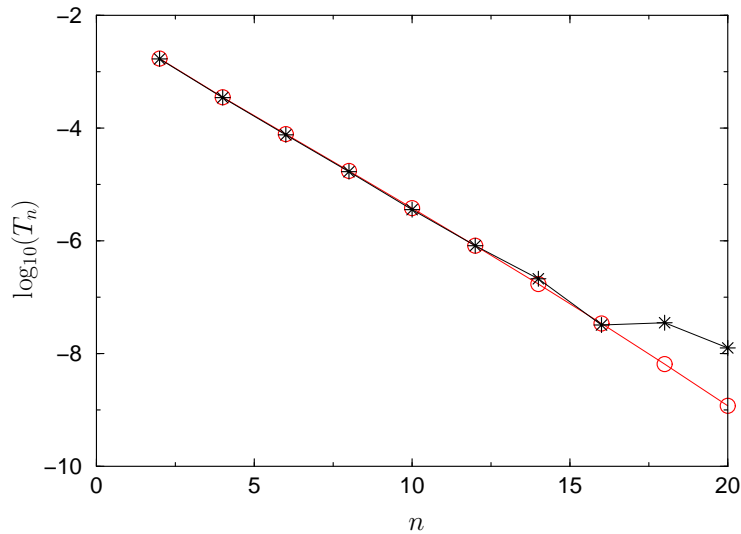
where  $p$  is an integer,  $\eta = w_y/2a_{\text{ho}}$ ,  $a_{\text{ho}} = \sqrt{\hbar/(m\omega_\perp)}$  is the harmonic oscillator length, and  $g_{2p}(\eta)$  accounts for the matrix element of the potential  $U(x, y)$  between the transverse oscillator states (see Appendix A):

$$g_{2p}(\eta) = \langle 2p | u_g(y) | 0 \rangle = (-1)^p \frac{\sqrt{2(2p)!}}{2^p p!} \eta \left( \frac{1}{1+2\eta^2} \right)^{p+\frac{1}{2}}. \quad (13)$$

The parity of the potential with respect to the  $y$  variable cancels out the contributions of the odd terms.

### 2.2. Validity of the perturbative approach

The predictions of the Born approximation can be compared with the results of direct simulations of the scattering of wavefunctions by such Gaussian potentials. An incident ideal guided matter wave can be modeled by a wave packet or a statistical mixture of wave packets [34]. We thus use Gaussian packets as initial state for the numerical simulations. In order to test the robustness of the results of the Born approximation that involves an incoming plane wave, we have chosen the wave packet  $\pi(x)$  with a large but realistic longitudinal size,  $L_p$ , (i.e. a small momentum dispersion) defined as  $\pi(x) = (2/\pi)^{1/2} L_p^{-1} \exp(-2x^2/L_p^2)$ . The time evolution of the wave packet is performed using the split-operator technique, for which the evolution operator is approximated by



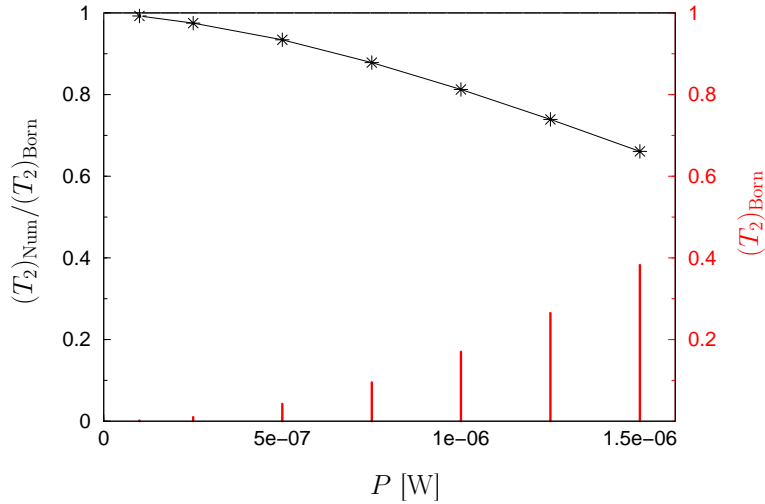
**Figure 1.** Logarithm (decimal) of the probability of transmission  $T_n = k_n |t_n|^2 / k_0$  (even states only) from the numerical simulations (black stars) and from the Born approximation (red circles), as a function of the transverse mode number  $n$  of the guide, for a wave packet after the interaction with a defect of width  $w = 1 \mu\text{m}$  and fixed power  $P = 10^{-7} \text{ W}$ . The initial wave packet of longitudinal width  $L_p = 63 \mu\text{m}$  and in the transverse mode  $n = 0$  of the guide potential moves towards the defect at a mean velocity of  $10 \text{ mm.s}^{-1}$ . The guide is generated by a dipole beam of waist  $45 \mu\text{m}$  and is characterized by a frequency  $\omega_{\perp} = 2\pi \times 203 \text{ Hz}$ .

the product of the potential and kinetic term for a succession of small time steps. The results depend on several parameters, in particular the depth of the potential (corresponding to the power,  $P$ , of the laser used to generate the defect) and its width  $w = w_x = w_y$ .

The wave packet is launched towards the localized potential, then interacts with it and the projections on the different transverse modes are eventually computed. Initially, the wave packet is entirely on the first transverse mode  $n = 0$ . For the simulations, we consider a matter wave of rubidium 87 atoms propagating, with a mean velocity of  $10 \text{ mm.s}^{-1}$ , in a guide provided by a far-off resonance dipole beam,  $\lambda = 1070 \text{ nm}$ , with a waist of  $45 \mu\text{m}$ . These values are consistent with recent experiments [3].

For small  $P$  and  $w$ , the projection of the scattered wavefunction on the different transverse modes is in very good agreement with the predictions of the Born approximation. Figure 1 shows that for  $P = 10^{-7} \text{ W}$  and  $w = 1 \mu\text{m}$  the projections on the first 16 transverse modes are well reproduced. Such widths of the defect, although small, are within reach of current experimental possibilities. For higher transverse modes, predicted values are so small that they are of no experimental relevance and, in addition, the numerical precision chosen precludes to check accurately the theoretical predictions.

For larger values of  $P$ , the Born prediction (12) is a priori interesting only in a certain range of values of  $w$ : for small  $w$  it predicts projections too large to be valid, while for large  $w$  the predictions are so small that they are practically useless (and almost



**Figure 2.** Ratio of transmissions  $T_2 = k_2|t_2|^2/k_0$  to the transverse state  $n = 2$  from the numerical simulations and from the Born approximation (black stars), as a function of the power of the defect  $P$  in W, for a wave packet with a defect of width  $w = 1 \mu\text{m}$ . The initial wave packet is the same as in Fig. 1. Red bars denote the value of  $T_2$  given by the Born approximation.

impossible to check within numerical accuracy). As an example, Born predictions are useful for a width of the order of  $12 \mu\text{m}$  with  $P = 10^{-3} \text{ W}$ , and or a width of the order of  $20 \mu\text{m}$  with  $P = 10^{-1} \text{ W}$ .

Numerical simulations allow one to determine quantitatively the range of validity of Born approximation. The role of the higher-order terms in the expansion (4) is clear for the power dependence since the localized potential is simply proportional to the power. For instance, we find that, for small widths of the defect such as  $w = 1 \mu\text{m}$  and  $w = 4 \mu\text{m}$ , the results of Born approximation remain approximately correct for the first transverse mode up to values of  $P$  where a significant part of the atoms ( $\approx 40\%$ ) is transferred from  $n = 0$  to  $n = 2$  (see Fig.2). The dependence of the higher order terms of the expansion (4) on the width of the localized potential is non trivial. We find that for larger values of the width, the agreement of Born predictions with the numerics is less good than for smaller width even when a comparable fraction of atoms is transferred (data not shown). This indicates that the higher-order terms in the expansion (4) grow faster with the size  $w$  than with the power  $P$  of the Gaussian potential.

In conclusion, the interaction of a guided matter wave with a localized potential enables one to investigate quantum scattering in confined environment both in the perturbative and non-perturbative regimes with accessible values for the power and the size of the dipole beam used to generate experimentally the defect.

### 2.3. Coherent control in the perturbative limit

When the transverse size of the localized potential is much larger than the oscillator length,  $\eta \gg 1$ , the excited levels of the transverse confinement are nearly not populated



after the interaction with the localized potential. For typical experimental conditions [1, 2, 3], the oscillator length is on the order of  $1 \mu\text{m}$ . Our simple calculation confirmed by numerical simulations thus suggests that, to control the population of the output scattering states, the defect size should be on the same order as the oscillator length. This conclusion remains valid for any localized potential. In practice, the realization of such defect by optical means can be achieved using large aperture optical elements as used in recent experiments, either to produce optical potentials or to image atoms [35, 36, 37].

By engineering the localized potential, it is possible to control the population in the different output channels. For instance, the following family of potentials

$$U_m(x, y) = U_0 u_g(x/w_x) u_g(y/w_y) [H_m(y/a_{\text{ho}}) + C] , \quad (14)$$

where  $H_m$  is the Hermite polynomial of order  $m$  and  $C$  a constant, permits one to populate only the  $m^{\text{th}}$  mode of the transverse guide in the large waist limit ( $\eta \gg 1$ ). Indeed, the  $g_p$  coefficients are given for  $p \neq 0$  by

$$g_p(\eta) = \langle p | u_g(y/w_y) [H_m(y/a_{\text{ho}}) + C] | 0 \rangle \propto \langle p | u_g(y/w_y) | m \rangle \simeq \langle p | m \rangle = \delta_{mp} , \quad (15)$$

where  $\delta_{mp}$  is the Kronecker delta function. A direct consequence is the possibility of creating propagating states in a linear superposition of transverse states by using an interacting potential of the form (14) where the Hermite polynomial  $H_m$  is replaced by a sum of Hermite polynomials.

### 3. Coherence length of a guided atom laser

#### 3.1. Thermodynamical model

The coherence properties of a guided continuous atom laser have been investigated in Ref. [34]. This study assumes the propagating beam to be transversally confined (with two transverse dimensions  $x$  and  $y$ ) and at thermal equilibrium in the frame moving at its mean velocity. To characterize the coherence properties, one has to compute the correlation functions for the atomic field operator  $\hat{\Psi}(x, y, z)$  in close analogy with their counterpart in optics [38]. The first order correlation function is defined by

$$g_1(X) = \langle \hat{\Psi}^\dagger(0, 0, 0) \hat{\Psi}(X, 0, 0) \rangle \quad (16)$$

and is sensitive to the coherence of the atomic field between two points on the axis separated by a distance  $|X|$ . For an ideal Bose gas, one finds an exponential decay with a characteristic length  $\xi$ :

$$g_1(X) \simeq \frac{m\omega_\perp n_1}{\pi\hbar} e^{-|X|/\xi}, \quad \text{where} \quad \xi = \frac{\lambda^2 n_1}{2\pi}, \quad (17)$$

$\lambda = h/\sqrt{2\pi m k_B T}$  is de Broglie wave length and  $n_1$  is the linear atomic density. For a weakly interacting Bose gas, the coherence length is magnified by a factor 2 [39]. The exponential decay of the first order correlation, in contrast to the result obtained for a three-dimensional homogeneous Bose-Einstein condensate, is due to thermal excitation

and intrinsically related to the fact that there is no Bose-Einstein condensation in a one-dimensional box in the thermodynamical limit. For the guided atom laser of Ref. [3], one finds  $\xi \sim 7 \mu\text{m}$ .

### 3.2. Scattering approach

However, it is not clear to which extent this thermodynamical model can be applied to the guided atom lasers generated so far by outcoupling atoms from Bose Einstein condensates. A different approach makes use of the scattering formalism described in Sec. 1. Indeed, formally one can write any incoming wave packet in terms of the scattering eigenfunctions  $\{|\psi_k\rangle\}$  in space representation as

$$\varphi_0(x, y) = \int_0^{+\infty} \frac{dk}{2\pi} \alpha(k) \psi_k(x, y) \quad \text{with} \quad \alpha(k) = \int_0^{+\infty} dx e^{-ikx} \varphi_0(x, y). \quad (18)$$

The time evolution of the wavefunction can then be written as

$$\varphi(x, y; t) = \int_0^{+\infty} \frac{dk}{2\pi} \alpha(k) \psi_k(x, y) \exp\left(-i \frac{\hbar^2 k^2}{2m} t\right). \quad (19)$$

Therefore, the correlation function of the wavefunction is obtained formally in the form:

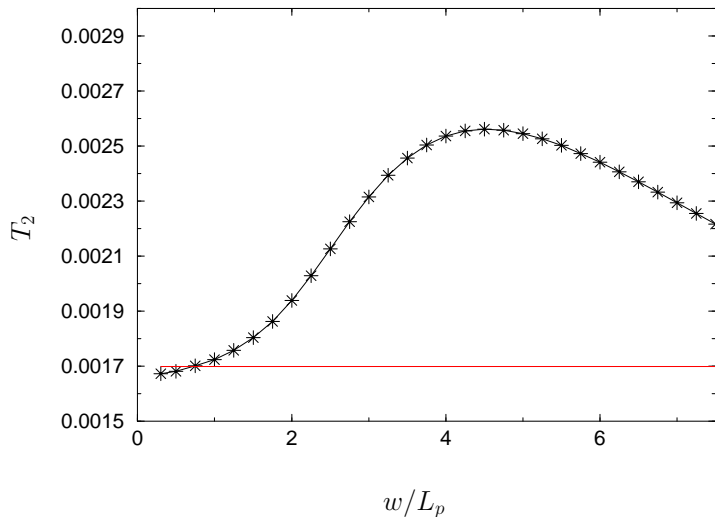
$$g_1(X) = \langle \varphi^*(x, y; t) \varphi(x + X, y; t) \rangle = \int_0^{+\infty} \int_0^{+\infty} \frac{dk}{2\pi} \frac{dk'}{2\pi} \langle \alpha^*(k) \alpha(k') \rangle \psi_k^*(x, y) \psi_{k'}(x + X, y) \exp\left(-i \frac{\hbar^2 (k'^2 - k^2)}{2m} t\right). \quad (20)$$

In the following, we show how the interaction of a guided atom laser with a defect of an adjustable size provides information on the coherence length.

### 3.3. Measuring the coherence length using a localized potential

As discussed above, the scattering of a wave packet can be described by the scattering of a coherent superposition of plane waves. The Born approximation remains valid for each plane wave of the wave packet when its dispersion  $\delta k$  is small compared to its mean wave vector  $k_0$ . In this regime the scattering turns out to be well described by the Born approximation result for a plane wave of wave vector  $k_0$ . In Sec. 2, we have used this regime of parameters.

Let us discuss the domain of validity of Born approximation by considering the first excited state (most populated). When the kinetic energy in this excited state tends to zero the Born approximation breaks down because of the  $1/k_2$  dependence of the reflection and transmission coefficients (see Eqs. (12)). This affects significantly the wave packet scattering. Indeed, in Fourier space, one can distinguish three different zones of wave vectors  $k$ : those sufficiently large so that Born approximation for  $k_0$  remains valid, those for which the incident energy is not sufficient to populate any excited states, and an intermediate zone where the Born approximation first increases the scattering to the excited state then breaks down because of the divergence in  $1/k_2$ . When the dispersion in  $k$  increases, one thus should expect an enhancement of the occupation of the excited state when the intermediate zone becomes significantly populated. A further increase



**Figure 3.** Transmissions  $T_2$  to the transverse state  $n = 2$  from the numerical simulations (black stars), as a function of the ratio of the width of the localized potential,  $w$ , over the longitudinal length of the initial wave packet,  $L_p$ , for  $w = 1 \mu\text{m}$  and power  $P = 10^{-7} \text{ W}$ . Except for  $L_p$ , the initial wave packet parameters are the same as in Fig. 1. Red horizontal line corresponds to the prediction of the Born approximation for an incoming plane wave of momentum  $\hbar k_0$ . We analyzed the scattering after the same evolution time for each  $L_p$ .

of the dispersion in  $k$  should eventually at some point decrease the population of the excited state as the momenta when no scattering occurs have more and more weight in the wave packet.

Figure 3 shows the results of the simulation of wave packets of different size compared to the Born approximation for  $k_0$ . One sees clearly an increase in the population of the excited state of more than 50 % starting from a longitudinal length  $L_p \approx 1 \mu\text{m}$ . This increase is followed by a decrease for smaller values of  $L_p$ , as predicted by the theory. Actually, in this non stationary regime, the precise maximum value obtained for  $T_2$  depends on the time at which the observation is made, since a part of the wave packet has very small velocity components. Larger  $L_p$  can be probed, for instance, by decreasing the initial velocity.

In summary, there is a regime of parameters in  $k$  for which the scattering strongly depends on the longitudinal size  $L_p$  of the wave packet. The breakdown of Born approximation in this regime may enable to probe the coherence length ( $\propto (\delta k)^{-1}$ ) of the atoms from measurements of the population of the transverse modes through the interaction of the matter wave. Note that other techniques, developed for quasi-condensate in very elongated geometry, could be envisioned to determine the coherence length such as Bragg spectroscopy [40] or ballistic expansion [41].

#### 4. Non-perturbative treatment

The results presented so far are valid only within the Born approximation. The higher order terms of the expansion (4) couples not only the ground state with the  $m^{\text{th}}$  mode, but also any modes  $i$  and  $j$  such that  $|i - j| = m$ . In the non-perturbative limit, the interaction of the matter wave with the potential (14) cannot selectively populate only one level. More generally, the complete calculations beyond the Born approximation can be performed by determining the contribution of the successive orders terms in the expansion (4). This strategy turns out to be cumbersome and, in addition, the convergence of the series is not necessarily ensured. In this section, we detail a matrix approach inspired by the theory of vibrational energy transfer between simple molecules in non-reactive collisions [31] or similarly by inelastic quantum scattering theory [42]. This method is non-perturbative with respect to the potential strength  $U_0$ , and therefore yields the non-perturbative response of the atom laser propagation while propagating through the localized potential.

##### 4.1. Matrix formalism

This approach consists of (i) expanding the scattering wave solution in terms of the transverse harmonic oscillator wave functions as  $\psi(x, y) = \sum_n \phi_n(x) \psi_n(y)$ , and (ii) taking the scalar product of the Schrödinger equation in the presence of the localized potential with a given  $m$  state of the transverse harmonic oscillator. In this way, we find that the longitudinal function  $\phi_n(x)$  obeys a set of coupled second-order linear equations:

$$\left[ \frac{d^2}{dx^2} + k_m^2 - \tilde{U}_{m,m}(x) \right] \phi_m(x) = \sum_{n \neq m} \tilde{U}_{m,n}(x) \phi_n(x) \quad (21)$$

with  $\tilde{U}_{m,n}(x) = 2m \langle m | U(x, y) | n \rangle / \hbar^2$ . The terms involving only the  $m$  index describe the “elastic” component of the scattering, while the term which involves  $\tilde{U}_{m,n}$  (with  $m \neq n$ ) is responsible for the coupling channel dynamics between the different transverse oscillator states. In the absence of the coupling term  $\tilde{U}_{m,n}$ , Eq. (21) provides an infinite set of one-dimensional scattering problems in the renormalized potentials  $\tilde{U}_{m,m}$ . The coupling between these 1D problems due to the right hand side terms of Eq. (21) gives rise to new resonances, as discussed in Sec. 4.4 on a particular example, that are reminiscent of the coupled channel theory used to describe Feshbach resonances [43].

The set of Eqs.(21) must be solved subject to the asymptotic conditions (equivalent to Eqs. (7) and (8)) that an incident flux is coming from the right with a wave vector  $k_0$  and in the transverse ground state, while reflected and transmitted fluxes of wave vectors  $-k_n$  and  $k_n$  respectively with a transverse wave function occupying the  $n^{\text{th}}$  oscillator state are moving out to the left and the right respectively:

$$\phi_n(x \rightarrow -\infty) = \langle x | k_0 \rangle \delta_{n,0} + r_n \langle x | -k_n \rangle, \quad (22)$$

$$\phi_n(x \rightarrow \infty) = t_n \langle x | k_n \rangle. \quad (23)$$

Through conservation of the probability current, the coefficients  $r_n$  and  $t_n$  are related by

$$k_0 = \sum_{n=0}^{N_p} k_n (|r_n|^2 + |t_n|^2), \quad (24)$$

where  $N_p$  denotes the number of propagating modes. Such a relation is particularly useful for checking the validity of numerical solutions, and permits one to define the level of contamination of a transverse “vibrational” state,  $n$ , both for the reflection  $R_n = k_n |r_n|^2 / k_0$  and the transmission  $T_n = k_n |t_n|^2 / k_0$  with the normalization rule  $\sum_{n=1}^{N_p} (R_n + T_n) = 1$ .

#### 4.2. Link with Green’s function formalism

In this section, we show how the matrix approach is consistent with the Green’s function formalism. The relation between both formalism can be made readily explicit within the Born approximation. Let us project Eq. (4) limited to the first power in  $U$  on the  $n^{\text{th}}$  oscillator state ( $n \neq 0$ )  $\langle \psi_n | \varphi \rangle(x) = \int dx' g^+(x, x'; E, n) \langle \psi_n | U | \psi_0 \rangle(x')$ . Since  $g^+(x, x'; E, n)$  is the Green’s function of the one-dimensional Schrödinger equation, the integral equation for  $\langle \psi_n | \varphi \rangle(x)$  means that  $\phi_n(x) = \langle \psi_n | \varphi \rangle(x)$  is solution of the equation:

$$\left[ \frac{d^2}{dx^2} + k_n^2 \right] \phi_n(x) \simeq \tilde{U}_{n,0}(x) \phi_0(x). \quad (25)$$

This equation is the same as Eq. (21) where higher order terms are neglected. Only the dominant contribution that involves  $\phi_0$  remains, since the wave function is marginally altered by the localized potential within the Born approximation. More elaborated approximation schemes such as the distorted wave approximation could also be worked out in this context [42].

#### 4.3. A simple example

Let us consider the following model potential

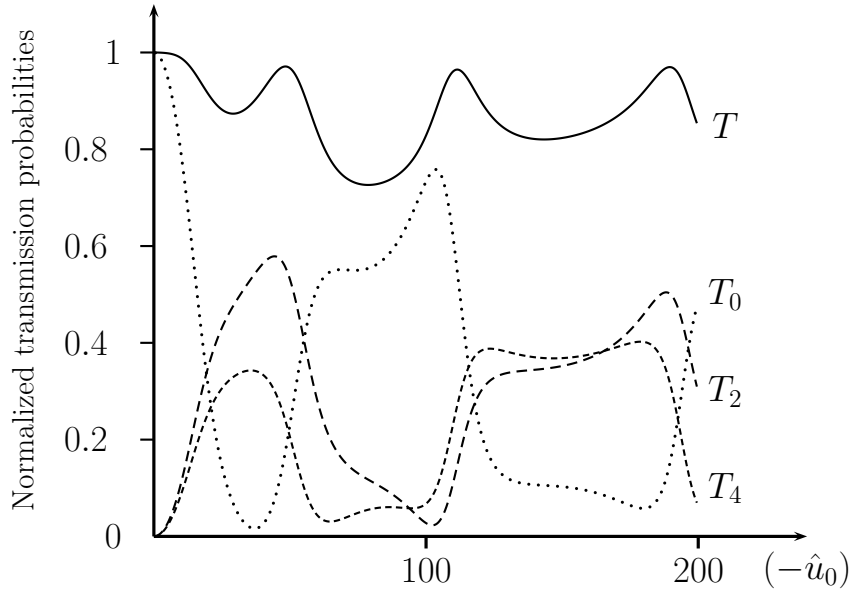
$$U(x, y) = -U_0 u_b(x; L_x) u_b(y - L_y; 2L_y), \quad (26)$$

where  $u_b$  is the square function  $u_b(x; L_x) = \Theta(x) \Theta(L_x - x)$  with  $\Theta(x)$  the Heaviside function. The localized potential is therefore centered transversally. In the regions  $x \leq 0$  and  $x \geq L_x$ , the wavefunction  $\phi_n$  is given by the Eqs. (22) and (23) respectively. In the region of the localized potential, one has to solve the equation:

$$\frac{d^2 \vec{f}}{dx^2} + \mathbf{M} \vec{f} = 0, \quad (27)$$

where  $\vec{f}$  is the vector of coordinate  $(\phi_0, \phi_1, \dots, \phi_n, \dots)$  and  $\mathbf{M}$  the matrix of elements  $\mathbf{M}_{n,n'} = k_n^2 \delta_{n,n'} - \tilde{U}_{n,n'}$ . The method used to solve this linear set of equations with the potential (26) is detailed in Appendix B

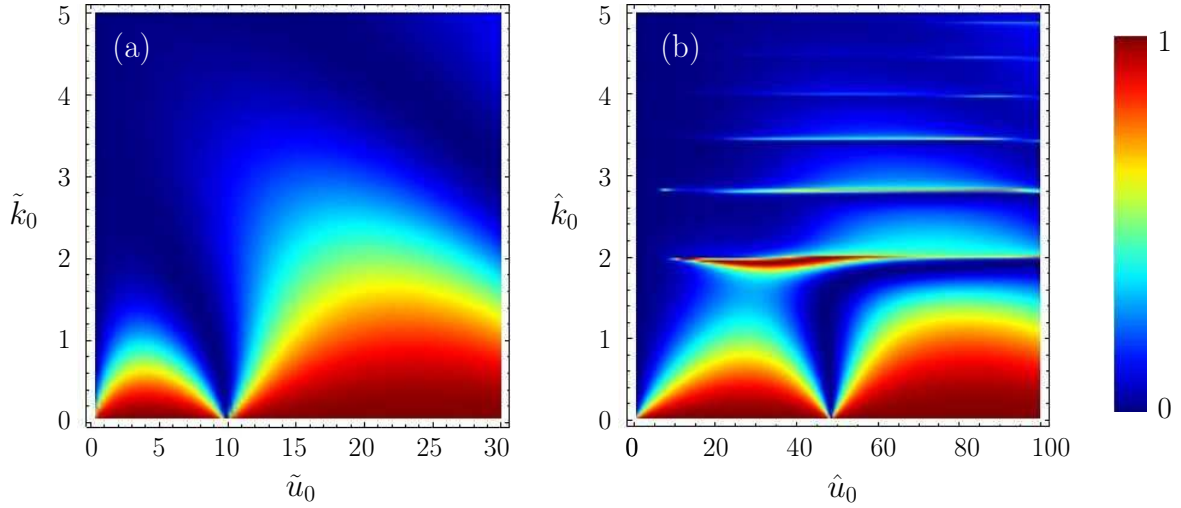
As an example, we have plotted in Fig. 4 the total transmission probability  $T$  along with the transmission probabilities,  $T_n$ , in each propagating mode ( $n = 0, 2$  and  $4$ ) as



**Figure 4.** Total probability of transmission  $T = \sum_n T_n$  (solid line), and the probabilities of reflection  $T_n$  in the transverse state  $n$  (dotted and dashed lines), as a function of the normalized depth  $\hat{u}_0 = 2ma_0^2 U_0 / \hbar^2$  as a result of the interaction of a guided matter wave with incoming longitudinal wave vector  $k_0 = 3.3/a_0$  with a square localized potential (see Eq. (26) with  $L_x = a_0$  and  $2L_y = 0.5a_0$ . In this example, there are  $N_p = 3$  even propagating modes.

a function of the normalized depth  $\hat{u}_0 = 2ma_0^2 U_0 / \hbar^2$ . In this example, the incident wave vector is  $k_0 = 3.3/a_0$  (there is therefore only  $N_p = 3$  propagating modes) and the potential is chosen of the form Eq. (26) with  $L_x = a_0$  and  $2L_y = 0.5a_0$ .

The interaction of the matter wave with the localized potential leads to nearly total transparency for some discrete specific values of the depth of the well ( $\hat{u}_0 \simeq -48.5, 111.5, 189.5$  in Fig. 4). This phenomenon is reminiscent of the “Ramsauer-Townsend” effect in one-dimensional scattering [44]. Conversely, resonances with a large fraction of the wave retro-reflected also occur for discrete values of the well depth. Those resonances correspond to “quasi bound states” for which the matter wave remains in the well for a maximum time. In the case studied in this article, with accessible excited oscillator states as output channels, new resonances occur with, for instance, a maximum probability of transmission  $T_2$ , i.e. with the transverse oscillator state  $n = 2$  more populated than the other modes. An example is provided in Fig. 4 for the transmission probabilities at  $\hat{u}_0 \simeq -44.5$ , where less than 5% of the wave is reflected and for which  $T_0 \simeq 0.08$ ,  $T_2 \simeq 0.58$  and  $T_4 \simeq 0.3$ . At the exit of the localized potential region, the state of the guided atom laser is a linear superposition of the propagating eigenvectors  $|k_n, n\rangle$ . The coefficients in front of each eigenvector are governed by the shape of the potential and can, therefore, be adjusted.



**Figure 5.** (a) Reflection probability for a one-dimensional square well of length  $L$  and depth  $U_0$  as a function of the incident wave vector  $\tilde{k}_0 = k_0 L$  normalized to  $L$  in ordinate and the potential depth  $\tilde{u}_0 = 2mL^2U_0/\hbar^2$ . Total reflection occurs when the incident energy is low compared to the potential depth. (b) Total reflection probability  $R = \sum_n R_n$  for a 2D scattering problem with a harmonic confinement in the transverse and a localized potential of the form (26) as a function of the incident wave vector,  $\hat{k}_0 = k_0 a_0$ , normalized to the oscillator length  $a_0 = (\hbar/m\omega_\perp)^{1/2}$  on the vertical axis and the potential depth  $\tilde{u}_0 = 2ma_0^2U_0/\hbar^2$ . Resonances in the reflection probabilities are observed for discrete values of the incident wave vector:  $k_0^{(n)} = (2n/a_0)^{1/2}$ , they correspond to resurgences of quantum reflection due to the coupling between transverse and longitudinal degrees of freedom.

#### 4.4. Total reflection resonances

Let us consider a one-dimensional square potential well of length  $L$  and depth  $U_0$ . The total reflection probability  $R$  for an incident wave vector  $k_0$  reads

$$R(\tilde{k}_0, \tilde{u}_0) = \frac{(\tilde{k}_0^2 - \tilde{q}^2)^2 \sin^2 \tilde{q}}{(\tilde{k}_0^2 + \tilde{q}^2)^2 \sin^2 \tilde{q} + 4\tilde{k}_0^2 \tilde{q}^2 \cos^2 \tilde{q}}, \quad (28)$$

where we have introduced the dimensionless parameters  $\tilde{k}_0 = k_0 L$ ,  $\tilde{u}_0 = 2mL^2U_0/\hbar^2$ , and  $\tilde{q} = (\tilde{k}_0^2 + \tilde{u}_0)^{1/2}$ . A total quantum reflection is obtained when the incident energy is low compared to the potential depth,  $\tilde{k}_0^2 \ll \tilde{u}_0$ , as illustrated in Fig. 5a.

One may wonder how this purely quantum effect is affected by the confinement. For this purpose, we consider the model potential of Eq. (26) with  $L_x = a_0$  and  $L_y = 0.1 a_0$ . The total reflection probability  $R = \sum_n R_n$  as a function of the normalized incident wave vector,  $\hat{k}_0 = k_0 a_0$ , and the potential depth,  $\tilde{u}_0 = 2ma_0^2U_0/\hbar^2$ , is represented in Fig. 5b. The matrix elements of the transverse potential renormalize the longitudinal potential, as it clearly appears in the set of Eqs. (21). In addition, we have chosen to normalize using the oscillator length  $a_0$ . The scales of the abscissa of the two figures 5a and 5b are therefore different. In Fig. 5b, one observes the appearance of new resonances for a set of discrete values of the incident wave vector,  $k_0^{(n)} = (2n/a_0)^{1/2}$ , that correspond to the opening of a new transverse channel accessible by the incident energy.

Our interpretation of these resonances is as follows; when the incident wave enters the localized potential zone, there is a strong coupling between transverse and longitudinal degrees of freedom. This coupling favors a virtual excitation of the transverse excited modes so that the longitudinal energy is, again, in a range for which total reflection occurs in 1D occurs. This effect is reminiscent of the confinement-induced resonances pointed out by M. Olshanii for atoms interacting through a Dirac potential under a strong transverse confinement [24, 25, 45].

The matrix approach carried out in this section can be readily generalized to a two dimensional transverse confinement at the expense of a much larger matrix  $\mathcal{M}$  for determining the transmission and reflection coefficients, since  $\mathcal{M}$  would be a  $2N(N+1) \times 2N(N+1)$  matrix.

## 5. Discussion and conclusion

The calculations described in this article are motivated by the recent realization of guided atom lasers in the ground state of the transverse confinement. The interaction of the matter wave with a localized potential where open and closed channels are accessible through the scattering of the matter wave on the potential is in direct analogy with non reactive chemical reaction and guided electronic wave propagation in mesoscopic physics.

The possibility of shaping the localized potential using techniques established in cold atom physics opens new perspectives:

- It allows for the generation and the manipulation of new kinds of entangled states that correlate longitudinal and external degrees of freedom. More complex potentials with a succession of interacting zones can be envisioned to code or stock information in the external degrees of freedom, or in both internal and external degrees. This latter prospect is reminiscent of the use of laser light for quantum computation with cold trapped ions [46].
- It provides a new method to determine the coherence length of a guided atom laser regardless of the thermodynamical equilibrium.
- It constitutes a new device to investigate coherent control of the population of the discrete energy levels after their interaction with the localized potential. As already emphasized, the control of the transmission output channels implies the shaping of the localized potential on the typical scale of the harmonic oscillator length corresponding to the transverse confinement§.
- It provides a test bed for inverse scattering problem in confined environment [47, 48]. For instance, it allows, in principle, to engineer potential with different shapes but with the same output after the interaction. It therefore enables the investigation

§ Another advantage of a very local action of the extra potential lies in the fact that the reflection or transmission effects become less sensitive to the de Broglie wavelength dispersion when the size of the potential decreases, and are therefore more robust with respect to the longitudinal monochromaticity of the incoming guided atom laser.



of the non linear functional relationship between the potential details and the scattering properties.

A natural extension of this work also lies in the inclusion of atom-atom interactions. Many new effects are expected. For instance, the propagation of an interacting beam through a constriction [6] (local increase in the strength of the transverse confinement) has no stationary solution if the compression is sufficiently high, but solitonic like solution [7]. This effect arises from the non linearity of the mean field term that describes the interactions. Other effects are connected to the quantum turbulent regime downstream the obstacle realized by the localized potential [49, 50]. Nonlinear atom optical effects are expected to arise from atom-atom collisional interactions in a single-mode atomic Fabry-Perot cavity driven by a coherent cw atom laser beam [51]. The role of interaction within the mean field description on quantum scattering problems is a fundamental issue related to the physics of non-linear Schrödinger equation that can be addressed with guided atom lasers [52].

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## Appendix A

In the Born approximation, the characterization of the interaction of a matter wave with a localized potential through the reflection and transmission amplitude coefficients requires the knowledge of the quantity  $\langle k_n, n | U | k_0, 0 \rangle$  (see Eq. 10). In this Appendix, we detail the calculation of this matrix element in the case of the Gaussian localized potential (11):

$$\langle k_n, n | U | k_0, 0 \rangle = \frac{U_0}{2\pi} \int_{-\infty}^{+\infty} e^{-i(k_n - k_0)x} e^{-2x^2/w_x^2} dx \underbrace{\int_{-\infty}^{+\infty} \psi_n^*(y) \psi_0(y) e^{-2y^2/w_y^2} dy}_{g_n}. \quad (29)$$

This expression contains two factors, the Fourier transform of the longitudinal Gaussian potential  $u_g(x/w_x)$  which can be easily calculated, and an integral  $g_n$  which involves the eigenfunctions of the harmonic oscillator, defined by:

$$\psi_n(y) = \frac{1}{\sqrt{a_{ho} n! 2^n \sqrt{\pi}}} H_n\left(\frac{y}{a_{ho}}\right) e^{-y^2/2a_{ho}^2} \quad (30)$$

where  $a_{ho} = (\hbar/m\omega_\perp)^{1/2}$  is the harmonic oscillator length, and  $H_n(u)$  are the Hermite polynomials of order  $n$ . The integral  $g_n$  can therefore be rewritten as

$$g_n = \int_{-\infty}^{+\infty} \frac{du}{\sqrt{2^n n! \pi}} H_n(u) e^{-u^2 \alpha^2}, \quad (31)$$

where we have introduced the two dimensionless parameters  $\eta = w_y/(2a_{\text{ho}})$  and  $\alpha^2 = 1 + 1/(2\eta^2)$ .

Let us calculate explicitly the generating function,  $f(z)$ , associated to the integrals  $g_n$ :

$$\begin{aligned} f(z) &= \sum_{n=0}^{+\infty} g_n \frac{z^n}{n!} = \frac{1}{\sqrt{2^n n! \pi}} \int_{-\infty}^{+\infty} \left( \sum_{n=0}^{+\infty} H_n(u) \frac{z^n}{n!} \right) e^{-\alpha^2 u^2} du \\ &= \frac{1}{\sqrt{2^n n! \pi}} \int_{-\infty}^{+\infty} e^{2uz - z^2} e^{-\alpha^2 u^2} du \\ &= \frac{1}{\sqrt{2^n n!}} \frac{1}{\alpha} \sum_{n=0}^{+\infty} \frac{z^{2n}}{n!} \left( \frac{1}{\alpha^2} - 1 \right)^n. \end{aligned} \quad (32)$$

Identifying the different terms of this last Taylor expansion with those of the definition of the generating function we deduce the expression for the integral,  $g_n$ :

$$\begin{aligned} g_{2p}(\alpha) &= \frac{1}{\sqrt{\pi(2p)!2^{2p}}} \frac{\sqrt{\pi}}{\alpha} \frac{(2p)!}{p!} \left( \frac{1}{\alpha^2} - 1 \right)^p \\ g_{2p+1}(\alpha) &= 0, \end{aligned} \quad (33)$$

where  $p$  is an integer. This calculation demonstrates equation (13).

Finally, we find:

$$\langle k_n, n | U_0 u_g(x/w_x) u_g(y/w_y) | k_0, 0 \rangle = \frac{U_0}{2\pi} \sqrt{\frac{\pi}{2}} w_x e^{(k_{2p}-k_0)^2 \frac{w_x^2}{8}} g_{2p}(\eta). \quad (34)$$

## Appendix B

To find the solution of Eq. (27), one needs to diagonalize the matrix  $\mathbf{M}$ . Let us introduce the matrix  $\mathbf{P}$  such that  $\mathbf{M} = \mathbf{PDP}^{-1}$  and the vector  $\vec{\ell} = \mathbf{P}^{-1} \vec{f}$ , Eq. (27) can be rewritten in the diagonal form  $\vec{\ddot{\ell}} + D\vec{\ell} = 0$  whose solution reads

$$\vec{f}(x) = \mathbf{P} e^{iD^{1/2}x} \vec{a} + \mathbf{P} e^{-iD^{1/2}x} \vec{b}, \quad (35)$$

where  $\vec{a}$  and  $\vec{b}$  are vectors that are determined by imposing the continuity of the wave functions and their derivatives. Introducing the matrices  $\mathbf{Q} = \mathbf{D}^{1/2}$ ,  $(\mathbf{K})_{n,n'} = k_n \delta_{n,n'}$ ,  $\mathbf{X} = \exp(i\mathbf{Q}L)$ ,  $\mathbf{Z} = \exp(i\mathbf{K}L)$  and the vectors  $\vec{\delta}_0 = (1, 0, \dots, 0, \dots)$ ,  $\vec{r} = (r_0, r_1, \dots, r_n, \dots)$ ,  $\vec{t} = (t_0, t_1, \dots, t_n, \dots)$ , we find:

$$\vec{\delta}_0 + \vec{r} = \mathbf{P}(\vec{a} + \vec{b}), \quad (36)$$

$$\mathbf{K}(\vec{\delta}_0 - \vec{r}) = \mathbf{PQ}(\vec{a} - \vec{b}), \quad (37)$$

$$\mathbf{Z}\vec{t} = \mathbf{P}(\mathbf{X}\vec{a} + \mathbf{X}^{-1}\vec{b}), \quad (38)$$

$$\mathbf{KZ}\vec{t} = \mathbf{PQ}(\mathbf{X}\vec{a} - \mathbf{X}^{-1}\vec{b}). \quad (39)$$

By combining, this set of matrix equations one determines the unknown vector

$$\vec{r} = -[\mathbf{A}_+ \mathbf{X}^{-1} \mathbf{B}_+ + \mathbf{A}_- \mathbf{X} \mathbf{B}_-]^{-1} [\mathbf{A}_- \mathbf{X} \mathbf{B}_+ + \mathbf{A}_+ \mathbf{X}^{-1} \mathbf{B}_-] \vec{\delta}_0, \quad (40)$$

and infer from it the other unknown vectors

$$\begin{aligned}\vec{a} &= (\mathbf{B}_+ \vec{\delta}_0 + \mathbf{B}_- \vec{r})/2, \\ \vec{b} &= (\mathbf{B}_- \vec{\delta}_0 + \mathbf{B}_+ \vec{r})/2, \\ \vec{t} &= \mathbf{Z}^{-1} \mathbf{P} (\mathbf{X} \vec{a} + \mathbf{X}^{-1} \vec{b}),\end{aligned}\tag{41}$$

with  $\mathbf{A}_\pm = \mathbf{K} \mathbf{P} \pm \mathbf{P} \mathbf{Q}$  and  $\mathbf{B}_\pm = \mathbf{P}^{-1} \pm \mathbf{Q}^{-1} \mathbf{P}^{-1} \mathbf{K}$ .

In practice, it is important to take into account a sufficient number of evanescent modes to ensure the convergence of the result. For the results of Fig. 5, the number of propagating modes is  $N_p = 3$  (modes 0,2,4) but we have solved the equations detailed in this appendix using 25 modes since the convergence on the probabilities  $R_i$  and  $T_i$  was obtained with typically 15 modes for our parameters.

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