Phase-matched matter wave collisions in periodic potentials

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Abstract. Quantum scattering of particles in a periodic potential differs from scattering of free particles because of the non-trivial relation between energy and momentum, and because the potential can extract or provide momentum in the form of integer multiples of the lattice momentum vectors. In this paper, we study solutions for the single-particle dynamics in periodic potentials in one and more dimensions, and we identify the possible final states for various collision processes. This analysis leads to an interpretation of recently performed experiments on four-wave mixing and collisions of Bose–Einstein condensates and to predictions for further collision experiments.

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1. Introduction

The solution to the Schrödinger equation and the resulting band spectrum for an electron moving in a periodic potential constitute the basis for our understanding of the physics of solids. With cold atoms in optical periodic lattices it has been possible to study another physical system governed by the same basic equations, but being in many ways easier to control and detect. The ability to work under ideal circumstances has led to fundamental experimental studies of numerous single-particle and many-body phenomena, e.g., Bloch oscillations of individual atoms [1], and the Mott-insulator transition of interacting particles [2]. The periodic potential has also been realized to be an ideal container for atoms, subject to, e.g., molecule formation [3, 4], quantum entanglement operations [5, 6], and quantum optical studies [7]. It has also been noted that a periodic potential can be used to modify the relation between energy and wavenumber and hereby increase the ratio between interaction and kinetic energy of the atoms, enabling the observation of a Tonks gas [8], and also to change the sign of the effective mass, $m^*$ of moving atoms, leading to the prediction of bright solitons of atoms with repulsive interactions [9].

We have recently studied the one-dimensional (1D) propagation of a Bose–Einstein condensate of interacting particles through a periodic potential and identified an efficient mechanism for conversion of almost the entire condensate at wavenumber $k_0$ into two new components at $k_1$ and $k_2$, which fulfill both energy conservation and quasi-momentum conservation (i.e., momentum conservation modulo the lattice momentum) [10]. This process cannot occur among free particles in one dimension, and it only occurs here if we carefully choose the wavenumbers so that the corresponding Bloch band energies match. The theory consists of an identification of matching energies and wavenumbers of the single particle band structure and of solutions to the Gross–Pitaevskii equation for the system, and it shows that a seed beam, hitting the $k_0$ condensate at appropriate values of the momentum $k_1$, is amplified and an accompanying component emerges at $k_2$. This theoretical prediction has been confirmed experimentally [11]. The predicted sensitivity of the amplification on the values of the condensate and seed wavenumbers $k_0$ and $k_1$ was verified, and the process was shown to also occur spontaneously without seeding. Both the theory and the experiments show that the accessible momenta $k_i$ are given to a very high precision by the phase matching condition imposed by the initial and final band structure solutions of the single-particle Schrödinger equation. The dynamics is thus well understood in terms of collisions between pairs of atoms where the total (quasi-) momentum is the same in the initial and final state $k_1 + k_2 = 2k_0$ (mod $2k_L$), and also the total band energy of the colliding atoms is conserved $\varepsilon(k_1) + \varepsilon(k_2) = 2\varepsilon(k_0)$. The lattice momentum is $2\hbar k_L$, twice the laser photon momentum, see below. It is the collisional interaction, and in particular the strength of the s-wave scattering, that accounts for the details of the process, but the single-particle band structure suffices to predict the possible final state of the process.

With this observation in mind, it is the purpose of the present paper to investigate further the possible phase matched processes in periodic potentials in one and more dimensions. We shall use simple band structure theory to make predictions for collision studies of atoms which have different initial momenta, for collisions within anisotropic external potentials, and for collisions occurring in time-dependent potentials. In section 2, we review 1D band structure theory for the relevant case of a simple cos-potential. In section 3, we move to higher dimensions, using simple separable potentials, and relying hence only on the 1D numerical solutions. In section 4, we discuss the dynamics in time-dependent periodic potentials. In section 5, we turn to a discussion of the full quantum scattering theory inside a periodic potential. Section 6 concludes the paper.

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2. 1D band structure

A laser standing wave with wavelength $\lambda = 2\pi/k_L$ generates a periodic potential for atomic motion. The potential is caused by the AC-Stark shift of the internal atomic ground state due to the off-resonant coupling to one or more excited states by the laser field. This shift is proportional to the local light intensity, and it therefore has half the period of the laser electric field, and hence the lattice wavenumber is twice the photon wavenumber, in agreement with the microscopic picture of the atom undergoing absorption and stimulated-emission cycles of counter propagating photon pairs from the laser field, conserving its momentum modulo $2\hbar k_L$. The atomic motion is described by the Schrödinger equation

$$i\hbar \frac{d\psi}{dt} = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} - \beta E_R \cos(2k_L z) \right) \psi,$$

where $\beta$ indicates the strength of the light-induced potential in units of the recoil energy $E_R \equiv \hbar^2 k_L^2 / 2m$. Bloch’s theorem applies to the solutions of equation (1), and the eigenvalues constitute a band structure shown in figure 1 for atoms moving in a weak and a strong laser field, respectively.

The information in this figure is the basis for the discussions and all further plots in this paper.

The band structure is computed for a single particle, and when more particles are present their collisional interaction cause transitions between the Bloch band states. We have two physical pictures of the collision processes occurring within or between matter waves: a particle description in which the total energy and (quasi-) momentum of the two particles involved must be conserved, and a wave description in which phase matching is needed for the nonlinear coupling of waves to yield a finite amplitude at the final wavenumbers. Both pictures yield the same
2.1. Break-up of a single condensate in 1D

In [10], we noted that the lowest Bloch band shows a relationship between energy and wavenumber which allows a moving condensate to break up because two condensate atoms can collide and one atom emerges at a lower wavenumber and the other emerges with a correspondingly higher wavenumber inside the next Brillouin zone. This is clearly not possible for a condensate at rest and also not for a freely moving condensate where the high momentum atom would have a too high energy to fulfil energy conservation in the process.

The process is very selective. Given the initial wavenumber \( k_0 \), only a specific pair of final state wavenumbers is allowed in our simple 1D band structure because lowering of the low momentum component and the corresponding raising of the high momentum component leads to a lowering of the energy of both particles, cf, figure 2. Such pairs of final states can only be identified for values of \( k_0 \) in the interval: \( k_L/2 < k_0 < k_{zm} \), where \( k_{zm} \) is the point of inflection (zero curvature) in the band structure (\( \frac{d\epsilon}{dk} \mid_{k_{zm}} = 0 \)). When the potential gets very deep, the band structure converges to a simple cosine function, and \( k_{zm} \) coincides with \( k_L/2 \), and the four-wave mixing process is not possible.

If the potential is shallow, however, \( k_{zm} \) is closer to the band edge. In figure 3, we present an alternative picture of the band structure of figure 2 shown as a function of the momenta of the two...
Figure 3. Lowest energy band for motion of two atoms in the ‘weak’ optical lattice ($\beta = 0.04$) of figure 1. The figure indicates the total energy contours, and by a diagonal dashed line, momentum pairs $k_1$ and $k_2$, with the same total momentum. The crossing between this line and contours with the same energy (possibly in different Brillouin zones) reveals initial and final momentum states coupled by energy and momentum conserving processes. The black dots indicate such a pair with an incident pair of atoms with the same momentum and outgoing atoms with the momenta indicated in figure 2.

In this figure, we can identify pairs of momenta having the same total energy (same energy contour) and same total quasi momentum (same diagonal lines). In figure 3, the momentum and energy conserving splitting processes are identified by varying $k_0$ along the $(k_0, k_0)$ diagonal, and searching along the perpendicular lines with $k_1 + k_2 = 2k_0$ for a $(k_1, k_2)$ pair, possibly in a neighbouring Brillouin zone with the same energy (a crossing with the same energy contour as the one going through $(k_0, k_0)$).

In a mean field description of the many body system, $k_0, k_1$ and $k_2$ waves interfere, and the collision process cannot occur without breaking the translational symmetry of the system state. One has to seed the system with a weak $k_1$ component to break the symmetry and get the process started. The full many-body state with quantum correlations between the momentum components allows the process without seeding, and indeed, experiments have revealed both the spontaneous process and the stimulated process [11]. With Bose–Einstein condensates, the collision process is coherently amplified and is eventually reversed into a coherent transfer of the atoms from $k_1$ and $k_2$ back to $k_0$ [10]. For a finite system, the different momentum components only overlap in space for a finite time, and this oscillatory collisional exchange still awaits experimental confirmation.

We recall that the analysis is for the case, where the atomic motion is restricted to one dimension only. This condition may be assured by a harmonic trapping potential that confines the particles, $\varepsilon_2(k_1, k_2) = \varepsilon(k_1) + \varepsilon(k_2)$. In this figure, we can identify pairs of momenta having the same total energy (same energy contour) and same total quasi momentum (same diagonal lines).
Figure 4. Momentum states of motion of two atoms in the ‘weak’ optical lattice as in figure 3. The two ‘boomerang-shaped’ regions show the initial momentum states \(k_1, k_2\) in the lowest energy band that can collide and form atoms at different final momenta.

the transverse atomic motion, but the results may also apply without such trapping for the case of seeding along the direction of motion of the condensate. A careful analysis of the instability of a moving condensate due to coupling to a range of transverse excitations is given in [12], and a closer study of the competition between a seeded collision channel and a range of spontaneous channels is clearly relevant.

2.2. Scattering of different momentum components

Figure 3 enables also a straightforward analysis of the possibilities for scattering of atoms with different initial momenta \(k_1, k_2\) into final momenta \(k'_1, k'_2\). As described above, one draws in figure 3 a line through the point \((k_1, k_2)\) along the diagonal with constant \(k'_1 + k'_2\) and identifies (possibly within neighbouring Brillouin zones) the final momentum states with same total energy. As with the case of identical initial momenta \(k_0\) there are values of the momenta where such collisions, and therefore effective four-wave mixing, are allowed and other values that are robust against collisions, i.e., where colliding condensates in a 1D lattice should be able to travel through each other or simply exchange their momenta \(((k_1, k_2) \rightarrow (k_2, k_1))\), which does not lead to new momentum components. In figure 4, we show the regions of momentum pairs \((k_1, k_2)\) in the first Brillouin zone which may collide and lead to other momentum states (which are also, possibly by a full lattice translation to be found in the depicted regions of the plot). The intersection between the boomerangs and the diagonal \((k_0, k_0)\), reveal the momentum interval where the 1D condensate is unstable against four-wave mixing, [10].

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So far, the analysis was based on the first Bloch band only. This is in accord with the cited experimental investigations, where the initial states were in the lowest band, and hence energy conservation does not allow promotion to the excited band. It will of course be of interest to study collisions where one or both matter waves populate higher Bloch bands, and where both intra-band and inter-band processes are possible. It should be expected that the collisions will occur according to simple propensity rules based on the nodal structures and the spatial overlap of the Bloch states. For deep lattices, the Bloch states are essentially plane waves multiplied with functions that resemble the harmonic oscillator eigenstates. The matrix element of a short range atomic interaction therefore becomes proportional to the spatial integral of the product of two such initial and two final oscillator states. From parity considerations, we expect that collisions of particles staying in the same band are allowed, but also, e.g., atoms in the second band may collide and lead to a state with one atom in the first and one in the third band, provided energy is conserved.

3. Scattering in higher dimensions

We turn first to the simple case of particles colliding along a single direction, but having the possibility to scatter in all directions. For freely colliding condensates, this process has been studied in experiments showing the first examples of four wave mixing processes of matter waves [13, 14]. Seen in the centre-of-mass frame of two colliding atoms, energy and momentum can only be conserved if the length of the wave vectors of the atoms are conserved, giving rise to the ‘scattering sphere’ of atoms coming out in all directions. The dominant contribution to scattering at low energies is $s$-wave scattering giving rise to a uniform spherical distribution of collision products, but by tuning to a $d$-wave shape resonance, it has also been possible to observe $s$- and $d$-wave interference and non-trivial angular distributions of the collision products [15]. In a periodic potential, we also need to conserve total (quasi-) momentum and energy, but this is no longer done by preserving the length of the wave vectors.

3.1. 2D and 3D scattering in a 1D lattice

The effect of extra dimensions on the scattering in a 1D lattice, is to provide the possibility to conserve energy in the process by allowing motion with momentum components in the perpendicular directions of motion. Thus, if the band structure rules out collisions in the 1D case, because the final states of motion have too little energy compared to the initial state, we can simply provide the scattered atoms with suitably matched equal and opposite momentum components in the orthogonal direction to make up for the difference.

The consequence of this is for example that a single condensate moving with wavenumber $k_0$ in an optical lattice can break up into many collision channels for all values of $k_0 > k_L/2$, which is intimately linked with the observed instability of condensates in that momentum range [16].

Another striking consequence of the interplay between energy and momentum conservation has been observed in experiments [17], where two opposite momentum components at $-k_L$ and $k_L$ (created by Bragg diffraction in the very same lattice) collide while the lattice is still present, and the angular distribution of particles is observed. Momentum conservation ensures that the atoms leave the collision with equal and opposite momenta, and with their energies unchanged.
Figure 5. Longitudinal quasi-momentum and transverse momentum after a head-on collision of atoms with momenta ±k_L along the direction of the lattice. The figure shows which transverse momentum is required as a function of the final longitudinal quasi-momentum to conserve energy in the scattering process. Atoms will emerge in pairs with equal and opposite momenta (on the upper and lower branches in the figure). The transverse component represents two directions in space, and seen from a single direction in 3D, the atomic cloud will fill the area between the two curves.

But, due to the lattice, the energy of an atom is not given by the length of its wave vector squared, but rather by a sum of the 1D band energy evaluated at the quasi-momentum component k_p along the lattice plus the free particle kinetic energy for a particle with the transverse momentum components k_t, so that energy conservation implies

$$\varepsilon(k_L) = \varepsilon(k_p) + \hbar^2 k_t^2 / 2m. \quad (2)$$

Since the lowest energy band bends down from the free particle quadratic energy dependence of momentum when the momentum approaches the band edge, see figure 1, there is less energy available for transverse motion in the collision process, and the solution of equation (2) predicts that the spherical scattering halo is ‘squeezed’ as depicted in figure 5 in the weak (solid line) and strong (dashed line) lattices of figure 1. The figure shows the momentum available for the transverse degree of freedom as a function of the longitudinal quasi-momentum of the scattered atoms. In 3D, this momentum has to be shared between two directions, and observing the atomic cloud from one direction, one should expect to see a filled ‘Zeppelin’ with the boundaries sketched in the figure. This is in very good agreement with the observations in [17].

By switching off the lattice after preparation, one should expect the spherical scattering halo, and by switching on, for example a lattice in the transverse direction, it should be possible to

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Figure 6. Longitudinal momentum and transverse quasi-momentum after a head-on collision of atoms with momenta \( \pm k_L \). After the collision, the atoms may be scattered towards the orthogonal direction, in which they move in a lattice potential. The figure shows which transverse quasi-momentum is required as a function of the final longitudinal momentum to conserve energy in the scattering process. Scattering cannot occur to small momentum components along the initial direction, because the associated transversal energy falls in the band gap. The solid (dashed) line is for the weak (strong) potential.

have atoms colliding along a free direction and scatter into a transverse direction along a periodic potential. For small incident collision wavenumbers \( \pm k \), the solution of the energy conservation equation

\[
\hbar^2 k^2 / 2m = \varepsilon(k_t) + \hbar^2 k_p^2 / 2m,
\]

has only solutions with transverse motion in the lowest Bloch band of the lattice. In figure 6, we show the possible final momentum states, when free atoms collide with momenta \( \pm k_L \), half the lattice momentum of the lattice in the orthogonal direction. The atoms may leave with smaller momentum \( k_p \) along the original direction, but due to the band structure, the transverse direction cannot pick up energies above the lowest energy band, and therefore final states with small \( k_p \) are not produced, as seen in figure 6 with the results in the weak (strong) lattice shown with solid (dashed) lines.

If the incident energy is high enough, it is also possible to populate higher Bloch bands of the transverse motion in the collision. In figure 7, we show results for atoms with initial momenta \( \pm 1.5k_L \), \( \pm 1.7k_L \) and \( \pm 1.9k_L \). Small changes of the longitudinal components can be accommodated by scattering into a transverse quasi-momentum state in the lowest Bloch band. For a range of changes, the energy difference lies in the band gap, and thus scattering is not
possible, and for larger changes, the energy loss can be accommodated by scattering into a transverse quasi-momentum state in the first excited Bloch band. In the figure, we show the results for both the weak and the strong potential, and for three different sets of initial momenta. For clarity, we show the transverse quasi-momentum of states in the lowest Bloch band in the first Brillouin zone, and in the excited Bloch band in the neighbouring Brillouin zones. In the weak potential, the scattering here tends to the spherical distribution known for free particles.

### 3.2. 2D and 3D lattice

In 2D and 3D, we need the solutions to the Schrödinger equation

\[ i\hbar \frac{d\psi}{dt} = \left( -\frac{\hbar^2}{2m} \nabla^2 - \beta_x E_R \cos(2k_L x) - \beta_y E_R \cos(2k_L y) - \beta_z E_R \cos(2k_L z) \right) \psi, \tag{4} \]

where we assume lattices along all three axis directions with the same periodicity, but potentially different strengths. To eliminate interference effects between the laser fields along different directions, the three lattices are often prepared with different optical frequencies.

This equation is separable, and the complete band structure is given by \( \epsilon(\vec{k}) = \epsilon_x(k_x) + \epsilon_y(k_y) + \epsilon_z(k_z) \), where the 1D band structure along each coordinate direction provides the full
solution to the 2D and 3D problem. Collision processes are always governed by the energy and quasi-momentum conservation, and as above we just have to take into account the possibility of redistribution of energy among the different directions.

For the case of two dimensions, with the same potential strength along both directions, figure 2 is now useful because it shows the energy of a single particle as function of its wave vector. The products from a collision can then be analysed, and we can determine all final states from given input states.

4. Temporally modulated lattice potential

So far, we described collisions in a static lattice. A time-independent Hamiltonian conserves energy, and we therefore find a restricted class of states coupled by the collisional interactions between the atoms. If the lattice is modulated, the atomic energy is no longer conserved and a wide range of physical processes becomes possible. Already single-particle dynamics in a modulated potential shows a number of interesting features [18], but since we focus in this paper on collisions, it may be relevant to point out cases where the modulation has particular consequences for collision processes, and the experimental signature is not dominated by complex single-particle dynamics in a time-dependent potential.

Imagine a lattice potential which is being modulated harmonically in time with frequency Ω but retaining at all times the spatial periodicity with wavenumber 2kL. The modulation cannot change the quasi momentum of the atoms, but Floquet theory gives rise to a coupling of states differing in energy by an integer multiple of ħΩ. If we imagine that the atoms populate initial Bloch states with momenta k1 and k2, and that the modulation frequency is not resonant with the energy gap between Bloch states with same quasi-momentum, to lowest order the modulation cannot resonantly excite the atoms. It is possible, however, that in a collision process, (k1, k2) → (k′1, k′2), the total energy can absorb a number of modulation quanta, ε(k′1) + ε(k′2) = ε(k1) + ε(k2) + n ħΩ. The modulation thus opens new collision channels, discernible in experiments by new final momentum states.

In another regime, the modulation can be thought of as a perturbation of the single particle Hamiltonian in the Schrödinger equation (1,4), and we may identify the new eigenstates and energies of this Hamiltonian first, and subsequently study collision processes among them. A modulated or shaken lattice couples states in different bands having the same quasi-momentum, and if this interaction is not resonant, it may in perturbation theory lead to a shift of the energy eigenvalues similar to the AC Stark shift of atomic levels in an off-resonant laser field (like the one giving rise to our optical lattice potential in the first place). A modulation with a frequency slightly smaller than the gap between the ground and first excited band, thus couples non resonantly all the Bloch states in the lowest band to states in the first excited band. The coupling is off-resonant and affects most states only slightly, but close to the band edges, the coupling is more resonant than at k = 0, cf, figure 1, and hence the level shift due to the coupling is larger here. We note that also the coupling matrix element, equivalent to the Rabi frequency in laser–atom interactions, may depend on the k-values. We hereby modulate the dispersion relation ε(k) and thus the final states of collision processes. Note that unlike in the previous paragraph, the total energy is conserved in this case, but the use of new dressed state energies lead to new final states. In [19], experiments are reported on condensates at rest in a shaken optical lattice, where, after a number of oscillation cycles of the lattice, new momentum components appear at ± ħkL. This is
at half of the lattice momentum and, in a mean field sense, breaks the lattice symmetry (the full many-body state still retains this symmetry, because the atoms are created in pairs at those momenta by the collisions). The same paper [19] offers simulations which support the dressed state interpretation of the results.

5. Scattering theory

So far, our analysis has focused entirely on the identification of the possible final states that can be populated without violating energy and momentum conservation. It would be useful, however, to know also something about the distribution of particles, when more final states are possible.

The Schrödinger equation describing the scattering of two particles in free space is effectively solved by separation of the centre-of-mass motion and the relative motion, and for a spherically symmetric scattering potential, the asymptotic properties of the relative position wave function is expanded as a sum of a plane wave \( \exp(\textbf{i} \cdot \textbf{r}) \), corresponding to the incident relative momentum, and a spherical outgoing wave \( f(\theta) \exp(\text{i}kr)/r \), where the scattering amplitude \( f(\theta) \) provides the cross-section for scattering into different directions. The asymptotic form of the scattering state, and hence the scattering amplitude, are conveniently found by solving the Lippman–Schwinger equation, which specifies explicitly the initial relative momentum of the two particles.

Scattering theory for particles in periodic potentials is generally very complicated, intimately linked with the fact that already the band structure calculation is non-trivial in higher dimensions and general periodic potentials. This is not the place to develop such a theory, but a few observations about the structure of the exact solutions are in order. The problem no longer separates in centre-of-mass and relative motion, so one would have to deal with a full 6D Schrödinger equation, or the equivalent 6D Lippman–Schwinger integral equation. Even if the motion did separate, the fact that the energy is not just a quadratic function of momentum invalidates the simple spherical wave ansatz \( f(\theta) \exp(\text{i}kr)/r \) with the same wavenumber in all directions, which has also been explicitly included in the above analysis, in particular figures 5–7. To quantify this a bit further and to introduce part of a more elaborate scattering theory, let us consider scattering on an impurity potential \( U(\textbf{x}) \) within a periodic potential. Here the Lippman–Schwinger equation for the exact scattering state \( \psi^+(\textbf{k}, \textbf{x}) \),

\[
\psi^+(\textbf{k}, \textbf{x}) = \phi^+(\textbf{k}, \textbf{x}) + \int \text{d}^3 \textbf{y} \mathcal{G}^+(E; \textbf{x}, \textbf{y}) U(\textbf{y}) \psi^+(\textbf{k}, \textbf{y}),
\]

(5)

differs from the usual Lippman–Schwinger equation in two important ways: the usual ‘free’ plane wave state is replaced by Bloch eigenstate \( \phi^+(\textbf{k}, \textbf{x}) \), renormalized by a factor \( \sqrt{\frac{\hbar k}{m}}/v \), where \( v \) is the speed of particles at quasimomentum \( k \). And the Green’s function \( \mathcal{G}^+(E; \textbf{x}, \textbf{y}) \) in (5) is the crystal Green’s function solution to the equation

\[
\left( \nabla^2 - \frac{2m}{\hbar^2} V(\textbf{x}) + \frac{2m}{\hbar^2} E \right) \mathcal{G}^+(E; \textbf{x}, \textbf{y}) = \delta(\textbf{x} - \textbf{y}),
\]

(6)

for all \( \textbf{x}, \textbf{y} \). It follows from the properties [20] of the Green’s functions, that far away from the impurity, the scattering state can be developed as a linear combination of the incident renormalized Bloch wave and a scattered wave with a wavenumber whose modulus depends
on the detection angle. The differential cross-section, defined as the ratio of the outward flux per solid angle in direction $\vec{k}'$ to the incoming flux per unit area in direction $\vec{k}$ is given by [20]

$$\frac{d\sigma(\vec{k}', \vec{k})}{d\Omega'} = \frac{|A(\vec{k}', \vec{k})|^2}{k^2},$$  \hspace{1cm} (7)

where

$$A(\vec{k}', \vec{k}) = -\frac{|\Omega|}{4\pi} \int d^3\vec{x}\phi(\vec{k}', \vec{x})^*U(\vec{x})\psi(\vec{k}, \vec{x}),$$  \hspace{1cm} (8)

can be determined once the scattering state is known from equation (5).

Turning now to the case of collisions between two atoms we expect that for example atoms with incident momenta $\vec{k}$ and $-\vec{k}$ scatter back-to-back and propagate away from the interaction zone and must asymptotically obey the Schrödinger equation of independent particles in the periodic potential and have the same energy as in the initial state. These properties are similar to the ones of the impurity scattering solution (5), and the use of wave vectors that fulfil energy conservation in the previous sections are thus in agreement with this aspect of the formal scattering theory.

The calculation of the angular distribution of the colliding particles, i.e., the probability distribution over the different available scattering channels, remains a challenge, and it may be interesting to compare experimental data with a simple ansatz, where for example $\psi(\vec{k}, \vec{x})$ in (8) is replaced by the free space scattering wave function. The recent scattering experiments with both an s-wave and a resonantly tunable d-wave contribution and therefore highly anisotropic distributions [15] may be performed in lattices to yield an ideal test case for such an ansatz and for more elaborate theories.

To study the dynamics of colliding Bose–Einstein condensates, the full Gross–Pitaevskii equation has to be solved, and the angular distribution will here be a complicated function of time because scattered atoms may recollide and populate other states with the same energy and momentum. In 1D, we observed [10] that $k_1$ and $k_2$ components in the 1D case couple back into the condensate state $k_0$ in a Rabi-oscillatory manner. In higher dimensions, the states may scatter into other directions, and distribute the total energy between them in a more continuous manner. A further analysis of this process needs an efficient method to propagate the Gross–Pitaevskii equation in higher dimensions and over a large number of lattice sites.

6. Discussion

Recent theory [10] and experiments [11, 17, 19] on colliding matter wave fields in periodic potentials can be well understood from the energy and momentum conservation in two-atom collision processes. We have in this paper reviewed this analysis and generalized the study of the possible outcome of collision processes with different initial states, higher dimensions and temporal modulation of the potential. The periodic potential offers means to engineer the dispersion relation of the system, and hence to obtain highly non trivial outcomes of such collision processes. When applied to Bose–Einstein condensates with many atoms, the mechanisms should become highly visible in the expanded clouds, and finer details of the collisions inside potentials may be studied with high precision in dilute systems. Four-wave mixing processes have been proposed as efficient means to produce new momentum components from existing condensates,
and non-trivial quantum correlations and entanglement of the collision output may be used in fundamental tests of quantum theory with massive particles. The inspiration for the theory work in [10] came from studies of nonlinear optics in crystal fibres, where a transversely structured fibre leads to a non-trivial dispersion relation for the longitudinal propagation of light, and phase matched four-wave mixing at specific frequencies was identified [21]. This is suggestive that also matter waves in more complicated, and not necessarily periodic, geometries may be steered in very non-trivial ways by analogy to recent studies in nano-photonics. By including Feshbach resonance theory, a host of collision processes and e.g., formation and dissociation of molecules become possible, which would indeed be very interesting to see in a setting where the molecules may be thus separated from the atoms by tunable momentum components.

As stated in the previous section, in a more elaborate theory, one needs the solution of the Gross–Pitaevskii equation, or a linearized Bogoliubov treatment, if adequate, to account for the dynamics of a Bose–Einstein condensate. And even more precise theories that do not rely on the mean field description should be investigated, e.g., in regimes approaching the Mott-insulator. Work along these lines is in progress.

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