

Reflection of matter waves in potential structures

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In this paper the behavior of matter waves in suddenly terminated potential structures is investigated numerically. It is shown that there is no difference between a fully quantum mechanical treatment and a semiclassical one with regards to energy redistribution. For the quantum case it is demonstrated that there can be substantial reflection at the termination. The neglect of backscattering by the semiclassical method brings about major differences in the case of low kinetic energies. A simple phenomenological model is shown to partially explain the observed backscattering using dynamics of reduced dimensionality.

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I. INTRODUCTION

Rapid advances in the fields of trapping and cooling of neutral atoms [1,2] and atom optics [3] have taken place during the past few years, especially after the first creation of a Bose-Einstein condensate (BEC) [4]. The experimental realization of traps for thermal clouds confined in one or more dimensions has been achieved using hollow glass tubes [5,6] and microfabricated current carrying structures [7]. Further progress has resulted in loading of a BEC into a waveguide using optical trapping [8], the creation of a BEC above a microcircuit [9], and loading of a BEC into a waveguide using optical tweezers [10].

Work is in progress to create the atom-optical analogs of standard optical components relying on waveguide structures like, for instance, directional couplers [11] and interferometers [12]. This development is partially spurred by the possibilities of utilizing matter-wave guides for quantum logic [13] and Bell state measurements [14].

Numerical wave packet dynamics [15] has proved to be very useful for studies of quantum dynamical systems, to devise phenomenological models and understand experimental results. In this work we consider propagation of wave packets on two-dimensional potential energy surfaces, the highest dimensionality comfortably available for numerical work at present. In the lowest approximation, the center of the wave packet may be assumed to propagate close to the classical minimum of the potential valley. In these systems it is natural to use a separation into channels or modes to simplify the problem as the dynamics is essentially one dimensional. In the quantum mechanical case this method was used early in chemical reaction theory [16], and is at present a standard method [17]. In previous work the limitations of this approach due to mode coupling were examined [18], and it was shown that the breakdown of adiabatic following of the transverse modes was connected to diffraction of matter waves. The connection with diffraction was shown also for the transition from adiabatic propagation to free expansion in [19]. Another technique commonly used takes advantage of assemblies of classical particles propagating in the force field given by the binding potential [20]. This method neglects

certain wavelike properties but stresses the similarities between classical and quantum dynamics. One major difference that is neglected is backscattering in the case of energetically allowed propagation. This was recently observed for Bose-Einstein condensates in waveguide geometries [10].

The main difference between classical and quantum dynamics is the influence of wave interference in the latter case. In this paper we show that the adiabatic redistribution of energy between longitudinal and transverse degrees of freedom does not differ between the classical and quantum cases. When the potential structure gives rise to backscattering, however, this derives solely from the wave features of propagation. This holds in both the adiabatic and nonadiabatic limits. When adiabaticity is negligible, the emergence of the wave packet from the potential structure can be viewed as a sudden release from guided propagation to free travel. In the adiabatic case, the scattering is essentially described by a one-dimensional potential model for the longitudinal propagation; the transverse degrees of freedom only act to set up the effective potential.

In Sec. II we discuss the problem of propagation in a waveguide that is terminated in a smooth manner. Both a fully quantum mechanical wave-packet treatment and a semiclassical one utilizing assemblies of particles are used. Section III discusses the presence of backscattering in the system under consideration. Finally, Sec. IV discusses the conclusions of the work.

II. PROPAGATION

We consider a general quantum mechanical problem with time independent Hamiltonian in a two-dimensional configuration space. The dynamics will then evolve according to the time dependent Schrödinger equation

$$i \frac{\partial \Psi(x, y, t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi(x, y, t) + V(x, y) \Psi(x, y, t). \quad (1)$$

Here, as in the rest of this paper, we use dimensionless quantities corresponding to $\hbar = 1$ and $m = 1$. In the case of guided matter waves the propagation will occur along the minimal valley of the potential energy surface, which for our purpose is taken to form a straight line with harmonic binding in the transverse direction,

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$$V(x,y) = V(x,0) + \frac{1}{2} \omega(x)^2 y^2. \quad (2)$$

In potential structures with minima it is common to use adiabatic approximations (see [18] and references therein), to gain insight into the dynamics and also to reduce the computational complexity of numerical simulations. In our case the potential allows us to separate the wave function, writing

$$\Psi(x,y,t) = \sum_{n=0}^{\infty} \phi_n(x,t) \eta_n(x,y), \quad (3)$$

where the set of transverse modes can be chosen to be the harmonic oscillator eigenfunctions

$$\eta_n(x,y) = \left(\frac{1}{\sqrt{\pi 2^n n!}} \Delta y(x) \right)^{1/2} e^{-(1/2)y^2/\Delta y(x)^2} \times H_n \left(\frac{y}{\Delta y(x)} \right) \quad (4)$$

with

$$\Delta y(x) = \frac{1}{\sqrt{\omega(x)}}. \quad (5)$$

The longitudinal wave functions $\phi_n(x,t)$ carry the time dependence. Inserting Eqs. (3) and (4) into Eq. (1), multiplying by $\eta_m(x)$ followed by integration over the transverse coordinate x , and using the orthonormality of the basis set, we arrive at

$$i \frac{\partial \phi_m}{\partial t} = -\frac{1}{2} \frac{\partial^2 \phi_m}{\partial x^2} + \left[V(x,0) + \frac{1}{2} \omega(x) \left(n + \frac{1}{2} \right) \right] \phi_m + \sum_{n=0}^{\infty} A_{nm}(x) \frac{\partial \phi_n}{\partial x} + B_{nm}(x) \phi_n, \quad (6)$$

where the kinetic couplings are given by

$$A_{n,m}(x) = -\frac{1}{2} \int_{-\infty}^{\infty} \eta_n(x,y) \frac{\partial \eta_m(x,y)}{\partial x} dy, \quad (7)$$

and the potential couplings by

$$B_{n,m}(x) = -\frac{1}{2} \int_{-\infty}^{\infty} \eta_n(x,y) \frac{\partial^2 \eta_m(x,y)}{\partial x^2} dy. \quad (8)$$

If the potential energy surface changes sufficiently slowly over lengths comparable with the de Broglie wavelengths of the wave packet, we expect the couplings between transverse states to be negligible. As a consequence, the corresponding one-dimensional equations decouple, resulting in adiabatic following of the transverse states as the wave packet propagates in the longitudinal direction. For most cases, the expansion of a smooth wave packet in the adiabatic eigenbasis $\{\eta_n(x,y)\}$ converges rapidly, and allows us to retain only a limited, in many cases small, number of transverse modes.

Ignoring the coupling between the modes, the full problem can be described by the set of equations

$$i \frac{\partial \phi_n}{\partial t} = -\frac{1}{2} \frac{\partial^2 \phi_n}{\partial x^2} + A_{nn}(x) \frac{\partial \phi_n}{\partial x} + \left[\frac{1}{2} \omega(x) \left(n + \frac{1}{2} \right) + B_{nn}(x) \right] \phi_n, \quad (9)$$

where the potential energy variation along the minimal curve has been omitted. The transverse eigenenergies together with the diagonal potential couplings, i.e., $\frac{1}{2} \omega(x) (n + \frac{1}{2}) + B_{nn}(x)$, act as effective one-dimensional potentials in the adiabatic limit, and they are referred to as adiabatic energies here. If, on the other hand, the transverse curvature changes rapidly, the different modes will not have sufficient time to experience adiabatic following. As a result, the wave packet is left in a coherent superposition where the expansion coefficients are given by projection on the new eigenstates. In the case of a sudden widening of the potential, causing the oscillator frequency to be significantly lower than initially, the guided wave essentially starts to behave like a free wave packet. This is considered as the case when the new eigenstates are given by plane waves. Such an event looks like the collimated ejection of a wave packet, retaining its shape from before the abrupt opening. The wave packet starts to expand in the transverse direction immediately after the ejection. If the oscillator frequency $\omega(x)$ starts to approach zero exponentially with the longitudinal distance, the adiabatic following ceases, and free spreading starts. If significant adiabatic adjustment takes place, the emerging momentum spread is much smaller than initially, causing a slower spreading. The transverse energy will then be converted into longitudinal kinetic energy and the wave packet will in general be accelerated during the process. In [19] the termination of matter-wave guides was investigated numerically in order to test how sensitive the dynamics is to the parameters involved in the transition. The oscillator frequency $\omega(x)$, as a function of distance, was taken to be

$$\omega(x) = \frac{\omega_0}{2} \left[1 - \tanh \left(\frac{x}{L} \right) \right]. \quad (10)$$

For large negative values, this potential allows adiabatic propagation according to Eq. (6), whereas, beyond a transition region around $x=0$, it goes to zero exponentially and allows the wave packet to expand freely. The length L is here taken to be the distance over which the transverse oscillator frequency decreases enough to cause a transition from adiabatic guiding to free propagation.

Physically the wave function describes an ensemble of identically prepared quantum systems. According to Ehrenfest's theorem [21], we have

$$\frac{d\langle x \rangle}{dt} = \langle k_x \rangle,$$

$$\frac{d\langle y \rangle}{dt} = \langle k_y \rangle,$$

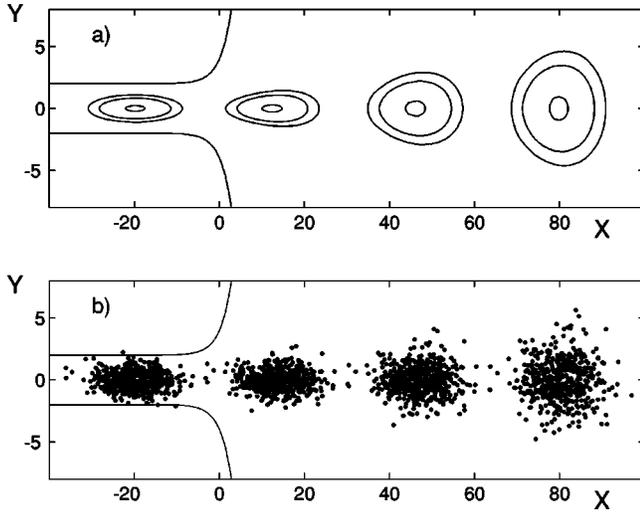


FIG. 1. Snapshots, taken at four equidistant times, of a wave packet propagating with momentum $k=40$ in the potential given by Eqs. (2) and (10) with the parameters $\omega_0=1$, $L=5$. The Fresnel number here is $N=4/\pi \approx 1.3$. It is seen from Fig. 2 below that there is almost negligible adiabatic redistribution in the transverse direction before exit. In (a) results from a wave-packet simulation are shown; in (b) an assembly of classical particles. The units have been chosen dimensionless.

$$\frac{d\langle k_x \rangle}{dt} = - \left\langle \frac{\partial V(x,y)}{\partial x} \right\rangle \approx - \frac{\partial V(\langle x \rangle, \langle y \rangle)}{\partial \langle x \rangle},$$

$$\frac{d\langle k_y \rangle}{dt} = - \left\langle \frac{\partial V(x,y)}{\partial y} \right\rangle \approx - \frac{\partial V(\langle x \rangle, \langle y \rangle)}{\partial \langle y \rangle}. \quad (11)$$

In other words, the center of mass motion can approximately be described by classical equations of motion. This implies that another way to simulate the system is using an assembly of classical particles with positions and velocities distributed as for the corresponding wave packet. Equation (11) has the advantage of being a small set of ordinary differential equations whereas both Eqs. (1) and (9) are partial differential equations whose numerical solution is considerably more demanding [15]. On the other hand, solution of Eqs. (11) has to be repeated until the statistical fluctuations in the quantities of interest have been reduced enough. As for general Monte Carlo methods, the inaccuracies decay as $1/\sqrt{M}$, where M is the number of events used.

In Fig. 1, the time evolution for wave packets initially in the transverse ground state of the potential given by Eqs. (2)–(10) is shown at four different times, in (a) for a quantum mechanical wave packet and in (b) for an assembly of particles propagating according to Eq. (11). The snapshots show the propagation out and away from the guiding region. The distributions, of both the quantum mechanical (QM) wave packet and the classical (CL) assembly, start spreading with time after exit. There appears to be little difference between the two cases as the spreading takes place at the same rate. Also, the propagation in the longitudinal direction occurs at equal speeds, indicating that the difference in speedup is negligible. The similarity between the behavior of the QM

and CL assemblies is to be expected under circumstances when wavelike behavior like, for instance, interference and reflection can be ignored. Using a fully quantum mechanical wave packet treatment, it was found in [19] that the amount of redistribution of energy at the exit is a function of a single parameter only. The relevant quantity, here shown in dimensional units for clarity, is defined as

$$Q \equiv \frac{\hbar \Delta k_y^2}{m \omega_0}. \quad (12)$$

This quantity Q is a measure of the adiabatic redistribution of transverse binding energy into longitudinal kinetic energy before the propagation ceases to be adiabatic. The adiabaticity properties of guided matter waves with respect to changes in the confining potential are determined by a single dimensionless parameter, the Fresnel parameter

$$N = \frac{\hbar}{m L \lambda \omega_0} = \frac{\Delta y_0^2}{L \lambda}, \quad (13)$$

where λ is the longitudinal de Broglie wavelength and Δy_0 denotes the transverse width of the ground state in the guiding region. It was found that adiabatic propagation takes place when the changes are such that the Fresnel parameter is small, $N \ll 1$. Equation (13) is for clarity given in dimensional units including the particle mass and Planck's constant. In [19] it was further shown that this parameter also determines the behavior at the transition from adiabatic to completely nonadiabatic propagation, i.e., free propagation. In order to investigate whether or not there is any difference between the quantum mechanical treatment based on wave packet propagation and a classical treatment using assemblies of particles as described above, the amount of adiabatic redistribution as a function of the Fresnel parameter has been determined numerically for assemblies of classical particles with positions and velocities distributed according to the Wigner functions of the initial states used in [19]. This simulation was repeated for different values of the potential parameters and longitudinal momentum. After propagation at least two Rayleigh lengths away from the potential opening, the transverse momentum width was determined numerically according to

$$\Delta k_y^2 = \langle k_y^2 \rangle = \frac{1}{M} \sum_{i=0}^M \langle k_y \rangle_i^2, \quad (14)$$

where the sum is over the individual particles in the assembly. In order to achieve negligible variance in the results, assemblies with $M=10^7$ particles were used.

In Fig. 2 the value of Q as defined in Eq. (12) is plotted versus the Fresnel parameter N . The solid line shows results of the wave packet calculation of [19] and the open circles show results from classical assemblies as described above. No difference can be seen between the two approaches. It can thus be concluded that the transition from adiabatic propagation in the guiding region to free spreading is similar for the quantum mechanical and classical cases. It should

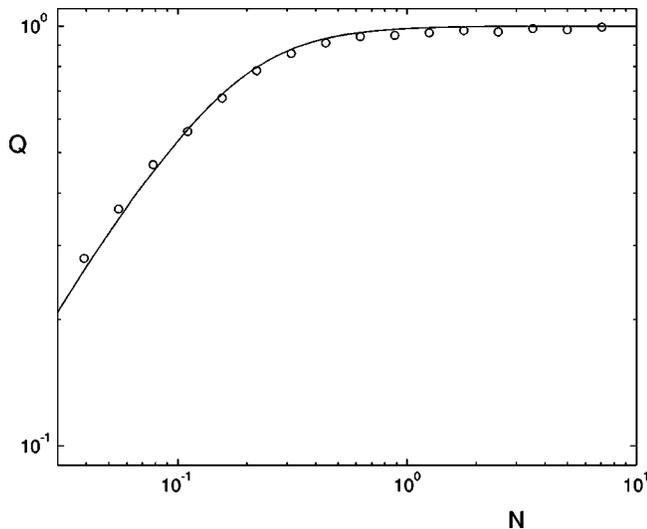


FIG. 2. Relative change in transverse energy after exit from adiabatic propagation, as defined by Eqs. (12)–(14), versus the Fresnel parameter. Open circles correspond to results due to assemblies of classically propagated particles, the solid line to a wave-packet calculation. The quantity Q is the ratio between the transverse energy after the wave packet has ceased to perform adiabatic following in the widening potential and the incoming oscillator energy. This has been computed for wave packets propagating in the potential given by Eqs. (2) and (10). The change is found to be a function of the dimensionless Fresnel parameter only, due to scaling invariance of the time dependent Schrödinger equation. The curve is seen to approach unity for large values of N , indicating that very little energy redistribution takes place. For smaller values of N , the relative change in energy can be substantial as is seen in the left part of the graph.

however be noted that the simulations have been carried out in a region where backscattering is expected to be very small.

III. BACKSCATTERING

In the framework of adiabatic propagation of wave packets, the governing equations contain all features of the potential locally around the minimal path. They enter either as sources of nonadiabatic transitions or as changes in the effective one-dimensional potentials for the different transverse modes. A narrowing will cause a steepening of the effective potentials, thus decreasing the wave-packet kinetic energy in the longitudinal direction. During propagation, in a one-dimensional potential, all changes of the potential may cause considerable backscattering of probability amplitude. Parts of a wave packet propagating adiabatically along a constant potential minimum in two or more dimensions may thus be backscattered due to changes in the transverse curvature. We can distinguish between three different sources of backscattering within our framework.

(1) Homogenous backscattering due to barriers that simply raise the bottom level $V(x,0)$ of the potential without affecting the transverse dynamics.

(2) Adiabatic backscattering due to rapid changes in the transverse curvature under the constraint $N \ll 1$. This requires

the longitudinal kinetic energy to be very small.

(3) Nonadiabatic backscattering due to more complex phenomena involving transitions between transverse modes. As total energy is conserved, transitions to higher modes will also cause conversion of kinetic energy into potential energy, thus affecting the longitudinal propagation.

The first and second sources can be understood using a one-dimensional picture without mode coupling, implying that backscattering will be negligible if the changes over one de Broglie wavelength in the potential minima and/or transverse energy are sufficiently small. If the kinetic energy is sufficiently low, the propagating wave packet will be very sensitive to changes in the transverse oscillator energy. It is known that reflection may occur in this case even for a decreasing potential, given that the change is rapid enough. To cause non-negligible reflection, the change in potential energy should be larger than the kinetic energy. If this is the case, the excitation to higher transverse modes will be classically forbidden and thus exponentially suppressed. In the potential structure under consideration here, this will be the case until the oscillator frequency has decreased enough to open the possibility for excitation as the energies of the excited states decrease with the frequency. Appreciable backscattering can thus occur for large changes in the transverse oscillator frequency given that these occur over distances long enough to be treated as adiabatic. The third case is the most difficult one as it includes coherent transfer between different states and will probably necessitate a thorough investigation of how the nonadiabatic couplings alter longitudinal dynamics. It is thus seen that in the full treatment, where all the couplings and all energetically allowed transverse modes are used, backscattering will be treated correctly, as is expected since the separation of variables introduced does not include any approximations. If the couplings are neglected, the third source of backscattering will be left out and only the first two will be modeled correctly. This approach will give correct results as long as there is negligible interaction between the different modes, i.e., when we have adiabatic propagation. We can also conclude that the amount of nonadiabatic backscattering can at most equal the total probability transferred between the modes, although it is likely to be much smaller than this unless the change in kinetic energy involved is considerable. As an example we can consider nonadiabatic transitions into higher transverse modes resulting in lower kinetic energy, which in turn might lead to homogeneous or adiabatic backscattering of probability of the higher mode even though the lower modes can propagate unreflected.

In Fig. 3 we see five snapshots of a wave packet with low kinetic energy taken at equidistant times during propagation toward an abrupt termination. As the termination around $x = 0$ is reached, part of the wave packet is reflected and is superposed on the incoming portions. As a result interference peaks are clearly seen. An asymmetry with respect to time is seen as the reflection is only partial, resulting in about 60% of the incoming wave packet remaining in the guided region.

To show the difference from classical mechanics, an assembly of particles was propagated through the same potential. The resulting dynamics is seen in Fig. 4 for the same

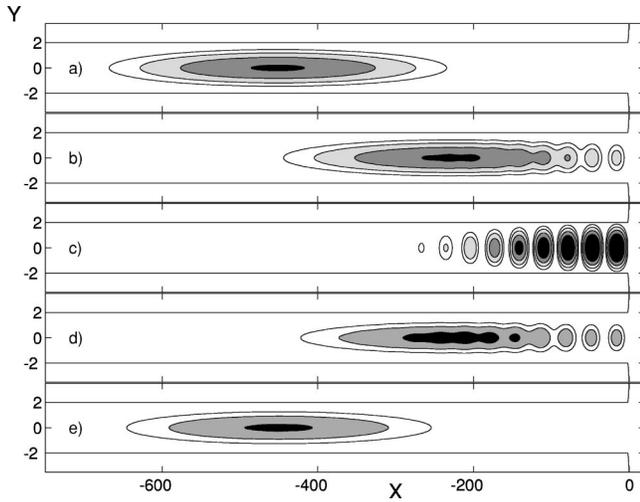


FIG. 3. Snapshots of the probability density for a wave packet with longitudinal momentum $k_x=0.1$ which is partly reflected and partly transmitted. The parameters for the potential, which is given by Eqs. (2) and (10), where $L=0.2$ and $\omega_0=1$. The initial Gaussian is shown together with subsequent times when it scatters against the waveguide termination. The final time has been chosen as twice the propagation time to the termination in order to make the initial and final wave packets overlap. In (b)–(d) the scattering against the termination takes place and interference between the incoming and backscattered parts of the wave packet is formed. From (a) and (e) it can be seen that the reflected probability density is smaller than the incoming. For these parameter values the backscattering amounts to about 60%. Due to energy conservation the reflection must occur back into the ground state mode as the kinetic energy is smaller than the gap between the ground and second excited states. The units have been chosen dimensionless.

times as in Fig. 3. All the particles in the assembly propagate out of the potential as is expected since the force field [right-hand side of Eq. (11)] is directed in the positive x direction everywhere.

In order to investigate the full longitudinal dynamics of this system we integrate the wave packet over the transverse direction:

$$p_{1D}(x,t) = \int_{-\infty}^{\infty} |\Psi(x,y,t)|^2 dx. \quad (15)$$

As a result we reduce the dynamics to a single spatial dimension. The reflection can be viewed in the reduced variables to extract more information. In Fig. 5 the projected probability density is shown as a function of longitudinal distance and time. The incoming Gaussian wave packet is seen to be partially reflected and partially transmitted. From the slope of the equiprobability contours in the (x,t) plane we see that the incoming and reflected wave packets have the same momentum, whereas the transmitted one has been accelerated due to transfer of energy from the transverse to the longitudinal degrees of freedom. There is a strong similarity between the reduced dynamics shown in Fig. 5 and one-dimensional potential scattering against a rapidly decreasing potential. In both cases there will, under the right circumstances, be partial reflection and partial transmission of an

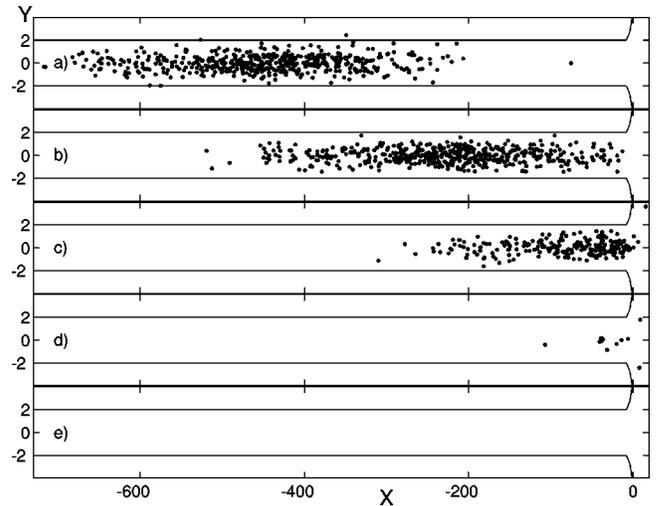


FIG. 4. Snapshots of an assembly of particles propagating in the potential given by Eqs. (2) and (10). The potential parameters are the same as used for the wave-packet propagation shown in Fig. 3. The initial conditions for the particles were chosen to mimic the propagation of the wave packet in Fig. 3. Although the adiabatic redistribution of energy for a quantum mechanical wave packet and for an assembly of particles is identical, the resulting dynamics are very different. In the classical case there is no reflection at the termination of the guiding structure.

accelerated component. This suggests that the reflection might be quantitatively described by a simple model in one dimension. To model this we may assume the propagation to be completely adiabatic up to the point of exit and thus the effective potential to be given by the diagonal elements of the coupling matrix. Beyond that point, there will be no redistribution of energy from transverse to longitudinal degrees of freedom, and the effective potential is taken to be constant. The value of the constant potential is taken to be the contribution from the transverse ground state energy at the point of exit. In this way we can enquire if the reflection observed is mainly adiabatic or nonadiabatic as described above. We thus take the potential to be

$$V_{1D}(x) = \begin{cases} \frac{1}{2} \omega(x) & \text{if } x \leq x_c, \\ \frac{1}{2} \omega(x_c) & \text{if } x > x_c, \end{cases} \quad (16)$$

where the exit point x_c is chosen such that

$$\frac{\omega(x_c)}{\omega_0} = Q(N). \quad (17)$$

This choice of potential is motivated by the observation that the change in transverse energy as noted in [19] and in Sec. II is a function of the Fresnel parameter only. A tacit assumption, in this model, is that the transition from adiabatic propagation to free expansion effectively takes place in a region much smaller than the length scale L . In effect the transition region is here taken to be pointlike. The exclusion

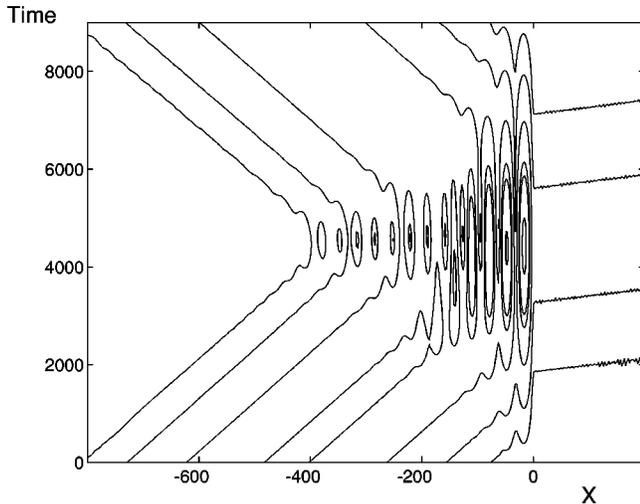


FIG. 5. A contour plot of total longitudinal probability density, as defined by Eq. (15), versus time for the same physical situation as in Fig. 3. A Gaussian wave packet can be seen impinging on the termination from the left resulting in partial transmission and partial reflection. The transmitted part is seen to have acquired a higher longitudinal momentum due to the adiabatic following of the transverse state that has taken place up to the exit point. The transition from adiabatic propagation to free expansion here takes place on a length scale much shorter than the de Broglie wavelengths of the incoming wave packet. As a result of this, the dynamics shows a close similarity to one-dimensional scattering off a rapidly decreasing potential. The units have been chosen dimensionless.

of the energy renormalization $B_{00}(x)$ from Eq. (16) is motivated as this term is of the same size as the off-diagonal terms, which can be neglected in the adiabatic limit. When the term $B_{00}(x)$ no longer can be neglected it is necessary anyway to include the couplings to higher modes for consistency. Using Eq. (16) for a single mode with the potential given by Eqs. (16) and (17), one-dimensional wave packets have been propagated under conditions identical with the two-dimensional simulations. The results for this simple *ad hoc* model are shown as solid lines in Fig. 6. It is seen that there is good agreement for $L=4$ and $L=2$ whereas the results for $L=1$ are overestimated by up to 5%. For smaller lengths the discrepancy grows even larger as most of the backscattering will be nonadiabatic due to the stronger interaction between the modes for shorter lengths. In Fig. 7 the reflection coefficient for $L=0.2$ is plotted versus longitudinal momentum for different choices of the initial oscillator frequency ω_0 . For the largest value $\omega_0=10$ the reflection is as large as $R=0.91$, and thus considerable. Only the results from the full two-dimensional propagation are shown as the simple model of Eqs. (16) and (17) fails for this length. It appears that arbitrarily large amounts of backscattering can be achieved for the system under consideration. The only limit is the available computational resources. The final propagation time is inversely proportional to the longitudinal momentum as a fixed distance has to be covered by the wave packet. In the adiabatic regime, the dynamics is dominated by the fast transverse motion that has to be resolved. This results in the execution time being directly proportional to

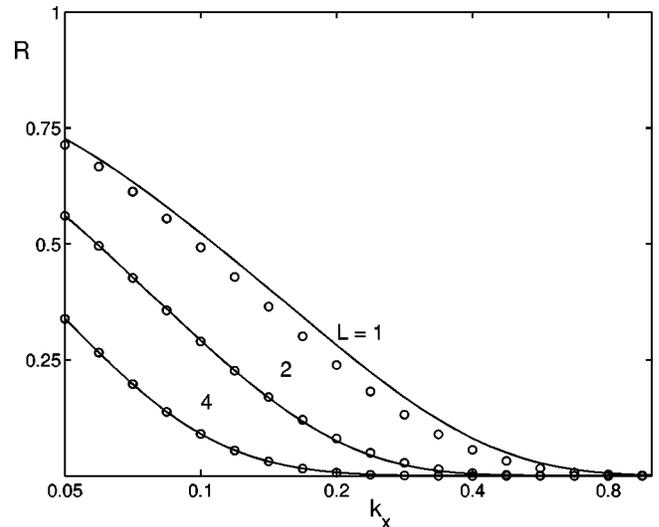


FIG. 6. The circles show the reflection coefficient, as calculated from the full numerical two-dimensional wave-packet simulations, vs longitudinal momentum. Results are plotted for different transition lengths L , as indicated in the figure. The initial harmonic oscillator frequency is here $\omega_0=1$. Shorter transition lengths give rise to more backscattering at a certain momentum k_x , as one would expect from a one-dimensional analogy. Shown as solid lines are reflection coefficients for the simple analytic model for adiabatic backscattering described by Eqs. (16) and (17). The agreement is good for lengths $L>1$, but there is a slight overestimate by up to 5% for $L=1$. For even shorter lengths the simple model deviates even more as the interaction region can no longer be considered to be small compared to the region where adiabatic backscattering takes place. The units have been chosen dimensionless.

ω_0 , the oscillator frequency, as faster oscillations have to be resolved. The total time for a single wave-packet simulation will then be proportional to ω_0/k_x , making the adiabatic limit progressively more expensive in computational time. This conclusion holds for both the classical and quantum mechanical cases.

IV. DISCUSSION

The adiabatic theorem in the old quantum mechanics is due to Ehrenfest [22] who also derived the theorem [21] that bears his name, Eqs. (11). Both of these results stress the classical features inherent in quantum mechanics, the former by the conservation of an adiabatic invariant and the latter by classical-like evolution equations for center of mass positions of particles. Heisenberg stressed the close connection between the uncertainty relations and diffraction of matter waves [23]. In a previous paper [18] we investigated the applicability of adiabaticity to wave-packet dynamics in potential structures and found connections with diffraction. In the adiabatic regime, changes in the binding potential are made slowly compared with the Rayleigh length of the matter waves, which implies that adiabatic propagation occurs when the Fresnel parameter (13) is smaller than unity. In Sec. II we showed that there is no difference between a full quantum mechanical wave-packet treatment and one based on as-

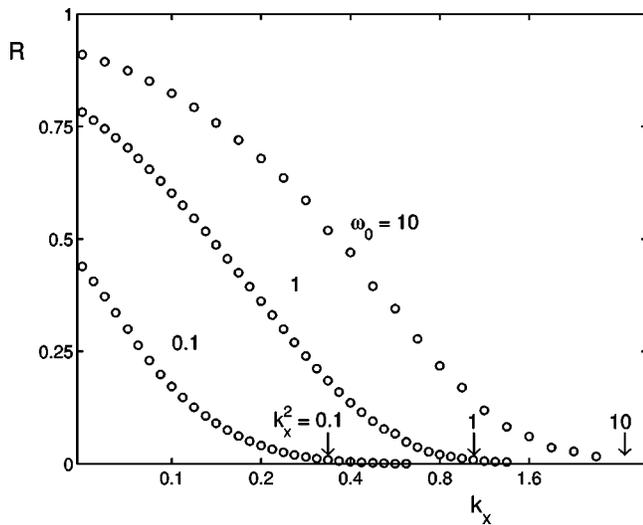


FIG. 7. The reflection coefficient as calculated in the full numerical two-dimensional wave-packet simulations for different values of ω_0 . The transition length has been taken to be $L=0.2$. As a result of this, the simple analytic model for adiabatic backscattering described by Eqs. (16) and (17) is inapplicable here. The maximal backscattering achieved for $\omega_0=10$ is 91%. The arrows indicate the points on the k_x axis that correspond to $k_x^2=\omega_0$, i.e., the momentum value where the kinetic energy equals the transverse binding energy, for the three curves. For all cases shown here, appreciable amounts of backscattering start to occur when $k_x^2 \ll \omega_0$. The units have been chosen dimensionless.

semblies of particles obeying Eqs. (11) when it comes to the redistribution of energy between longitudinal and transverse degrees of freedom during a transition from an adiabatic propagation to free expansion. The amount of adiabatic readjustment is a function of the Fresnel parameter only. The connections between adiabaticity, diffraction, and the uncertainty relations are fundamental and may seem self-evident. It is, however, worth stressing their importance as they give a clearer picture of the complementary properties of adiabaticity

taken together with wave phenomena versus classical adiabaticity combined with the uncertainty relations. The fact that we can reproduce the wave mechanical results by using assemblies of classical particles obeying the uncertainty relations, which in themselves include wavelike behavior to some extent, only stresses that quantum adiabaticity, as we have explored it, does not rely on any effects using phase coherent properties in the dynamics. There will, however, appear a major difference in the case of very low kinetic energy

$$k_x^2 \ll \omega_0. \quad (18)$$

In this case there will be considerable backscattering for small transition lengths. In the case when the reflection takes place during the adiabatic propagation, this can be explained using the simple model of Eqs. (16) and (17). The complete two-dimensional dynamics will thus be classical-like with respect to the adiabatic following of the transverse degrees of freedom. For the longitudinal propagation the nonclassical phenomenon of reflection against a decreasing potential will take place. In the case when the transition length is very short, the backscattering, to a large degree, takes place within the region of strong involvement of higher transverse modes. In this case, the simple model of adiabatic propagation fails. We have in this work shown the occurrence of backscattering of matter waves in changing potential structures. Adiabaticity can be achieved by moving to lower kinetic energies or higher transverse binding energies. In the adiabatic regime, it seems clear that the transverse binding energy will dominate the dynamics and Eq. (18) will be satisfied. The risk of unwanted reflection is then overwhelming as the length scales cannot be made arbitrarily long since the total propagation times must be within the coherence times of these systems [24]. The use of matter-wave optical structures will thus have to take backscattering into account during the design process. Unfortunately, no simple criteria for when backscattering occurs exist, and detailed simulations together with experiments will have to be used.

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