Examensarbete

Targeted Energy Transfer in Bose-Einstein Condensates
Robin Karhu
Examensarbetet utfört vid IFM
2013-09-30

LITH-IFM-A-EX--13/2835—SE
Targeted Energy Transfer in Bose-Einstein Condensates

Robin Karhu

Examensarbete utfört vid IFM

2013-09-30

Handledare
Peter Jason

Examinator
Magnus Johansson
Targeted Energy Transfer is a resonance phenomenon in coupled anharmonic oscillators. In this thesis we investigate if the concept of Targeted Energy Transfer is applicable to Bose-Einstein condensates in optical lattices. The model used to describe Bose-Einstein condensates in optical lattices is based on the Gross-Pitaevskii equation. Targeted Energy Transfer in these systems would correspond to energy being transferred from one lattice site to another.

We also try to expand the concept of Targeted Energy Transfer to a system consisting of three sites, where one of the sites are considered a perturbation to the system.

We have concluded that it is possible to achieve Targeted Energy Transfer in a three-site system. The set-up of the system will in some of the cases studied lead to interesting properties, such as more energy being transferred to the acceptor site than what was initially localized on the donor site.
Targeted Energy Transfer in Bose-Einstein Condensates

Robin Karhu

September 30, 2013
Abstract

Targeted Energy Transfer is a resonance phenomenon in coupled anharmonic oscillators. In this thesis we investigate if the concept of Targeted Energy Transfer is applicable to Bose-Einstein condensates in optical lattices. The model used to describe Bose-Einstein condensates in optical lattices is based on the Gross-Pitaevskii equation. Targeted Energy Transfer in these systems would correspond to energy being transferred from one lattice site in the optical lattice to another site, this energy transfer would in this system correspond to bosons transferring from one site to another.

We also try to expand the concept of Targeted Energy Transfer to a system consisting of three sites, where one of the sites are considered a perturbation to the system.

We have concluded that it is possible to achieve Targeted Energy Transfer in a three-site system. The set-up of the system will in some of the cases studied lead to interesting properties, such as more energy being transferred to the acceptor site than what was initially localized on the donor site.
# Contents

1 Introduction ........................................... 1  
   1.1 Bose-Einstein Condensates ......................... 1  
   1.2 Targeted Energy Transfer .......................... 2  
   1.3 Aim ............................................. 2  
   1.4 Method .......................................... 2  
   1.5 Outline ......................................... 3  

2 Theory .................................................. 4  
   2.1 Theoretical Background ............................ 4  
      2.1.1 Hamilton’s Equations of Motion ............... 4  
      2.1.2 Action-Angle Variables ........................ 7  
   2.2 Physical Background ......................... 8  
      2.2.1 Bose-Einstein Condensates ...................... 8  
      2.2.2 Optical lattices ............................. 13  
      2.2.3 Targeted Energy Transfer ...................... 14  

3 Two-site system ...................................... 15  

4 Three-site system .................................... 20  
   4.1 Configurations .................................... 20  
   4.2 Targeted Energy Transfer ....................... 21  
      4.2.1 Linear configuration ......................... 24  
      4.2.2 Triangular configuration ..................... 36  

5 Conclusions ............................................ 48  

6 Future Works .......................................... 50
Chapter 1

Introduction

1.1 Bose-Einstein Condensates

Bose-Einstein condensates were first proposed in 1925 by Albert Einstein. Satyendra Nath Bose had in 1924 used statistical arguments to derive the black-body photon spectrum. Einstein extended Bose’s argument to the case of noninteracting bosonic atoms (bosons are particles with integer spin) [1]. This resulted in Bose-Einstein statistics. Einstein noticed that at temperatures very close to absolute zero a macroscopic fraction of the atoms would be located at the same energy level. This phenomenon is called Bose-Einstein Condensation (BEC). The first BEC to be observed experimentally was created in 1995. This was done with a dilute gas of rubidium atoms by Eric Cornell and Carl Wieman [1]. For this they were awarded the Nobel prize in physics together with Wolfgang Ketterle in 2001 [2].

The content of this thesis is about energy transfer in BECs in optical lattices. An optical lattice is a standing wave created from the interference of two or more laser beams. The interference pattern of the laser beams will form a set of potential wells. These wells can be used to spatially confine atoms. The confinement will occur due to the electric field of the light inducing a dipole moment in the atoms. These atoms will be trapped in the oscillating electrical field of the lasers [3]. BEC trapped in an optical lattice is interesting to study for various reasons. One of which is that the system has a lot in common with condensed matter physics, where electrons are trapped in the periodic potential of a crystal lattice [3]. Some experiments that have been successfully performed in BEC in optical lattices are for example the quantum phase transition from a superfluid to a Mott-insulator [4] and negative absolute temperatures in the condensate [5].
We will assume that the number of atoms is very large, which makes it possible to neglect atom number fluctuations, this will enable us to use a mean-field approach to model the BEC in an optical lattice. This means that the atoms will be acted upon by the mean force of all the other atoms, it has been chosen to only consider atoms in the same lattice site when determining the mean force [3].

1.2 Targeted Energy Transfer

In this thesis resonance will refer to the complete transfer of energy back and forth between two oscillators, where one of the oscillators is initially at rest. Resonance will occur between two coupled harmonic oscillators if they have the same frequency. In the case of anharmonic oscillators the frequency depends on the amplitude of the oscillation. So if the oscillators begin resonant, as the energy is transferred the amplitude of the oscillators will change and thus change the frequency of the oscillators. The change of frequency will generally interrupt the resonance, since the frequencies will no longer be the same on both sites. There has however been found that in special situations the resonance can persist through out the entire transfer [6]. This phenomenon is called Targeted Energy Transfer (TET).

Even though the connection between anharmonic oscillators and BECs in optical lattices may not be obvious, the mathematical models describing the systems are the same. This is the motivation for why we believe that the theory of TET could be carried over from systems of anharmonic oscillators to BECs in optical lattices.

1.3 Aim

This thesis investigates if it is possible to apply the theory of TET to a model describing a BEC in an optical lattice. TET has been shown to exist in a system of two anharmonic oscillators [6]. The aim of this thesis is to investigate if TET can be achieved in a system of three anharmonic oscillators, and how the configuration and coupling of the oscillators influence the energy transfer between the oscillators.

1.4 Method

Systems consisting of three sites have been studied with a few different configurations of the coupling between the sites. A MATLAB program has
been written to numerically solve the equations of motion for the systems and plot the results.

1.5 Outline

This thesis has the following outline. In chapter 2 we review the basic theory. We discuss Hamilton’s equation of motion and action-angle variables. We will then have a discussion about Bose-Einstein condensates in optical lattices and Targeted Energy Transfer. In chapter 3 we review Targeted Energy Transfer in a system consisting of two sites. In chapter 4 we extend what has been done in the previous chapter, to study if it is possible to achieve Targeted Energy Transfer in a system consisting of three sites. Chapter 5 contains summary of the results and concluding remarks. In chapter 6 we have a brief discussion about possibilities to continue on this work.
Chapter 2

Theory

2.1 Theoretical Background

2.1.1 Hamilton’s Equations of Motion

We start the discussion about Hamilton’s equations of motion with Hamilton’s principle, which has been formulated in [7] as

"The motion of the system from time $t_1$ to time $t_2$ is such that the line integral (called the action or the action integral),

$$I = \int_{t_1}^{t_2} L dt,$$

where $L = T - V$, has a stationary value for the actual path of the motion." Where $T$ is the kinetic energy and $V$ is the potential energy.

Hamilton’s principle will correspond to the variation of the action integral being equal to zero (for a more detailed review of the calculus of variation, see for example [7])

$$\delta I = \delta \int_{t_1}^{t_2} L(q_1, q_2, ..., q_n, \dot{q}_1, \dot{q}_2, ..., \dot{q}_n, t) dt = 0,$$

where $q_i$ are the generalized coordinates and $\dot{q}_i$ are the time derivatives of the generalized coordinates. $\delta I$ is the infinitesimal variation about the action’s correct path. In mechanics the boundary conditions for $q_i$ need to be known in order to specify a trajectory. This means that their variation at the boundary will be zero

$$[\delta q_i(t)]_{t=t_1} = [\delta q_i(t)]_{t=t_2} = 0, \ (i = 1, 2, ..., n).$$
We can write (2.2) on the form

$$\delta I = \int_{t_1}^{t_2} [L(q_1 + \delta q_1, ..., q_n + \delta q_n, \dot{q}_1 + \delta \dot{q}_1, ..., \dot{q}_n + \delta \dot{q}_n, t)$$

$$- L(q_1, ..., q_n, \dot{q}_1, ..., \dot{q}_n, t)] dt = 0. \quad (2.4)$$

Expanding the first term of (2.4) in a Taylor series and neglecting second and higher order terms, we obtain

$$\delta I = \int_{t_1}^{t_2} [L(q_1, ..., q_n, \dot{q}_1, ..., \dot{q}_n, t) + \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} (q_i + \delta q_i - q_i)$$

$$+ \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} (\dot{q}_i + \delta \dot{q}_i - \dot{q}_i) - L(q_1, ..., q_n, \dot{q}_1, ..., \dot{q}_n, t)] dt \quad (2.5)$$

$$= \int_{t_1}^{t_2} \sum_{i=1}^{n} (\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i) dt = 0.$$

Using the relation that

$$\delta \dot{q}_i = \frac{d}{dt} \delta q_i \quad (2.6)$$

and integrating by parts the last term of (2.5), we obtain

$$\int_{t_1}^{t_2} \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} \frac{d}{dt} \delta q_i dt = \left[ \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} \delta q_i \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \sum_{i=1}^{n} \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i dt. \quad (2.7)$$

Using (2.3) in (2.7) and inserting this back in (2.5) gives us

$$\delta I = \int_{t_1}^{t_2} \sum_{i=1}^{n} \left[ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) \right] \delta q_i dt = 0. \quad (2.8)$$

Since the generalized coordinates $q_i$ and their variation $\delta q_i$ are independent of each other, the only way we can ensure that (2.8) is zero is to demand that the terms inside the brackets vanish. That is,

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0, \quad (i = 1, 2, ..., n). \quad (2.9)$$

Eq. (2.9) are called the Euler-Lagrange equations which are the equations of motion in Lagrange’s formulation of mechanics.

In Lagrangian formulation of mechanics, a system with $n$ degrees of freedom are described by $n$ equations of motion. As the equations are of
second order $2n$ initial values need to be specified in order to solve the equations.

The Hamiltonian formulation is instead based on describing the motion in terms of first order equations. Since the number of initial values determining the motion still need to be $2n$, we need to find $2n$ independent first order equations formulated in $2n$ independent variables. Now we have doubled our set of independent quantities (for a detailed discussion see [7]). We can now choose half of them to be the $n$ generalized coordinates $q_i$. The other half will be chosen as the conjugate momentum $p_i$ defined as

$$p_i \equiv \frac{\partial L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t)}{\partial \dot{q}_i} \quad (i = 1, 2, \ldots, n). \quad (2.10)$$

The set of $(q, p)$ is called canonical variables. Differentiating the Lagrangian, $L(q, \dot{q}, t)$, we obtain

$$dL = \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} dq_i + \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial t} dt. \quad (2.11)$$

Using the definition of conjugate momentum (2.10) and substituting this into the Euler-Lagrange equation (2.9) results in

$$\dot{p}_i = \frac{\partial L}{\partial q_i} \quad (i = 1, 2, \ldots, n). \quad (2.12)$$

Eq. (2.11) can now be written as

$$dL = \sum_{i=1}^{n} \dot{p}_i dq_i + \sum_{i=1}^{n} p_i d\dot{q}_i + \frac{\partial L}{\partial t} dt. \quad (2.13)$$

Let us now introduce a new function called the Hamiltonian

$$H(q_1, \ldots, q_n, p_1, \ldots, p_n, t) = \sum_{i=1}^{n} \dot{q}_i p_i - L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t). \quad (2.14)$$

Differentiating (2.14) and using the result (2.13), we obtain

$$dH = \sum_{i=1}^{n} \dot{q}_i dp_i - \sum_{i=1}^{n} \dot{p}_i dq_i - \frac{\partial L}{\partial t} dt. \quad (2.15)$$

We can also write $dH$ as

$$dH = \sum_{i=1}^{n} \frac{\partial H}{\partial q_i} dq_i + \sum_{i=1}^{n} \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt. \quad (2.16)$$
Comparing (2.15) with (2.16) gives us

\[ \dot{q}_i = \frac{\partial H}{\partial p_i} \]  
(2.17a)

\[ -\dot{p}_i = \frac{\partial H}{\partial q_i} \quad (i = 1, 2, \ldots, n) \]  
(2.17b)

\[ -\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \]  
(2.17c)

Eq. (2.17) are Hamilton’s equations of motion, and the first two sets of equations are the 2n equations of motion we were searching for. For a more in-depth derivation of Hamilton’s equations of motion see [7].

### 2.1.2 Action-Angle Variables

Action-angle variables can be used in order to find the frequency of periodic motion without completely solving the equations of motion.

In our discussion we deal with periodic motion and can thus introduce an action variable \( I \),

\[ I = \frac{1}{2\pi} \int pdq, \]  
(2.18)

where the integration limits are taken over a complete period. We can perform a canonical transformation to a new set of variables \((q, p) \rightarrow (I, \theta)\) where \( \theta \) is the conjugate variable to \( I \), known as the angle variable. \( \theta \) is defined through the transformation equation

\[ \theta = \frac{\partial W}{\partial I}, \]  
(2.19)

where

\[ W = W(q, I) \]  
(2.20)

is Hamilton’s characteristic function (for more information on Hamilton’s characteristic function and canonical transformations see for example [7]). Since the transformation is canonical the equation of motion will be

\[ \dot{\theta} = \frac{\partial H(I)}{\partial I} \]  
(2.21)

which gives the angular frequency as

\[ \omega(I) = \dot{\theta} = \frac{\partial H(I)}{\partial I} \Leftrightarrow \theta = \omega(I)t + \beta, \]  
(2.22)

where \( \beta \) is a constant of integration.
2.2 Physical Background

2.2.1 Bose-Einstein Condensates

BEC is a state of matter which can be realized from a gas of bosons where a macroscopic part of the bosons is in the same single-particle quantum state. BEC can be achieved if the thermal de Broglie wavelength of the bosons becomes large enough to overlap with the neighbouring bosons. The thermal de Broglie wavelength is given by

\[ \lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}, \]  

(2.23)

where \( m \) is the mass of the boson, \( k_B \) is Boltzmann’s constant and \( T \) is the temperature. Lowering the temperature of the bosons is a way to increase the thermal de Broglie wavelength, and it turns out that extremely low temperatures (nano-Kelvin) are required in order to obtain BECs. The main point of interest for studying BECs is for the peculiarity that a macroscopic fraction of bosons is occupying the same single-particle quantum state, this means that the BEC will have one coherent wavefunction. An object consisting of a macroscopic fraction of bosons and with a coherent wavefunction will exhibit an assortment of quantum mechanical properties [1, 8].

Two cooling techniques are used in order to reach the temperatures required for BEC. These techniques are laser cooling and evaporative cooling [3]. Laser cooling utilizes the Doppler effect and the thermal motion of the atoms in a gas. Atoms moving towards the laser source will detect a shorter wavelength than atoms moving away from the laser source. Since the photon energy is \( E = \frac{hc}{\lambda} \), where \( h \) is Planck’s constant, \( c \) is the speed of light and \( \lambda \) is the wavelength of the photon, this results in atoms moving towards the laser source being bombarded by higher energy photons than atoms moving away from the source. Tuning the lasers photon energy just below an energy transition of the atoms, it is then possible to excite atoms moving towards the laser. Excited atoms will eventually relax back to a lower energy state and thus cooling the gas. With this method it is possible to achieve temperatures in the micro-Kelvin range. This temperature is however not low enough to achieve BEC. Lower temperatures can be reached by evaporative cooling. This is done by trapping the gas in a magnetic trap, and successively lowering the depth of the trap. This will allow for the most energetical atoms to escape the trap, thus lowering the overall temperature of the gas. Using first laser cooling and then evaporative cooling, it will be possible to
reach temperatures of a few nano-Kelvin. At such low temperatures it is possible under favourable conditions to achieve BEC [3].

Model

In this section we are going to review the model used in this thesis, for a more detailed discussion about the model see for example [9]. We have assumed that the number of bosons is very large, which enables us to use a mean-field approximation to describe the BEC in an optical lattice. This means that every atom in one of the lattice points will feel the mean force of all the other atoms in that lattice point. Between the lattice points different couplings have been introduced to model which sites that interact with each other. The strength of these couplings are proportional to how far the optical lattice points are from each other. In this work a few different configurations of three lattice sites and couplings have been considered. The configurations of the sites will be introduced properly at a later point in this thesis.

A BEC may be treated as a set of weakly interacting particles. We can assume that the interaction between two low energy particles are given by (see for example [9] for a more detailed discussion)

\[ U = \frac{4\pi\hbar^2 a}{m}, \]

(2.24)

where \( a \) is the scattering length. Since in a BEC a macroscopic fraction of the particles occupy the same quantum state, we can consider the wavefunction as a product of \( N \) single-particle wavefunctions \( \phi(r) \), where \( N \) is the number of particles in the state. We can thus write the wavefunction as

\[ \Psi(r_1, r_2, ..., r_N) = \prod_{i=1}^{N} \phi(r_i). \]

(2.25)

Where the many-particle wavefunction is normalized,

\[ \int |\Psi(r)|^2 dr = 1. \]

(2.26)

We can choose to consider only contact interactions between low energy particles as \( U\delta(r - r') \), where \( r \) and \( r' \) are the positions of the two particles, and \( \delta \) is Dirac’s delta function. The total Hamiltonian will thus be

\[ H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V_{\text{ext}}(r_i) \right] + \frac{1}{2} U \sum_{i=1}^{N} \sum_{j\neq i}^{N} \delta(r_i - r'_j), \]

(2.27)
where $V_{\text{ext}}$ is the external potential, which could include periodical optical lattice, external trap potential and double/triple-well potential. The energy for the many-particle state is given by

$$E = \frac{\int \Psi^*(r)H\Psi(r)\,dr}{\int |\Psi(r)|^2\,dr},$$  \hspace{1cm} (2.28)

where the denominator is given by (2.26). The nominator of (2.28) can be solved in parts as

$$\int \sum_{i=1}^{N} \phi^*(r_i)\frac{p_i^2}{2m} \phi(r_i)\,dr_i = \sum_{i=1}^{N} \frac{\hbar^2}{2m} \int \nabla \phi^*(r_i) \nabla \phi(r_i)\,dr_i$$  \hspace{1cm} (2.29)

and

$$\int \sum_{i=1}^{N} \phi^*(r_i)V_{\text{ext}}(r_i)\phi(r_i)\,dr_i = N \int V_{\text{ext}}(r)|\phi(r)|^2\,dr.$$  \hspace{1cm} (2.30)

For the interaction term we get

$$\int \int \sum_{i=1}^{N} \sum_{j\neq i}^{N} \phi^*(r_i)\phi^*(r_j)U \frac{1}{2} \delta(r_i - r_j')\phi(r_i)\phi(r_j')\,dr\,dr'$$

$$= U \frac{N(N-1)}{2} \int \phi^*(r)\phi^*(r')\delta(r - r')\phi(r)\phi(r')\,dr\,dr'$$  \hspace{1cm} (2.31)

in the last step we assume that the number of particles is large enough so that $N - 1 \approx N$. Combining eqs. (2.29), (2.30), (2.31) with (2.28) gives us the energy for the many-particle state as

$$E = N \int \left[ \frac{\hbar^2}{2m} |\nabla \phi(r)|^2 + V_{\text{ext}}(r)|\phi(r)|^2 + \frac{N}{2} U |\phi(r)|^4 \right] \,dr.$$  \hspace{1cm} (2.32)

We want to write this in terms of the wavefunction of the condensed state,

$$\psi(r) \equiv \sqrt{N}\phi(r).$$  \hspace{1cm} (2.33)
We should notice here that $\psi(r)$ is the condensed state wavefunction and $\Psi(r)$ is the many-particle wavefunction.

Now we can rewrite (2.32) as

$$E = \int \left[ \frac{\hbar^2}{2m} |\nabla \psi(r)|^2 + V_{\text{ext}} |\psi(r)|^2 + \frac{1}{2} U |\psi(r)|^4 \right] \, dr. \quad (2.34)$$

We assume that the total number of particles is constant

$$N = \int |\psi(r)|^2 \, dr. \quad (2.35)$$

Using the techniques of Lagrange multipliers (for more information on Lagrange multipliers, see for example [7]) we can write $\delta E - \mu \delta N = 0$, where $\mu$ is the chemical potential and is used as the Lagrange multiplier. This procedure is equivalent to minimizing $E - \mu N$ with respect to $\psi^*$ (see [9] for more details). This gives

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V_{\text{ext}}(r)\psi(r) + U |\psi(r)|^2 \psi(r) = \mu \psi(r), \quad (2.36)$$

which is the time-independent Gross-Pitaevskii (GP) equation. To include the time dependence in this equation we can use a similar technique as the one used to include the time dependence in the Schrödinger equation (for details see for example [9, 10]). The result is the time dependent GP equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r,t) + V_{\text{ext}}(r)\psi(r,t) + U |\psi(r,t)|^2 \psi(r,t) = i\hbar \frac{\partial \psi(r,t)}{\partial t}, \quad (2.37)$$

where

$$\psi(r,t) = \psi(r)e^{-i\mu t/\hbar}. \quad (2.38)$$

**Discretization**

From here, we assume that the potential $V_{\text{ext}}$ consists of several potential wells with sufficient depth to localize the wavefunction to one of the potential wells. By this assumption we can use the tight binding approximation (for more information about the tight binding approximation see for example [11, 12]) and the condensate wavefunction can be written as

$$\psi(r,t) = \sum_n \psi_n(t) \Phi(r - r'_n) \quad (2.39)$$
where $\Phi(r-r'_n)$ is the condensate wavefunction localized at site $n$. In this thesis we will later assume that the wavefunction is sufficiently localized at site $n$ so that we only need to consider nearest neighbour interactions. Some properties of this function are

\[
\int \Phi(r-r'_n)\Phi(r-r'_{n+1})dr = 0 \quad (2.40a)
\]
\[
\int |\Phi(r-r'_n)|^2 dr = 1. \quad (2.40b)
\]

\[
\psi_n(t) = \sqrt{N_n(t)e^{i\theta(t)}} \quad (2.41)
\]

is the amplitude on site $n$, where $N_n$ is the number of particles and $\theta(t)$ is the phase at site $n$. Substituting (2.39) into (2.37) gives us

\[
\frac{i}{\hbar}\frac{\partial}{\partial t}\left( \sum_n \psi_n(t)\Phi(r-r'_n) \right) = -\frac{\hbar^2}{2m}\nabla^2 \left( \sum_n \psi_n(t)\Phi(r-r'_n) \right) + V_{\text{ext}}(r) \left( \sum_n \psi_n(t)\Phi(r-r'_n) \right) + U|\sum_n \psi_n(t)\Phi(r-r'_n)|^2 \sum_n \psi_n(t)\Phi(r-r'_n). \quad (2.42)
\]

Multiplying (2.42) with $\Phi(r-r'_n)$, where the index $n$ is the same index as in (2.42) (actually it is $\Phi^*(r-r'_n)$ but $\Phi(r-r'_n)$ is real [11]) and integrating we obtain after some work

\[
\frac{i}{\hbar}\frac{d\psi_n(t)}{dt} = J_n(\psi_{n+1}(t) + \psi_{n-1}(t)) + U\Lambda|\psi_n(t)|^2\psi_n - E_n\psi_n(t). \quad (2.43)
\]

Where

\[
J_n = \int \left[ \frac{\hbar^2}{2m}(\nabla\Phi(r-r'_n)\nabla\Phi(r-r'_{n+1})) + \Phi(r-r'_n)V_{\text{ext}}(r)\Phi(r-r'_{n+1}) \right] dr, \quad (2.44a)
\]

\[
E_n = -\int \left[ \frac{\hbar^2}{2m}(\nabla\Phi(r-r'_n))^2 + V_{\text{ext}}(r)(\Phi(r-r'_n))^2 \right] dr, \quad (2.44b)
\]

\[
\Lambda = \int \Phi(r-r'_n)^4 dr. \quad (2.44c)
\]
In eq. (2.43) we have assumed that \( \Phi(r - r'_n) \) are sufficiently localized so that we only need to consider the nearest neighbor interactions. Eq. (2.43) is the discrete nonlinear Schrödinger (DNLS) equation [13]. We can consider the set of variables and conjugate variables \((\psi_n, i\psi_n^*)\), this makes it possible to express Hamilton’s equations of motion (2.17) as

\[
\dot{\psi}_n = -i \frac{\partial H}{\partial \psi_n^*}.
\]  

(2.45)

**Final model**

Equation (2.43) has the Hamiltonian

\[
H = \sum_n \left[ J_n (\psi_n(t)\psi_{n+1}^*(t) + \psi_{n}^*(t)\psi_{n+1}(t)) - E_n |\psi_n(t)|^2 + \frac{\Lambda U}{2} |\psi_n(t)|^4 \right],
\]

(2.46)

where the first term is the coupling between sites. Later on we will introduce two different couplings as \( J = -\lambda \) and \( J = -\Delta \), we will for the time being omit the index \( n \) on these couplings since this will vary with the configurations of the system. We will be able to vary the strength of the \( \lambda \)- and \( \Delta \)-couplings individually by adjusting the distance between the two sites the coupling connects. The Hamiltonian for one site \( n \) would be

\[
H_n = -E_n |\psi_n(t)|^2 + \frac{\Lambda U}{2} |\psi_n(t)|^4,
\]

(2.47)

the Hamiltonian for the coupling between two sites \( n \) and \( n + 1 \) would be

\[
H_{n \to n+1} = J_n (\psi_n(t)\psi_{n+1}^*(t) + \psi_{n}^*(t)\psi_{n+1}(t)).
\]

(2.48)

Exploiting the phenomenon of Feshbach resonance [9] it is possible to tune the value of the scattering length \( a \). This makes it possible to experimentally choose a value of the factor \( \Lambda U/2 \). In our discussion we will mainly take an interest in two values of the factor, namely \( \pm 1/2 \), this does not limit the discussion since it corresponds to a normalization of the energy scale.

### 2.2.2 Optical lattices

An optical lattice is basically a standing wave created by the interference between laser beams. The regions of the standing wave where the atoms are trapped will be the lattice sites of the optical lattice. Atoms are trapped at the lattice sites by a force exerted on the atoms by the oscillating electrical
field of the laser beams [3]. In this thesis optical lattices consisting of three lattice sites have been considered, see 4.1 for a discussion about experimental realization of such systems.

The three sites will be referred to as the donor, acceptor and third site. The donor site will be the site initially injected with energy and the acceptor site will be the site that the energy is transferred to. The third site is introduced to the system as a perturbation, by starting with a very low coupling strength and studying how the system behaves when the coupling strength is increased. The couplings between the sites have been divided into two different types, the $\lambda$-coupling which is the coupling between the donor and acceptor, and the $\Delta$-coupling which is the perturbation coupling that introduces the third site to the system. If the $\Delta$-coupling is zero we will end up with a two-site system. In this thesis we have considered a few different configurations of the sites and the couplings.

2.2.3 Targeted Energy Transfer

In a system of two coupled identical harmonic oscillators resonance will occur when the frequency of both oscillators are the same. Resonance in such a system will correspond to any amount of energy injected to one of the oscillators being tunneled back and forth between the oscillators. This becomes significantly more complicated when the oscillators in question are anharmonic. Anharmonic oscillators have their amplitude of oscillation dependent on the frequency of oscillation (For a detailed derivation of the motion of both harmonic and anharmonic oscillators, see for example [7]). This will generally cause a system of oscillators initially at resonance to break the resonance as soon as some energy has been transferred from one oscillator to the other [14].

In [6, 15] it is shown that TET can occur in a system of two chains of oscillators modeled using the DNLS equation. We will study if TET can occur in BEC in a triple-well potential.
Chapter 3

Two-site system

In this section a review of the results already obtained for a two-site system is presented (for a more in depth presentation of the theory see [6]). We need to search for a condition for complete energy transfer from the donor site with action $I_{Tot}$ to the acceptor site. In a DNLS model the total action $I_{Tot}$ is conserved and the action for a site is $I = \psi^* \psi$. This gives us

$$I_{Tot} = I_D + I_A = |\psi_D|^2 + |\psi_A|^2. \quad \text{(3.1)}$$

Using (2.41) with (3.1) we can see that the action $I$ corresponds to the number of bosons, for $I_{Tot}$ it is the total number of bosons in the system and for $I_D(I_A)$ it is the number of bosons on the corresponding site. The total energy of the system needs to be conserved, this gives us

$$E_{Tot} = H_D(I_D) + H_A(I_A) + H_C(I_D, I_A, \theta_D, \theta_A),$$

where $H_D$ and $H_A$ are the Hamiltonian given by (2.47) and the index D and A are used to denote the donor and acceptor site respectively, $H_C$ is the Hamiltonian given by (2.48) where the index C is used to denote the coupling between the sites. In this work we assume that the coupling between the two sites is very weak. The reason why we choose to study the weak coupling is that there exists almost exact solutions localized to one site. This assumption makes it possible to approximate the total energy to 

$$E_{Tot} = H_D(I_D) + H_A(I_{Tot} - I_D), \quad \text{(3.2)}$$

Differentiating (3.2) with respect to $I_D$ results in

$$\frac{dH_D(I_D)}{dI_D} + \frac{dH_A(I_{Tot} - I_D)}{dI_D} = 0 \Leftrightarrow \left| \frac{dI_A}{-dI_D} \right|$$

$$\Leftrightarrow \omega_D = \frac{dH_D(I_D)}{dI_D} = \frac{dH_A(I_A)}{dI_A} = \omega_A, \quad \text{(3.3)}$$
where $\omega_D$ and $\omega_A$ are the frequencies of the donor and acceptor. This shows that the frequencies of both sites will remain identical during the entire energy transfer, i.e., the two sites remain resonant.

From eq. (2.47) we can construct the Hamiltonians for the two sites as

$$H_D = E_D = -E_{osD}|\psi_D|^2 - \frac{1}{2}|\psi_D|^4$$  \hspace{1cm} (3.4)

$$H_A = E_A = -E_{osA}|\psi_A|^2 + \frac{1}{2}|\psi_A|^4$$  \hspace{1cm} (3.5)

where $E_{osD}$ and $E_{osA}$ are the on-site energies. $E_{osD}$ and $E_{osA}$ have been chosen arbitrary to be 0.98 and 2.26 respectively. $E_{osD}$ and $E_{osA}$ can be chosen arbitrarily since it will only influence the initial conditions of the equations of motion. These two quantities will be related to the depth of the optical lattice potential.

![Figure 3.1: Energy $E_{D,A}$ versus action $I_{D,A}$ for donor and acceptor site.](image)

In figure 3.1 the energy $E_D$, $E_A$ given by eq. (3.4) and (3.5) are plotted as a function of the action $I_D$, $I_A$. At the point of intersection is where TET can be expected to occur. The intersection takes place at $E_{D,A} = -2.0736$ and $I_{D,A} = 1.2800$. The coupling between the two sites has the Hamiltonian

$$H_C = -\lambda(\psi_A^*\psi_D + \psi_A^*\psi_D)$$  \hspace{1cm} (3.6)
where $\lambda$ is the strength of the coupling. In [6] it is shown that in a DNLS model, if the signs of the nonlinear terms in (3.4) and (3.5) are opposite to each other, TET can occur for any value of $\lambda \neq 0$. Since we have also assumed that $\lambda$ is weak, we have arbitrarily chosen $\lambda = 0.001$. The total Hamiltonian for this system is thus

$$H = H_D + H_A + H_C =$$

$$= -E_{osD}|\psi_D|^2 - \frac{1}{2}|\psi_D|^4 - E_{osA}|\psi_A|^2 + \frac{1}{2}|\psi_A|^4 - \lambda(\psi_A\psi_D^* + \psi_A^*\psi_D).$$

(3.7)

Using the Hamiltonian (3.7) in eq. (2.45), gives us

$$i\dot{\psi}_D + |\psi_D|^2\psi_D + E_{osD}\psi_D + \lambda\psi_A = 0$$

(3.8a)

$$i\dot{\psi}_A - |\psi_A|^2\psi_A + E_{osA}\psi_A + \lambda\psi_D = 0.$$  (3.8b)

Solving the differential equations (3.8) gives the time evolution of the system.
Figure 3.2: (a) \((E_D - E_A)/E_{Tot}\) and (b) \((I_D - I_A)/I_{Tot}\) versus time. The time unit is the period \(t_b = 2\pi/\omega_D\) of the initial conditions on D. The coupling constant used here is \(\lambda = 0.001\).

In figure 3.2 we have the ratios \((E_D - E_A)/E_{Tot}\) and \((I_D - I_A)/I_{Tot}\) plotted against time. The initial condition is energy on site D, the amount of energy is decided from the intersection of the curves in fig. 3.1. The ratios oscillate between 1 (here \(E_D = E_{Tot}, I_D = I_{Tot}, E_A = 0, I_A = 0\)) and -1 (here \(E_D = 0, I_D = 0, E_A = E_{Tot}, I_A = I_{Tot}\)). This shows that for this system both the energy and action oscillates between the donor and acceptor site. This transfer of energy back and forth between the donor and acceptor corresponds to TET. It is also interesting to see what happens if we choose an initial condition that is slightly off the intersection of the curves in fig 3.1, to see how TET is effected by the initial condition.
Figure 3.3: (a) \((E_D - E_A)/E_{Tot}\) and (b) \((I_D - I_A)/I_{Tot}\) versus time. The time unit is the period \(t_b = 2\pi/\omega_D\) (\(\omega_D = 2.2597\)) of the initial conditions on D. The coupling constant used here is \(\lambda = 0.001\).

In fig. 3.3, the initial conditions used are \(E_D = -2.072922045\), \(I_D = 1.279700000\), \(E_A = 0\) and \(I_A = 0\). In this figure we can see that we no longer have perfect resonance in the system. If we compare the initial conditions used in fig. 3.2 and 3.3, we can notice that the difference in action is \(3\times10^{-4}\).
Chapter 4

Three-site system

In this chapter we extend on the work done previously on two-site systems to three-site systems.

4.1 Configurations

Figure 4.1: Two different configurations of systems. The top one will be referred to as the linear system and the bottom one as the triangular system.

In fig. 4.1 the two configurations used in this chapter are schematically described. D and A stands for the donor and acceptor sites respectively, these sites are coupled together as in the two-site case by a coupling $\lambda$. T
stands for the third site, which will be introduced as a perturbation by the coupling constant $\Delta$.

There have been suggestions for experimental realization of the linear and triangular configuration for three sites. One suggestion for the linear configuration can be found in [16], where the idea is to take a one-dimensional optical lattice and superimposing a harmonic dipole potential to select the number of sites wanted in the experiment. Realization of the triangular configuration is suggested in [17], here the idea is to instead take a Kagome lattice [18] and superimposing a harmonic dipole potential to just select one of the triangles making up the Kagome lattice.

### 4.2 Targeted Energy Transfer

In this section we will investigate if it is possible to achieve TET in a system of three sites. We will use a very similar approach to the one used in the case of the two-site system.

First we need to define what we mean with TET in a three-site system. TET will correspond to complete energy transfer from the donor site to the acceptor site, while a perturbing third site is present. We will consider both the case when the transfer only happens once and when the transfer repeats itself several times.

Analogous to the two-site system, we can define three complex-valued variables as $\psi_D = \sqrt{I_D}e^{-i\theta_D}$, $\psi_A = \sqrt{I_A}e^{-i\theta_A}$ and $\psi_T = \sqrt{I_T}e^{-i\theta_T}$.

From eq. (2.47) we can construct the Hamiltonians for the three sites as

\begin{align*}
H_D & = -E_{osD}|\psi_D|^2 - \frac{1}{2}|\psi_D|^4 \quad (4.1) \\
H_A & = -E_{osA}|\psi_A|^2 + \frac{1}{2}|\psi_A|^4 \quad (4.2) \\
H_T & = -E_{osT}|\psi_T|^2 \pm \frac{1}{2}|\psi_T|^4 \quad (4.3)
\end{align*}

where $E_{osD}$, $E_{osA}$ and $E_{osT}$ are the on-site energies of the donor, acceptor and third site respectively. Using what has been shown in [6] we choose the signs of the nonlinear term in eqs. (4.1) and (4.2) opposite to each other. We will investigate how the system is affected by the sign of the nonlinear term in (4.3).

In the systems used in this thesis the on-site energies have been chosen as $E_{osD} = 0.98$, $E_{osA} = 2.26$ to coincide with the discussion we had about two-site system, we will investigate how the value of $E_{osT}$ influences the system.
We will limit our discussion to two values of $E_{osT}$, namely $E_{osT} = E_{osD}$ and $E_{osA}$.

Since $H_D$ and $H_A$ are the same as in the two-site system we can conclude from figure 3.1 that the two cases when the third site is either equivalent to the acceptor or donor sites, there exists a point where $\omega_D = \omega_T = \omega_A$. In both cases this occurs at $E_{D,A,T} = -2.0736$ and $I_{Tot} = 1.2800$ just as in the case for the two-site system. We also need to consider the two other cases, namely when the third site is $E_{osT} = E_{osD}$ and the sign of the nonlinear term in (4.3) is chosen as positive (4.4), and the third site is $E_{osT} = E_{osA}$ and the sign is chosen as negative (4.5). This means that the Hamiltonians for these two cases will be

\[
H_T = -E_{osD}|\psi_T|^2 + \frac{1}{2}|\psi_T|^4 \tag{4.4}
\]

\[
H_T = -E_{osA}|\psi_T|^2 - \frac{1}{2}|\psi_T|^4 \tag{4.5}
\]
Figure 4.2: Energy $E_{A,T}$ versus action $I_{A,T}$ for: a) Acceptor (red), donor (green) and third (blue) site for the case when the third site is $E_{osT} = E_{osD}$ and the sign of the nonlinear term in (4.3) is chosen as positive. b) Acceptor, donor and third site for the case when the third site is $E_{osT} = E_{osA}$ and the sign of the nonlinear term in (4.3) is chosen as negative.

Figure 4.2 is made in the same way as 3.1. In figure 4.2 we can see that there is no point where $\omega_A = \omega_T$ except for $I = 0$. In both of these cases $H_D$ and $H_A$ will still fulfill the condition for resonance, namely that $\omega_D = \omega_A$. This will be investigated further to conclude if it is possible to achieve resonance in these systems.
The $\lambda$-coupling between the sites is the same for all cases discussed in this thesis. But we need to consider different Hamiltonians of the $\Delta$-coupling to account for the different configurations. The Hamiltonian for the $\lambda$-coupling is

$$H_\lambda = -\lambda(\psi_D^*\psi_A + \psi_A^*\psi_D).$$

(4.6)

We chose the parameter $\lambda = 0.001$ to coincide with the discussion had about the two-site system.

### 4.2.1 Linear configuration

The $\Delta$-coupling in the linear configuration has Hamiltonian

$$H_\Delta = -\Delta(\psi_T^*\psi_D + \psi_D^*\psi_T).$$

(4.7)

The total Hamiltonian for the system is

$$H = H_D + H_A + H_T + H_\lambda + H_\Delta$$

$$= -E_{osD}|\psi_D|^2 - \frac{1}{2}|\psi_D|^4 - E_{osA}|\psi_A|^2 + \frac{1}{2}|\psi_A|^4 - E_{osT}|\psi_T|^2$$

$$\pm \frac{1}{2}|\psi_T|^4 - \lambda(\psi_D^*\psi_A + \psi_A^*\psi_D) - \Delta(\psi_T^*\psi_D + \psi_D^*\psi_T).$$

(4.8)

Using eq. (4.8) in combination with eq. (2.45) gives us

$$\dot{\psi}_D - i|\psi_D|^2\psi_D - iE_{osD}\psi_D - i\lambda\psi_A - i\Delta\psi_T = 0$$

(4.9a)

$$\dot{\psi}_A + i|\psi_A|^2\psi_A - iE_{osA}\psi_A - i\lambda\psi_D = 0$$

(4.9b)

$$\dot{\psi}_T \pm i|\psi_T|^2\psi_T - iE_{osT}\psi_T - i\Delta\psi_D = 0$$

(4.9c)

In this chapter we choose the initial conditions of (4.9) to be energy on site D and T while A is unoccupied. We chose the phase difference between site D and T to be 0. The initial conditions are determined by the intersection of the curves in figure 3.1. Which gives $E_D = E_T = -2.0736$, $I_D = I_T = 1.2800$, $E_A = 0$ and $I_A = 0$ just as in the two-site system. These initial conditions will be used for all configurations of the system studied in this chapter. We also define two new quantities, $E_{Tot} = E_D + E_A$ and $I_{Tot} = I_D + I_A$. Using these definitions $E_{Tot}$ and $I_{Tot}$ will not be conserved quantities.
Figure 4.3: This figure is for the case when the third site is equivalent to the donor site. a) $\min((E_D - E_A)/E_{Tot})$ versus $\Delta$, where the equations of motion have been solved for one period of oscillation. b) $\min((E_D - E_A)/E_{Tot})$ versus $\Delta$, where the equations of motion have been solved for three periods of oscillation.
Figure 4.4: This figure is similar to figure 4.3 but for the case when the third site is equivalent to the acceptor site.

In figures 4.3 and 4.4, $\min((E_D - E_A)/E_{Tot})$ is plotted versus the coupling strength $\Delta$. The figures are generated by solving equations (4.9) for approximately one respectively three periods of oscillation of the localized energy for $\Delta = 10^{-7}$. The reason for solving the equations for one respectively three periods are that for one period we will get a good idea how the system behaves for different values of $\Delta$, three periods are chosen rather arbitrarily as we noticed that we could get complete transfer of energy early on in the time evolution of the system even if it did not happen in the first period of oscillation. The equations (4.9) are solved for values between $\Delta = 10^{-7}$ and $\Delta = 10^{-5}$ the values used are spaced $10^{-7}$ apart. We should notice that the scale of the $\min((E_D - E_A)/E_{Tot})$-axis is vastly different in figure 4.3 and 4.4. When $\min((E_D - E_A)/E_{Tot})$ is -1 the energy has at least transferred to the acceptor once, making these values of $\Delta$ interesting.
for further investigation. It does not take into account $E_T$ but the plot is used to determine values for the coupling to further investigate. Interesting values to study are those where $\min((E_D - E_A)/E_{Tot})$ are very close to -1 since this is where resonance can occur. We also want to study how the system behaves outside of resonance and we chose to look at the system at a value of $\Delta$ where $\min((E_D - E_A)/E_{Tot})$ is not as close to -1.
Third site equivalent to the donor site

Figure 4.5: (a) \( \frac{(E_D - E_A)}{E_{\text{Tot}}} \), (b) \( \frac{(I_D - I_A)}{I_{\text{Tot}}} \), (c) \( I_D \), (d) \( I_A \) and (e) \( I_T \) versus time. The time unit is the period \( t_b = \frac{2\pi}{\omega_D} (\omega_D = 2.2600) \) of the initial condition on D. The coupling is \( \lambda = 0.001 \) and \( \Delta = 10^{-7} \). This figure is for the case when the third site is equivalent to the donor site.
Figure 4.6: This figure is similar to 4.5 but for $\Delta = 9.2 \times 10^{-6}$. 
Figure 4.7: This figure is similar to 4.5 but for $\Delta = 10^{-5}$.

Figure 4.5 has been chosen to represent the case when $\min((E_D - E_A)/E_{Tot})$ is very close to the value -1. 4.6 is chosen to represent a value of $\Delta$ that corresponds to one of the sharp spikes in 4.3 b), and 4.7 is used to represent when $\min((E_D - E_A)/E_{Tot})$ is not as close to the value -1. Figures 4.5, 4.6 and 4.7 are all for the case when the third site is equivalent with the donor site. Figures 4.5 and 4.7 are the solutions to the equations of motion plotted
for $\Delta = 10^{-7}$ and $\Delta = 10^{-5}$ respectively, in the first figure it looks like the energy is transferred back and forth between the donor and acceptor, while in figure 4.7 have a single transfer from the donor to the acceptor. This is also in line with fig. 4.3. Comparing figures 4.5 and 4.6 we can see in figure 4.5 that the energy is transferred back and forth between the donor and acceptor, while in figure 4.6 we can see that after some time the energy is transferred from the donor to the acceptor. The main difference between 4.7 and 4.6 is that in the second figure we predicted that the transfer would happen early in the time evolution. This is a good illustration of two different kinds of resonance that occur in the systems we study. The first one is when the energy is transferred back and forth between the donor and acceptor. The second one is when the energy is transferred from the donor to the acceptor after some time has passed.

Figure 4.8: $\min((E_D - E_A)/E_{Tot})$ plotted against $\Delta$, for very small values of $\Delta$. In this figure the equations of motion have been solved for approximately one period of oscillation, for the case when the third site is equivalent to the donor site.

Figure 4.8 is made in the same way as figures 4.3 and 4.4, but for other values of $\Delta$. In fig. 4.8 we can see that the function is tending towards -1 as $\Delta$ is going towards 0. This leads to the conclusion that there is no region
where the function is strictly -1. The noise in the figure is from the precision of the solver used to solve the differential equations. Figures similar to 4.8 have been made for all the other cases studied and they also show that there is no region for any of the cases where \( \min((E_D - E_A)/E_{Tot}) \) is strictly -1.

We can see in figure 4.5 that the transfer, while not being perfect, still persists through several periods. We have studied longer times (up to \( 3.5 \times 10^5 \)\(|t_b|\)) than the figures in this text show, and the transfer persisted through longer times as well. In figures 4.6 and 4.7 we can see that the time evolution of the systems become unpredictable. It may be interesting to notice that in figure 4.6 we have a transfer from the donor to the acceptor early in the figure, just as predicted by figure 4.3 b).
Third site equivalent to the acceptor site

Figure 4.9: This figure is similar to 4.5 but for the case when the third site is equivalent to the acceptor site and $\Delta = 10^{-7}$. 
Figure 4.10: This figure is similar to 4.5 but for the case when the third site is equivalent to the acceptor site and $\Delta = 10^{-5}$.

In figures 4.9 and 4.10 the solutions to equations (4.9) are plotted against time for the case when the third site is equivalent to the acceptor site, this have been done in figure 4.9 for $\Delta = 10^{-7}$ and in figure 4.10 for $\Delta = 10^{-5}$.

Figures 4.5, 4.6 and 4.7 are for the case when the third site is equivalent to the donor site, while 4.9 and 4.10 are for the case when the third site is
equivalent to the acceptor site. We can see that in the two cases where we have a resonance back and forth between the donor and acceptor site (4.5 and 4.9) the action of the third site ($I_T$) have very small variations. Figure 4.9 seems to have a consistent period of $I_T$ while in 4.5 we see a beat-like quality to the period. In figure 4.10 we can see that at the same time the action of the third site has a high value we also lose the perfect transfer of energy between the donor and acceptor. This is not so surprising since the energy of the system needs to be conserved.

Other cases

![Graph](image)

Figure 4.11: $\min((E_D - E_A)/E_{Tot})$ versus $\Delta$ for the case when $E_{osT} = E_{osD}$ and the sign of the nonlinear term is positive.
Figure 4.12: \( \min((E_D - E_A)/E_{Tot}) \) versus \( \Delta \) for the case when \( E_{osT} = E_{osA} \) and the sign of the nonlinear term is negative.

We can see that for the two cases mentioned in fig. 4.2 there are no choices of initial condition where \( \omega_A = \omega_T \). We can see in figures 4.11 and 4.12 that the values of \( \min((E_D - E_A)/E_{Tot}) \) varies very slowly. We have investigated these cases as well and can conclude that the transfer of energy back and forth between the donor and acceptor site will persist for any values of \( \Delta \lesssim \lambda \). These figures have been generated in the same way as 4.3 and 4.4, where the equations of motion have been solved for one period of oscillation. We should notice that the two figures look very similar to each other, this is due to very similar behaviour of the two systems.

4.2.2 Triangular configuration

The \( \Delta \)-coupling in the triangular configuration has Hamiltonian

\[
H_\Delta = -\Delta(\psi_T\psi_D^* + \psi_T\psi_A^* + \psi_D\psi_T^* + \psi_A\psi_T^*)
\]  

(4.10)
The Hamiltonian for the total system is

\[ H = H_D + H_A + H_T + H_\lambda + H_\Delta \]

\[ = -E_{osD}|\psi_D|^2 - \frac{1}{2}|\psi_D|^4 - E_{osA}|\psi_A|^2 + \frac{1}{2}|\psi_A|^4 - E_{osT}|\psi_T|^2 \]

\[ \pm \frac{1}{2}|\psi_T|^4 - \lambda(\psi_D^*\psi_A + \psi_A^*\psi_D) - \Delta(\psi_T^*\psi_D + \psi_T^*\psi_A + \psi_A^*\psi_T + \psi_D^*\psi_T) \]

(4.11)

Using eq. (4.11) with (2.45) gives us

\[ \dot{\psi}_D - i|\psi_D|^2\psi_D - iE_{osD}\psi_D - i\lambda\psi_A - i\Delta\psi_T = 0 \] (4.12a)

\[ \dot{\psi}_A + i|\psi_A|^2\psi_A - iE_{osA}\psi_A - i\lambda\psi_D - i\Delta\psi_T = 0 \] (4.12b)

\[ \dot{\psi}_T \pm i|\psi_T|^2\psi_T - iE_{osT}\psi_T - i\Delta\psi_A - i\Delta\psi_D = 0 \] (4.12c)

Choosing the initial conditions just as in the section 4.2.1.
Figure 4.13: This figure is similar to figure 4.3 but for the triangular configuration and the third site is equivalent to the donor site.
Figure 4.14: This figure is similar to figure 4.3 but for the triangular configuration and the third site is equivalent to the acceptor site.

In figure 4.13 and 4.14 $\min ((E_D - E_A)/E_{Tot})$ is plotted versus the coupling strength $\Delta$. These figures are generated in the same way as figures 4.3 and 4.4. We can see in figure 4.14 that this plot is very different from
the plots 4.3, 4.4 and 4.13. The difference is that \( \min((E_D - E_A)/E_{Tot}) \) has a lower value than -1. Lower values of \( \min((E_D - E_A)/E_{Tot}) \) than -1 means that there is more energy localized at the acceptor site than what was initially localized at the donor site, this indicates that some energy need to have transferred from the third site as well as from the donor site. We will investigate this further later on in this thesis.
Third site equivalent to the donor site

Figure 4.15: This figure is similar to 4.5 but for the triangular configuration and the third site is equivalent to the donor site and \( \Delta = 10^{-7} \).
Figure 4.16: This figure is similar to 4.5 but for the triangular configuration and the third site is equivalent to the donor site and $\Delta = 10^{-5}$.

Figures 4.15 and 4.16 are plots of the solutions of equations (4.12) against time. These equations are solved for the case when the third site is equivalent to the donor site. As can be seen in the figures the near resonance is present in fig. 4.15 but not in fig. 4.16. This is in line with fig. 4.13, and also very similar to the same case as in section 4.2.1.
Figure 4.17: \( \min((E_D - E_A)/E_{Tot}) \) plotted against \( \Delta \), for very small values of \( \Delta \). In this figure the equations of motion have been solved for approximately one period of oscillation, for the case when the third site is equivalent to the donor site.

Figure 4.17 is made in the same way as figure 4.8. In figure 4.17 \( \min((E_D - E_A)/E_{Tot}) \) is plotted against \( \Delta \) for small values of \( \Delta \). From this figure we can conclude that the value of \( \min((E_D - E_A)/E_{Tot}) \) does not reach -1. This is similar to the same case for the linear configuration in section 4.2.1. Just as in figure 4.8 the noise is from the solver used to produce the figure.
Third site equivalent to the acceptor site

Figure 4.18: This figure is similar to 4.5 but for the triangular configuration and the third site is equivalent to the acceptor site and $\Delta = 10^{-7}$.
Figure 4.19: This figure is similar to 4.5 but for the triangular configuration and the third site is equivalent to the acceptor site and $\Delta = 10^{-5}$.

Figures 4.18 and 4.19 are generated in the same way as 4.15 and 4.16, but for the case when the third site is equivalent to the acceptor site.

In fig. 4.18 we can see that the resonance seems to be present. While in fig. 4.19 it seems that the energy located at the donor site is transferred to the acceptor.
Figure 4.20: $\text{min}((E_D - E_A)/E_{Tot})$ plotted against $\Delta$, for very small values of $\Delta$. This figure is for the case when the third site is equivalent to the acceptor site.

Figure 4.14 is made in the same way as figure 4.8. The noise in the figure originates from the solver used, as in similar figures. We can see that figure 4.20 looks very different from 4.17 in that the quantity $\text{min}((E_D - E_A)/E_{Tot})$ takes values lower than -1. The system still tends towards -1 when $\Delta$ tends towards 0.

**Comparisons**

We have also made the calculations of the two cases when the third site is $E_{osT} = E_{osD}$, the sign of the nonlinear term of (4.3) is positive and $E_{osT} = E_{osA}$, the sign of (4.3) is negative for the triangular configuration. The result was very similar to the linear case with resonances persisting for values of $\Delta \lesssim \lambda$. 

46
We made changes to the on-site energies of the third site so that $E_{osT} \neq E_{osD}$ or $E_{osT} \neq E_{osA}$. This did not seem to influence the possibilities for resonance, but $I_T$ had minor variations with different values of $E_{osT}$. We also performed calculations for larger values of $\Delta$ but omitted them in this report, since the trend seemed to continue for values up to $\Delta \approx \lambda$. 
Chapter 5

Conclusions

In chapter 4 we expand on the concept of TET and try to apply it to a system of three sites. We have limited our discussion to \( \Delta \)-coupling strength of \( \Delta > 10^{-13} \). This is part due to the precision of the solvers used to solve the differential equations, and part due to physical significance of the coupling. It is hard to specify an exact limit for \( \Delta \) where it is of physical significance. But what can be said is at least that \( \Delta \) can not be too small or other effects will dominate the coupling. With this in mind we have limited the values to \( \Delta > 10^{-13} \). We have also limited the values we present in this text to \( \Delta < 10^{-5} \). This is mainly for editing and presentation purposes, we have seen that the trend continues for \( \Delta \)-values up to about \( \Delta \approx \lambda \).

In the figures plotting \( \min((E_D - E_A)/E_{Tot}) \) against \( \Delta \) for \( \Delta \) between \( 10^{-7} \) and \( 10^{-5} \) we can see in three of the cases, namely 4.3 (Linear configuration, third site equivalent to the donor site, \( \Delta \) between \( 10^{-7} - 10^{-5} \)), 4.4 (Linear configuration, third site equivalent to the acceptor site, \( \Delta \) between \( 10^{-7} - 10^{-5} \)) and 4.13 (Triangular configuration, third site equivalent to the donor site, \( \Delta \) between \( 10^{-7} - 10^{-5} \)) that for smaller values of \( \Delta \) the amount of energy transferred from the donor to the acceptor increases. But in the case for the triangular configuration with the third site equivalent to the acceptor site (fig. 4.14) we can see that the amount of energy transferred to the acceptor can exceed the amount of energy that was initially localized on the donor site. In the figures plotting \( \min((E_D - E_A)/E_{Tot}) \) against \( \Delta \) for small values of \( \Delta \) (\( 10^{-13} - 10^{-10} \)) 4.8 and 4.17, we can see that the transfer never reaches perfect resonance. As \( \min((E_D - E_A)/E_{Tot}) \) tends towards \(-1\) as \( \Delta \) is going towards zero.

In the figures plotting \( \min((E_D - E_A)/E_{Tot}) \) versus \( \Delta \) when the equations of motion are solved for three periods of oscillation, namely figures
4.3, 4.4, 4.13 and 4.14 b) (Triangular configuration, third site equivalent to the acceptor site, $\Delta$ between $10^{-7} - 10^{-5}$), we can see that it is possible to achieve a single transfer from the donor to the acceptor even at higher values of $\Delta$. This transfer is however not a continuous transfer back and forth. In figures 4.3 and 4.13 this single transfer is almost perfect.

In the end of section 4 we mentioned that if the values of $E_T$ does not coincide with the on-site energy $E_D$ or $E_A$, the system can still support resonances.

Even though we were not able to find a region of $\Delta$ where perfect TET could take place, in figures 4.5 (Linear configuration, third site equivalent to the donor site, solutions for the equations of motion plotted for $\Delta = 10^{-7}$) and 4.15 (Triangular configuration, third site equivalent to the donor, solutions for the equations of motion plotted for $\Delta = 10^{-7}$) we can see that there exist regions where the energy transfer between the donor and acceptor site could persist for a long time. We have not performed any in-depth studies of how the non-perfect nature of the resonance influences the time evolution of the system.

We have arrived at these conclusions for both configurations of the system studied in this thesis. And we only found some interesting cases. The triangular configuration when the third site is equivalent to the acceptor site (figure 4.14) is drastically different from the other cases considered in this work. We will thus come to the conclusion that the configuration of the system can drastically change the behaviour of the system. One question that has not been answered in this thesis is whether or not the values required of the $\Delta$-coupling to achieve TET is physically representative of a BEC in an optical lattice.
Chapter 6

Future Works

There are several ways to continue this work. We have in this thesis used the Gross-Pitaevskii equation as a starting point when describing BECs, this means that the condensate is treated as a classical field. But if the number of atoms in the sites would be small, we would have to consider quantum mechanical effects. This could be taken into account for example by modeling the system starting from the Bose-Hubbard model [3], which models the system as a set of interacting atoms instead of a field.

We never did in-depth investigations on how the non-perfect resonance in the three site system affects the time evolution of the system. We never studied how close to -1 the function $\min((E_D - E_A)/E_{Tot})$ needs to be in order to reach a state of resonance that is good enough for practical purpose. Both of these topics could be greatly improved upon in further works.

In this thesis we have not concerned ourselves with the physical significance of parameter values. This would be a very interesting topic for further discussions. The main parameters for this would be the on-site energies and the couplings between the sites.

Experimental continuation of this work is also possible, and could involve investigating how well it is possible to realize TET in a BEC in an optical lattice of both two and three sites.
Bibliography


Upphovsrätt

Detta dokument hålls tillgängligt på Internet – eller dess framtida ersättare – från publiceringsdatum under förutsättning att inga extraordinära omständigheter uppstår.

Tillgång till dokumentet innebär tillstånd för var och en att läsa, ladda ner, skriva ut enstaka kopior för enskilt bruk och att använda det oförändrat för icke-kommersiell forskning och för undervisning. Överföring av upphovsrätten vid en senare tidpunkt kan inte upphäva detta tillstånd. All annan användning av dokumentet kräver upphovsmannens medgivande. För att garantera äktheten, säkerheten och tillgängligheten finns lösningar av teknisk och administrativ art.

Upphovsmannens ideella rätt innefattar rätt att bli nämd som upphovsman i den omfattning som god sed kräver vid användning av dokumentet på ovan beskrivna sätt samt skydd mot att dokumentet ändras eller presenteras i sådan form eller i sådant sammanhang som är kränkande för upphovsmannens litterära eller konstnärliga anseende eller egenart.

För ytterligare information om Linköping University Electronic Press se förlagets hemsida http://www.ep.liu.se/

Copyright

The publishers will keep this document online on the Internet – or its possible replacement – from the date of publication barring exceptional circumstances.

The online availability of the document implies permanent permission for anyone to read, to download, or to print out single copies for his/hers own use and to use it unchanged for non-commercial research and educational purpose. Subsequent transfers of copyright cannot revoke this permission. All other uses of the document are conditional upon the consent of the copyright owner. The publisher has taken technical and administrative measures to assure authenticity, security and accessibility.

According to intellectual property law the author has the right to be mentioned when his/her work is accessed as described above and to be protected against infringement.

For additional information about the Linköping University Electronic Press and its procedures for publication and for assurance of document integrity, please refer to its www home page: http://www.ep.liu.se/.

© Robin Karhu.