Exact Theoretical Description of Two Ultracold Atoms in 3D Optical Lattices

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Abstract. A theoretical approach was developed that allows for a full numerical description of a pair of ultracold atoms trapped in a three-dimensional optical lattice. This approach includes the possible coupling between centre-of-mass and relative motion coordinates in a configuration-interaction type formulation. The atoms are allowed to interact by their full interaction potential that is, presently, only limited to be central. With the aid of the newly developed method deviations from the harmonic approximation are discussed for the heteronuclear $^{87}\text{Rb}-^{40}\text{K}$ pair.

1. Introduction
The physics of ultracold atoms has attracted a lot of interest since the experimental realization of Bose-Einstein condensation in dilute alkali atom gases [1]. Besides the exciting physics at ultracold energies by itself, a further important progress was the positioning of the ultracold gas in an optical lattice formed with the aid of counter-propagating laser fields [2, 3]. The optical lattice resembles in a certain sense the periodicity of a crystal potential. In contrast to real solids the lattice parameters are, however, easily tunable by a variation of the laser intensity (trap depth) or wavelength (lattice geometry). Furthermore, different atoms possess different interaction potentials that can be even either attractive or repulsive. While different kinds of atoms (Li, Na, . . .), isotopes ($^6\text{Li}, ^7\text{Li}, . . .$) or atoms in different electronic or spin states cover already quite some range of interaction strengths, a further tuning parameter is provided by magnetic Feshbach resonances. At the resonance energy, the interaction varies from strongly attractive to strongly repulsive, or vice versa.

In view of the experimentally accessible parameters (lattice and particle-particle interaction) ultracold atomic gases in optical lattices are of interest as quantum simulators for solid-state models or for quantum information related studies. Especially in the latter case it is of interest to study optical lattices with a very small (and almost constant) filling rate, optimally with one or two atoms per lattice site. These systems are nowadays experimentally accessible, and recently the observation of confinement induced molecules, repulsively interacting pairs and ”real” molecules for both homonuclear [4, 5] and heteronuclear [6] atomic species in optical lattices has been reported.

Stöferle et al. [5] compared the measured binding energies of confinement induced and ”real” molecules with the theory describing two particles in a harmonic oscillator potential for which analytical solutions exist in the case of homonuclear systems [7], if the interatomic interaction
is described by a delta-type pseudopotential. While in that experiment good agreement was found, a higher resolution spectroscopy together with the use of a heteronuclear system allowed to see first indications of a breakdown of the harmonic approximation [6]. In the present work a numerical approach was developed that allows an in principle exact description of two atoms trapped in an optical lattice. As is briefly outlined below, the anharmonic part of the optical lattice potential leads to a coupling of centre-of-mass and relative motion and requires therefore to solve the full six-dimensional problem. In fact, even in a harmonic trap different trapping potentials of the two atoms as they occur, e.g., for heteronuclear atom pairs or two atoms of the same kind but in different electronic states lead to a coupling of centre-of-mass and relative motion [8, 9]. This coupling is treated in a configuration-interaction (CI) like fashion (also called exact diagonalisation) which for sufficiently large expansion lengths leads to exact results. Motivated by the already mentioned experimental work described in [6] results of the current approach applied to the $^{87}$Rb-$^{40}$K system are presented in this report.

2. System and numerical approach

2.1. Hamiltonian

The Hamiltonian describing the interaction of two atoms (with coordinate vectors $\vec{r}_1$ and $\vec{r}_2$) in a 3D optical lattice is given by

$$\hat{H}(\vec{r}_1, \vec{r}_2) = \hat{T}_1(\vec{r}_1) + \hat{T}_2(\vec{r}_2) + \hat{V}_{\text{trap},1}(\vec{r}_1) + \hat{V}_{\text{trap},2}(\vec{r}_2) + \hat{U}(\vec{r}_1, \vec{r}_2)$$

(1)

where $\hat{T}_j$ is the kinetic energy operator for particle $j$, $\hat{V}_{\text{trap},j}$ the sinusoidal trapping potential for particle $j$, and $\hat{U}$ is the atom-atom interaction potential. A direct solution of Eq. (1) is complicated, since $\hat{U}$ depends on all six coordinates describing the two-particle system, even if the atom-atom interaction is central, i.e. $\hat{U} = \hat{U}(r)$ with $r = |\vec{r}_1 - \vec{r}_2|$. Furthermore, atom-atom interaction potentials (reducing in Born-Oppenheimer approximation to BO potentials) are in general only known numerically which leads to computationally very demanding six-dimensional integrals. In view of this complication, it is more convenient to treat the two-particle problem in centre-of-mass (COM) and relative (REL) motion coordinates. In the case of two identical atoms (in the same state) application of the harmonic approximation to the trap potential leads to a problem that is completely separable in COM and REL coordinates and thus to decoupled COM and REL motion [10]. If the true atom-atom interaction is furthermore replaced by one that reproduces only asymptotically the two-body zero-energy $s$-wave scattering the Schrödinger equation possesses an analytical solution for isotropic and anisotropic harmonic traps [7, 11].

Even within the harmonic approximation this separability is, however, lost, if the two atoms experience different trapping potentials. This is the case, if a heteronuclear system or two identical atoms in different electronic states are considered. Of course, the anharmonicity of a sinusoidal potential leads already for two indistinguishable atoms to a coupling of COM and REL coordinates. The transformation of the Hamiltonian in (1) into the COM and REL coordinate systems leads after performing a Taylor expansion of the sinusoidal trapping potential around the origin to a Hamiltonian of the form

$$\hat{H}(\vec{R}, \vec{r}) = \hat{h}_{\text{COM}}(\vec{R}) + \hat{h}_{\text{REL}}(\vec{r}) + \hat{W}(\vec{R}, \vec{r})$$

(2)

with

$$\hat{h}_{\text{COM}}(\vec{R}) = \hat{t}_{\text{kin}}(\vec{R}) + \hat{v}_{\text{OL}}(\vec{R}),$$

(3)

$$\hat{h}_{\text{REL}}(\vec{r}) = \hat{T}_{\text{kin}}(\vec{r}) + \hat{V}_{\text{OL}}(\vec{r}) + \hat{V}_{\text{int}}(\vec{r}).$$

(4)

Only the non-separable terms consisting of products of COM and REL coordinates are left in the coupling term $\hat{W}$. All separable (harmonic and higher-order) terms of the optical
lattice (OL) potential are included into the COM and REL Hamiltonians $\hat{H}_{\text{COM}}$ and $\hat{H}_{\text{REL}}$, respectively. The corresponding eigenfunctions $\psi(\vec{R})$ and $\phi(\vec{r})$ fulfilling $\hat{H}_{\text{COM}} |\psi_i\rangle = E_i |\psi_i\rangle$ and $\hat{H}_{\text{REL}} |\phi_j\rangle = \epsilon_j |\phi_j\rangle$, respectively, are then used for a configuration-interaction (CI) type solution of the full problem. Defining the configuration state functions $\Phi_k(\vec{R}, \vec{r}) = \psi_{i_k}(\vec{R}) \phi_{j_k}(\vec{r})$ the final wavefunction of $\hat{H}(\vec{R}, \vec{r})$ is obtained as $\Psi(\vec{R}, \vec{r}) = \sum_k c_k \Phi_k(\vec{R}, \vec{r})$. In the present stage of implementation the atom-atom interaction potential is limited to the case $\hat{V}_{\text{int}} = \hat{V}_{\text{int}}(r)$ with $r = |\vec{r}|$. However, as is evident from Eqs. (2) to (4), the extension to, e.g., atomic or molecular gases with dipolar interactions is straightforward.

2.2. Trap parameters

Despite the mentioned break-down of the harmonic approximation for heteronuclear systems, it is convenient to introduce for an isotropic trap the averaged harmonic oscillator frequency

$$\omega_{\text{ho}} = k \sqrt{\frac{2V_1 \mu_2^2 + V_2 \mu_1^2}{\mu}}. \quad (5)$$

In Eq. (5) $k$ is the wavenumber of the trapping laser, $\mu$ denotes the reduced mass of the two particles, $\mu_j$ is defined as $\mu_{1,2} = \mu/m_{2,1}$ where $m_j$ is the mass of atom $j$, and $V_j = I_0 \cdot \alpha_j$ is the optical lattice depth that is equal to the product of the laser intensity $I_0$ (for an isotropic geometry one has $I_0 = I_x = I_y = I_z$) and the polarisability $\alpha_j$ of atom $j$.

The trap parameters chosen in the present study were motivated by the recent experiment reported in [6]. In [6] a three-dimensional optical lattice generated by lasers with wavelength $\lambda = 1030$ nm was used for trapping ultracold bosonic $^{87}$Rb and fermionic $^{40}$K atoms. The two different lattice depths $V_{\text{Rb}} = 40 E_{\text{Rb}}^{\text{Rb}}$ and $V_{\text{Rb}} = 27.5 E_{\text{Rb}}^{\text{Rb}}$ were used where the individual recoil energy is defined as $E_{r}^{\text{Rb}} = k^2/2m_{\text{Rb}}$. Using the static dipole polarisability of rubidium $\alpha_{\text{Rb}} = 324$ a.u. [12] it is possible to estimate the intensities used in the experiment to be given by $I(27.5 E_{\text{Rb}}^{\text{Rb}}) \sim 2.8 \times 10^{-14}$ a.u. and $I(40.0 E_{\text{Rb}}^{\text{Rb}}) \sim 4.1 \times 10^{-14}$ a.u. (here $I = I_x + I_y + I_z$). Potassium possesses a different static polarisability $\alpha_{\text{K}} = 301$ a.u. [12]. Therefore, the lattice depths for this element are slightly different and amount to $V_{\text{K}} = 20.6 E_{r}^{\text{Rb}}$ and $V_{\text{K}} = 25.6 E_{r}^{\text{Rb}}$ for $V_{\text{Rb}} = 40 E_{r}^{\text{Rb}}$ and $27.5 E_{r}^{\text{Rb}}$, respectively. The averaged harmonic oscillator frequencies (5) are $\omega_{\text{ho}}(40) = 2\pi \times 20.6$ kHz and $\omega_{\text{ho}}(27.5) = 2\pi \times 17.1$ kHz.

2.3. Interatomic interaction potential

The interaction between rubidium and potassium atoms is modelled using the BO potential of the $a^3 \Sigma^+$ electronic state describing the interaction of two spin-polarised atoms. For the short-range part of the potential $V_{\text{SR}}$ in between $R \in [1.588 a_0, 18.2 a_0]$ data of [13] are used where $a_0$ is the Bohr radius. The data points at $R = 17.6 a_0$ and $R = 16.99998 a_0$ have, however, been omitted, because their inclusion results in a non-smooth potential curve. The data of [13] were analysed by Zemke et al. [14]. The long range part $V_{\text{LR}}$ of the $a^3 \Sigma^+$ electronic state is constructed in a similar way as was done by Zemke et al. Therefore, the long range part is defined as $V_{\text{LR}}(r) = D_e + \Delta V_{\text{disp}}(r) + \Delta V_{\text{ex}}(r)$ for all $R \geq 18.6 a_0$. Here $\Delta V_{\text{disp}}(r) = -C_6/r^6 - C_8/r^8 - C_{10}/r^{10}$ where the dispersion coefficient $C_6 = 4292 \pm 19$ a.u. is taken from a fit to experiment [17], while for $C_8$ and $C_{10}$ the theoretical values given in [15, 16] are adopted. The exchange interaction is given by $\Delta V_{\text{ex}}(r) = -C r^\alpha e^{-\beta r}$ with $C = 0.00231382$, $\alpha = 5.25603$, $\beta = 1.11892$ as given in [14]. To merge the short- and the long-range parts the short-range part is raised up by half of the value $\delta_{\text{merge}} = V_{\text{SR}}(18.2 a_0) - V_{\text{LR}}(18.6 a_0)$. According to [14] the $a^3 \Sigma^+$ state supports 32 bound states and the interaction of the atoms via the $a^3 \Sigma^+$ potential is strong and repulsive. The same amount of bound states and character of the interaction is obtained in the present calculation using the potential curve constructed the way described above.
2.4. Manipulation of the interatomic interaction

In the limit of zero collision energy the interaction between two atoms can be characterised by their s-wave scattering length \( a_{sc} \). Its sign determines the type of interaction (repulsive or attractive) and its absolute value the interaction strength. There is no agreement about the value of the triplet scattering length for the \(^{87}\text{Rb}-^{40}\text{K} \) system. The value \(-215 \pm 10 \, a_0\) appears to be the best value according to the ongoing discussion [18, 19, 17]. The standard way to match the calculated scattering length with experimental values is a smooth shift of the inner wall of the BO potential as described in [14]. This procedure can also be used for an effective variation of the scattering length, since a systematic variation of the inner wall allows to shift the least bound state supported by the potential curve. If the least bound state is close to the dissociation threshold or moves even into the dissociative continuum, the scattering length and thus the interaction between ultracold atoms is strongly influenced. In the present work, \( a_{sc} \) of the \(^{87}\text{Rb}-^{40}\text{K} \) atom pair was tuned by a variation of the inner wall of the BO curve. Instead of the scattering length \( a_{sc} \) itself one often introduces a scaled interaction parameter \( \xi = a_{sc}/a_{ho} \), where the characteristic length of a harmonic potential \( a_{ho} \) is defined by \( a_{ho} = 1/\sqrt{\mu \omega^2} \). In the case of a heteronuclear atom pair in an optical lattice one uses again the averaged frequency that is obtained in the harmonic approximation (5).

Experimentally, a strong variation of the interaction strength can be realized by the aid of magnetic Feshbach resonances (MFR) [20, 21]. The MFR technique was also used to tune the interatomic interaction from strong repulsive to strong attractive in the already mentioned experiments with atoms in optical lattices [4, 5, 6]. In general, the correct theoretical description of a MFR in alkali atom systems requires a multi-channel scattering treatment which in the present case would have to incorporate also the optical lattice. In the analysis of the experiments in [4, 5, 6] it is, however, assumed that it is possible to model the MFR in an effective two-channel picture. Within this model it is straightforward to relate the applied magnetic field to a scattering length and thus to its scaled variant \( \xi \).

2.5. Computational details

The eigenfunctions of the Hamiltonians \( \hat{h}_{\text{COM}} \) and \( \hat{h}_{\text{REL}} \) are obtained by expressing both \( \psi(\vec{R}) \) and \( \phi(\vec{r}) \) as a linear combination of products of radial \( B \)-spline functions times spherical harmonics. In general the lattice leads to a coupling of the angular momenta and the spherical harmonics are therefore no eigensolutions of the angular parts. Due to the isotropic trap geometry used in the experiment in [6] and thus for the present calculations, the coupling of different spherical harmonics is weak. In fact, the orbitals \( \psi(\vec{R}) \) and \( \phi(\vec{r}) \) describing the states discussed below are practically converged, if only \( l = 0 \) is considered. However, the coupling term \( \hat{W} \) in Eq. (2) leads to a stronger angular momentum coupling. Good convergence was found in the CI calculation, if all spherical harmonics up to \( l = 3 \) (and thus also \(-3 \leq m \leq +3\)) were included in the calculation of the orbitals \( \psi(\vec{R}) \) and \( \phi(\vec{r}) \). The required number of \( B \) splines and their knot sequence depends strongly on the behaviour of the wavefunction \( \psi(\vec{R}) \) or \( \phi(\vec{r}) \) that should be described. In the context of ultracold collisions one is mainly interested in the energetically low-lying COM orbitals \( \psi(\vec{R}) \) with small number of nodes. About 70 \( B \) splines were found to be sufficient for their description in the context of this work. Clearly, more complicated or highly anisotropic trap geometries (like double-wells) already implemented in the code require larger expansions.

The numerical description of the REL orbitals \( \phi(\vec{r}) \) is more demanding, if one is interested in the most weakly bound states or the low-lying dissociative states. The BO curves of alkali atom dimers support often a large number of bound states (in the present example of \(^{87}\text{Rb}-^{40}\text{K} \) it is already 32 bound states for \( l = 0 \)). The very long ranged weakly bound states consist therefore of a highly oscillatory inner part (covering the so-called molecular regime and providing orthogonality to all lower lying bound states) and a rather smooth long range
part. Correspondingly, it is useful to adopt two different knot sequences for the $B$ splines. In the present case convergence was found, if 200 $B$ splines expanded on a linear knot sequence covering $0 \leq r \leq 20 a_0$ are used together with about 70 $B$ splines covering the remaining $r$ range. The latter are expanded on a knot sequence in which the separation between the knot points increases in a geometric fashion. For the states of interest in this work it was sufficient to include in the CI calculations only configurations built from about 120 REL and 60 COM orbitals. Taking symmetry into account, this amounted to about 1060 configurations used in the CI expansions.

3. Results

In [6] the binding energy of the least bound state of the $^{87}$Rb-$^{40}$K molecule was measured as a function of the magnetic field strength close to a MFR by high-resolution rf association. The magnetic field dependence may be transformed into a dependence on the interatomic interaction strength (characterised in the case of ultracold collisions by the scattering length $a_{sc}$ or its scaled analogue $\xi$) using the two-channel model for MFR.

![Figure 1](image-url)

**Figure 1.** Energy of the least bound state ($E_{lb}$, insert) and the first trap-induced state ($E_{1ti}$) of $^{87}$Rb-$^{40}$K in an optical lattice of depth (a) $V_{Rb} = 27.5 E_{Rb}^{Rb}$ and (b) $V_{Rb} = 40.0 E_{Rb}^{Rb}$ as a function of the interatomic interaction parameter $\xi$. Shown are the energies obtained within the harmonic [sextic] approximation for the uncoupled COM and REL motion ($E_{sep}$, solid [dots]) and from the full CI calculation ($E_{CI}$, dashes [chain]).

For an ultracold gas in an optical lattice the initial (atom pair) state is the lowest trap-induced state ($1_{ti}$), i.e. the first state above the trap-free dissociation threshold. In Fig. 1 the absolute energies $E_{1b}$ and $E_{1ti}$ (in units of the averaged harmonic trap frequency) of the least bound state and the first trap-induced state, respectively, are shown as a function of $\xi$. The effect of the anharmonicity of the optical lattice is investigated by a comparison of the results obtained within the harmonic and the sextic approximation in which the terms up to 2nd or 6th order of the Taylor expansion of the $\sin^2$ describing the optical lattice potential are included. In both cases, the full CI energies $E_{CI}$ of $\hat{H}$ are compared to the results obtained from the separable parts of the Hamiltonian, i.e. the sum $E_{sep}$ of the energies $E$ and $\epsilon$ of $\hat{h}_{COM}$ and $\hat{h}_{REL}$ respectively. Clearly, the energy of the least bound state is for the given parameters almost completely unaffected by the anharmonicity of the trap, since all energies are very similar. Although this state is very long-ranged it feels the trapping potential only very weakly. Therefore, the effect of the anharmonicity of the trap on the binding energy is only a result of the sensitivity of the energy of the first trap-induced state on the trap potential. Even within the harmonic approximation there is an evident difference between $E_{sep}$ and $E_{CI}$. This is due to the coupling of COM and
REL motion present in the harmonic approximation for a heteronuclear system. The inclusion of anharmonicity (sextic instead of harmonic approximation) leads to an even larger modification of the energy as can be seen by a comparison of $E_{\text{sep}}$ in the two approximations. Also the effect of the coupling of COM and REL motion increases, if the anharmonicity of the optical lattice is considered, as is evident from a comparison of the difference $E_{\text{CI}} - E_{\text{sep}}$ for either the harmonic or the sextic approximation. A comparison of the results for different trap depths in Figs. 1 (a) and (b) reveals that a deeper trap diminishes the effects. This is not unexpected, since for a deeper trap the low-lying states will experience less of the anharmonicity. On the absolute scale the effects of anharmonicity and coupling of COM and REL motion amount for the considered system and relatively large positive values of $\xi$ to about 11 kHz. This effect is visible in the experiment in [6] with a resolution of 1.7 kHz, but would not be resolvable with a ten times worse resolution as it occurs for a ten times shorter rf pulse as was used, e.g., in [5].

Besides a more detailed analysis of the influence of anharmonicity and COM-REL motion coupling for different homo- and heteronuclear systems future studies with the existing code will consider highly anisotropic, asymmetric (disordered) and double-well lattice geometries. Further extensions of the code should also allow to study the case of a pair of atoms or molecules interacting by non-centric, e.g., dipolar interactions. Finally, it is planned to extend the method for studying the time-dependent dynamics of atomic pairs in time-varying lattices.

During completion of the present work we became aware of a similar approach with somehow comparable conclusions [22]. While a detailed comparison will be given elsewhere, it may be remarked that [22] does not use the full interatomic interaction potential but applies the pseudopotential approximation. Furthermore, a different partitioning of the Hamiltonian and different, less flexible basis functions (eigensolutions of the harmonic oscillator) were adopted.

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References

[1] Anderson M H, Ensher J R, Matthews M R, Wieman C E and Cornell E A 1995 Science 269 198
[2] Jaksch D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 Phys. Rev. Lett. 81 3108
[3] Greiner M, Mandel O, Esslinger T, Hänsch T and Bloch I 2002 Nature 415 39
[4] Köhl M, Moritz H, Stöferle T, Günter K and Esslinger T 2005 Phys. Rev. Lett. 94 080403
[5] Stöferle T, Moritz H, Günter K, Köhl M and Esslinger T 2006 Phys. Rev. Lett. 96 030401
[6] Ospelkaus C, Ospelkaus S, Humbert L, Ernst P, Sengstock K and Bongs K 2006 Phys. Rev. Lett. 97 120402
[7] Busch T, Englert B G, Rzazewski K and Wilkens M 1998. Found. of Phys. 28 549
[8] Bolda E L, Tiezinga E and Julienne P S 2005 Phys. Rev. A 71 033404
[9] Grishkevich S and Saenz A 2007 Phys. Rev. A 76 022704
[10] Blume D and Greene C H 2002 Phys. Rev. A 65 043613
[11] Idziaszek Z and Calarco T 2005 Phys. Rev. A 71 050701(R)
[12] Lim I S, Pernpointner M, Seth M, Laerdahl J K and Schwerdtfeger P 1999 Phys. Rev. A 60 2822
[13] Rousseau S, Allouche A R and Aubert-Frécon M 2000 J. Mol. Spec. 203 235
[14] Zemke W T, Côté R and Stwalley W C 2005 Phys. Rev. A 71 062706
[15] Derevianko A, Babb J F and Dalgarano A 2001 Phys. Rev. A 63 052704
[16] Porsev S G and Derevianko A 2003 J. Chem. Phys. 119 844
[17] Ferlaino F, D’Errico C, Roati G, Zaccanti M, Inguscio M, Modugno G and Simoni A 2006 Phys. Rev. A 73 040702. Erratum: 2006 Phys. Rev. A 74 039903.
[18] Goldwin J, Inouye S, Olsen M L, Newman B, DePaola B D and Jin D S 2004 Phys. Rev. A 70 021601
[19] Inouye S, Goldwin J, Olsen M L, Ticknor C, Bohn J J and Jin D S 2004 Phys. Rev. A 93 183201
[20] Loftus T, Regal C A, Ticknor C, Bohn J J and Jin D S 2002 Phys. Rev. Lett. 88 173201
[21] Regal C A and Jin D S 2003 Phys. Rev. Lett. 90 230404
[22] Deuretzbacher F, Plassmeier K, Pfannkuche D, Werner F, Ospelkaus C, Ospelkaus S, Sengstock K and Bongs K arXiv:cond-mat/0703322v1

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