Exact theoretical description of two ultracold atoms in a single site of a 3D optical lattice using realistic interatomic interaction potentials

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A theoretical approach was developed for an exact numerical description of a pair of ultracold atoms interacting via a central potential that are trapped in a three-dimensional optical lattice. The coupling of center-of-mass and relative-motion coordinates is explicitly considered using a configuration-interaction (exact-diagonalization) technique. Deviations from the harmonic approximation are discussed for several heteronuclear alkali-metal atom pairs trapped in a single site of an optical lattice. The consequences are discussed for the analysis of a recent experiment [C. Ospelkaus et al, Phys. Rev. Lett. 97, 120402 (2006)] in which radio-frequency association was used to create diatomic molecules from a fermionic and a bosonic atom and to measure their binding energies close to a magnetic Feshbach resonance.

I. INTRODUCTION

The physics of ultracold atoms has attracted a lot of interest since the experimental observation of Bose-Einstein condensation in dilute alkali-metal atom gases [1, 2]. Besides the exciting physics at ultracold energies by itself, a further important progress was the loading of the ultracold gas into an optical lattice formed with the aid of standing light waves [3, 4, 5]. The optical lattice resembles in some sense the periodicity of a crystal potential [6, 7, 8]. 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). Moreover, different atoms possess different interaction potentials that can be either attractive or repulsive. While different kinds of chemical elements, their isotopes, or atoms in different electronic or spin states cover already quite some range of interaction strengths, a further tunability of the atom-atom interactions in optical lattices can be achieved using magnetic Feshbach resonances [9, 10]. Close to the resonance value of the magnetic field the interaction varies in a wide range of attractive and repulsive values.

Ultracold atoms deposited in light crystals are ideal systems for a realization of the Hubbard model [11]. This model takes into account a single band of a static lattice potential and assumes the interactions to be purely local [11] (low tunneling limit). In this case the optical lattice is considered as an array with a very small filling rate; optimally with one or two atoms per lattice site. The experimental study of a bosonic Mott insulator [4] and a fermionic band insulator [5] provided such a system. The fact that the analysis of a single site is sufficient for such systems simplifies their theoretical description drastically.

Another interesting aspect is that ultracold atoms can bind together to form ultracold molecules. The optical lattice can shield the often fragile, very weakly bound molecules from destructive three-body collisions. The physics of ultracold atom pairs in optical lattices with controllable interactions is thus presently an intensively investigated research area. Recently the observation of confinement-induced molecules, repulsively interacting pairs, and real molecules for both homonuclear [3, 12] and heteronuclear [13] atomic species in optical lattices has been reported.

In order to describe the behavior of atoms in an optical lattice the latter is usually considered as an array of harmonic traps. In such an approach some important features of the optical lattice can be lost. For example, the correct sinusoidal potential exhibits an energy band with a spread of transition energies while the harmonic potential possesses a discrete equidistant spectrum. Nevertheless, the experiment of Stöferle et al. [12] showed good agreement with a simplified theoretical description based on the harmonic approximation. In their analysis, Stöferle et al. compared the measured binding energies of confinement-induced molecules and real molecules to the ones predicted by a simplified theory in which two atoms are trapped in a harmonic potential and interact via a δ-function pseudopotential. Within such a model an analytical solution exists in the case of two identical atoms (in the same quantum states) [14]. However, another experiment that adopted higher resolution spectroscopy and considered a heteronuclear system was interpreted to clearly indicate a break-down of the harmonic approximation [13].

From the theoretical point of view, the description of two atoms in an optical lattice beyond the harmonic approximation is very laborious. The anharmonic part of the optical lattice potential leads to a coupling of center-of-mass and relative motion and requires therefore to solve the full six-dimensional problem. In fact, even within the harmonic approximation different trapping potentials experienced by the two atoms lead to a coupling of center-of-mass and relative motion [15, 16]. This situation occurs, e.g., for heteronuclear atom pairs or two atoms of the same kind but in different electronic states.

In this work a numerical approach is developed that allows in principle to describe two atoms trapped in an optical lattice in an exact way, if the interatomic interaction potential is central (isotropic) and can be given
in terms of a single potential curve. The fact that this latter curve stems usually from a full molecular calculation and is only given in numerical form is explicitly considered. Extensions to non-central (like dipolar) interactions are rather straightforward and planned for the near future. The anharmonic coupling is treated in a configuration-interaction (CI) like fashion also known as exact diagonalization. It leads for sufficiently large expansion lengths to exact results. Although the approach allows to consider multiple-well potentials and thus more than a single site of an optical lattice [17], the present work focuses on results obtained for two atoms in a single site. Motivated by the experiment reported in [13] the heteronuclear atom pair formed by fermionic $^{40}$K and bosonic $^{87}$Rb was used as a generic system in the present study. In order to investigate the influence of the atomic interaction strength, its value was varied artificially by a controlled manipulation of the inner wall of the corresponding potential curve. For the investigation of the influence of the mass difference on the results, two other heteronuclear pairs, $^{6}$Li-$^{7}$Li (almost equal masses) and $^{6}$Li-$^{133}$Cs (very large mass difference) were considered. After a systematic investigation of the effects of anharmonicity and coupling of center-of-mass and relative motion a comparison to the experimental data [12] as well as to a subsequent theoretical analysis [18] performed in parallel to the present work is given.

The paper is organized in the following way. In Sec. II the theoretical approach is described. This includes the formulation of the problem in Sec. II A as well as a description of the trap parameters (Sec. II B), the used interatomic interaction potentials (Sec. II C), and its systematic variation in Sec. II D. The section ends with the computational details described in Sec. II E. The results presented in Sec. III are first discussed in terms of energies (and their differences) for the generic $^{87}$Rb-$^{40}$K dimer in Sec. III A and for other dimers in Sec. III B. This is followed by an analysis of the radial pair densities (Sec. III C 1) and the wavefunctions in absolute coordinates (Sec. III C 2). This is followed by a comparison to the experimental and recent alternative theoretical results in Sec. III D. Finally, a conclusion and outlook is given in Sec. IV. All equations and quantities in this paper are given in atomic units unless otherwise specified.

II. SYSTEM

A. Hamiltonian

The Hamiltonian describing the interaction of two atoms with coordinate vectors $\vec{r}_1$ and $\vec{r}_2$ trapped in a three-dimensional optical lattice is given by

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

(1)

where $\hat{T}_j$ is the kinetic energy operator for particle $j$, $\hat{U}$ is the atom-atom interaction potential, and $\hat{V}_{\text{trap},j}$ is the trapping potential for particle $j$. For optical lattices $\hat{V}_{\text{trap},j}$ is often (and also in the present work) given by

$$
\hat{V}_{\text{trap},j} = \sum_{c=x,y,z} V_c^j \sin^2(k_c\vec{c}_j),
$$

(2)

where $V_c^j$ is the potential depth which particle $j$ experiences along direction $c$, and $k_c = 2\pi / \lambda_c$ is the wave vector and $\lambda_c$ the wavelength of the laser creating the lattice potential along the (Cartesian) coordinate $c$.

A direct solution of the Schrödinger equation with the Hamiltonian given in the form of Eq. (1) is complicated, since $\hat{U}$ depends in general 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 $r = |\vec{r}_1 - \vec{r}_2|$. For realistic interatomic interaction potentials (that are usually even only known numerically), there is no separability and this leads to very demanding six-dimensional integrals. Therefore, it is more convenient to treat the two-particle problem in center-of-mass (COM) and relative (REL) motion coordinates. If spherical coordinates are adopted, a central interaction potential leads to a function of the radial coordinate only.

On the other hand, the formulation of the two-particle problem in COM and REL coordinates complicates the treatment of the trap potential, since its separability in Cartesian coordinates is lost in the COM and REL coordinate system. However, performing a Taylor expansion of the sinusoidal trapping potential [2] around the origin simplifies the problem drastically, because the angular parts can be analytically solved for in the case of a central interatomic interaction potential. For two identical atoms in the same state the use of the harmonic approximation for the trapping potential leads even to a problem that is completely separable in COM and REL coordinates [13]. If the true atom-atom interaction is, furthermore, replaced by a $\delta$-function pseudopotential that reproduces only asymptotically the two-body zero-energy s-wave scattering, the Schrödinger equation possesses an analytical solution for both isotropic or anisotropic harmonic traps [14, 20]. Noteworthy, even within the harmonic approximation the separability is 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.

After performing the Taylor expansion of the sinusoidal trapping potential [2] around the origin, the transformation of the Hamiltonian $\hat{H}$ into the COM and REL coordinate systems leads to a Hamiltonian of the form

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

(3)

with

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

(4)

$$
\hat{h}_{\text{REL}}(\vec{r}) = \hat{\imath}_{\text{kin}}(\vec{r}) + \hat{\imath}_{\text{OL}}(\vec{r}) + \hat{\imath}_{\text{int}}(\vec{r}^\prime).
$$

(5)
It is worth emphasizing that in the present formulation only the truly non-separable terms (represented by products of COM and REL coordinates) are left in the coupling term $W$. All separable 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.

In a first step, the eigenstates and -values of the COM and REL Hamiltonians are obtained independently of each other by means of a numerical solution of the corresponding stationary Schrödinger equations,

$$\hat{h}_{\text{COM}} |\psi_i\rangle = \varepsilon_i |\psi_i\rangle \quad \text{and} \quad \hat{h}_{\text{REL}} |\phi_i\rangle = \varepsilon_i |\phi_i\rangle . \quad (6)$$

The wavefunctions $\psi(\vec{R})$ and $\phi(\vec{r})$ are then used to form the configuration state functions $\Phi_k(\vec{R}, \vec{r}) = \psi_i(\vec{R}) \phi_j(\vec{r})$. The stationary Schrödinger equation with the full Hamiltonian given in Eq. (5),

$$\hat{H} |\Psi_i\rangle = \varepsilon_i |\Psi_i\rangle , \quad (7)$$

is then solved by expanding $\Psi$ as $\Psi(\vec{R}, \vec{r}) = \sum_k C_k \Phi_k(\vec{R}, \vec{r})$. Insertion of this expansion into Eq. (7) leads (after the usual manipulations) to a matrix eigenvalue problem that is solved numerically and yields the energies $\varepsilon_i$ and eigenvector coefficients $C_k$.

### B. Trap parameters

Despite the already mentioned breakdown of the harmonic approximation especially for heteronuclear systems it is still convenient to introduce the mean harmonic-oscillator frequencies $\omega_{\text{ho}}$ and $\Omega_{\text{ho}}$ of a single lattice site for the REL and COM motion respectively,

$$\omega_{\text{ho}} = k \sqrt{\frac{V_1 \mu_2^2 + V_2 \mu_1^2}{\mu}} \quad (8)$$

$$\Omega_{\text{ho}} = k \sqrt{\frac{V_1 + V_2}{M}} . \quad (9)$$

In Eqs. (8) and (9) $\mu$ and $M$ denote the reduced mass and total mass of the two particles respectively, $\mu_j$ is defined as $\mu_{1,2} = \mu / m_{1,2}$ where $m_j$ is the mass of atom $j$, and $V_j = I_0 \alpha_j$ is the optical lattice depth that is equal to the product of the laser intensity $I_0$ (for an isotropic geometry $I_0 = I_x = I_y = I_z$) and the polarizabilities $\alpha_j$ of atom $j$. Finally, one has $k = k_x = k_y = k_z$ for an isotropic geometry of the lattice. This isotropy is in fact assumed in Eqs. (8) and (9). For identical particles of mass $m$ Eq. (8) reduces to the well-known relation $\omega_{\text{ho}} = k \sqrt{2V_0 / m}$.

Some parameters of the trap chosen in the present study were motivated by the recent experiment reported in [13]. Therein a three-dimensional optical lattice generated by lasers with wavelength $\lambda = \lambda_x = \lambda_y = \lambda_z$ of 1030 nm was used for the trapping of ultracold bosonic $^{87}$Rb and fermionic $^{40}$K atoms. The two different lattice depths $V_{\text{Rb}} = 40 E_{\text{Rb}}^\text{SR}$ and $V_{\text{Rb}} = 27.5 E_{\text{Rb}}^\text{SR}$ were considered where the individual recoil energy is defined, e.g., as $E_{\text{Rb}}^\text{SR} = k^2 / (2m_{\text{Rb}})$. Since the static dipole polarizabilities of rubidium and potassium are different, $\alpha_{\text{Rb}} = 324 \text{ a.u.}$ and $\alpha_{\text{K}} = 301 \text{ a.u.}$ [21], the two atoms experience different potentials: $V_{\text{K}} = 37.2 E_{\text{Rb}}^\text{SR}$ and $V_{\text{K}} = 25.5 E_{\text{Rb}}^\text{SR}$ for $40 E_{\text{Rb}}^\text{SR}$ and $27.5 E_{\text{Rb}}^\text{SR}$ respectively. The mean harmonic-oscillator frequencies [23] are $\omega_{\text{ho}}(40 E_{\text{Rb}}^\text{SR}) = 2 \pi \times 35.7 \text{ kHz}$ and $\omega_{\text{ho}}(27.5 E_{\text{Rb}}^\text{SR}) = 2 \pi \times 30 \text{ kHz}$. While most of the results of this work are obtained for these frequencies, some other values are also considered in order to investigate the influence of the trap frequency in more detail.

### C. Interatomic interaction potential

The interaction between rubidium and potassium atoms is modeled using the Born–Oppenheimer (BO) potential of the $a^3 \Sigma^+$ electronic state describing the interaction of two spin-polarized atoms. In general the atom-atom interaction potentials are only known numerically. For the short-range part $V_{\text{SR}}$ of the potential in between $R \in [1.588 a_0, 18.2 a_0]$ the data of [22] are used ($a_0$ is the Bohr radius). The data points at $R = 17.6 a_0$ and $R = 16.99998 a_0$ have been omitted, because their inclusion results in a non-smooth potential curve. 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. [23]. Therefore, this long range part is defined as $V_{\text{LR}}(r) = D_c + \Delta V_{\text{disp}}(r) + \Delta V_{\text{ex}}(r)$ for $R \geq 18.6 a_0$ where $\Delta V_{\text{disp}}(r) = -C_6 / r^6 - C_8 / r^8 - C_{10} / r^{10}$ and the dispersion coefficients $C_n$ are the values of Derevianko and co-workers [24, 25], except $C_0 = 4292 \pm 19 \text{ a.u.}$ which was taken from [20]. The exchange interaction is given by $\Delta V_{\text{ex}}(r) = -C_6 e^{-\beta r}$ with $C = 0.00231382$, $\alpha = 5.25603$, $\beta = 1.11892$ as given in [23]. To merge the short- and the long-range parts the short-range part is raised by half of the value $\Delta V_{\text{merge}} = V_{\text{SR}}(18.2 a_0) - V_{\text{LR}}(18.6 a_0)$.

According to [23] 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 the same character of the interaction are observed in the present calculation using the potential curve constructed the way described above.

In order to study the influence of different masses, polarizabilities, different interaction potentials, and also to check the generality of the conclusions of this work other systems are also analyzed. In particular, the heteronuclear $^4\text{Li} - ^7\text{Li}$ and $^6\text{Li} - ^13\text{Cs}$ pairs interacting via their respective $a^3 \Sigma^+$ electronic state are considered. The potential curves for $^4\text{Li} - ^7\text{Li}$ and $^6\text{Li} - ^13\text{Cs}$ were constructed according to [16] and [27], respectively.

### D. Manipulation of the interatomic interaction

In the limit of zero collision energy the interaction between two atoms can be characterized by their s-wave
scattering length $a_{sc}$. The sign of $a_{sc}$ determines the type of interaction (repulsive or attractive) and the absolute value determines the interaction strength. Experimentally it is difficult to accurately measure the scattering length. For example, there is no agreement about the value of the triplet scattering length for the $^{87}\text{Rb}^{40}\text{K}$ system. According to the ongoing discussion [26, 28, 29, 30] the value $-186(4)\ a_0$ appears to be the most reliable one. A standard way to match the calculated scattering length with the experimental value is a smooth shift of the inner wall of the BO potential as is described in [23]. 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 (lb) state supported by the potential curve as is shown in Fig. 1. 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 the ultracold atoms are strongly influenced. Therefore, a small variation of the inner wall of the potential can modify the interatomic interaction potential from strongly repulsive to strongly attractive. This procedure is adopted in the present work in order to investigate the influence of the interatomic interaction potential. The scattering length is only well-defined for zero-energy scattering and thus the underlying concept is in principle not applicable to trapped particles with a non-vanishing zero-point energy. Therefore, the scattering-length values (for a given inner-wall shift) are determined for the trap-free situation. In this case $a_{sc}$ can be uniquely determined from the analysis of the shape of the zero-energy scattering wave function [31].

Ignoring the formal problems of defining a scattering length within a trap (that will be discussed in some more detail below), it is often considered useful to introduce a dimension-free interaction parameter $\xi$ that reflects the relative magnitude of the interaction strength with respect to the confinement by the trap. If this confinement is approximated within the harmonic approximation, the relative magnitude of the interaction strength with respect to the confinement by the trap. If this confinement is approximated within the harmonic approximation, the interaction parameter is naturally defined as $\xi = a_{sc}/a_{ho}$ where $a_{ho}$ is the characteristic length of a harmonic potential given by $a_{ho} = 1/\sqrt{\mu \omega_{ho}}$. For a heteronuclear atom pair $\omega_{ho}$ is again the mean harmonic frequency defined in Eq. (8).

Experimentally, a strong variation of the interaction strength can be realized with the help of magnetic Feshbach resonances (MFR) [5, 32]. The MFR technique was also used to tune the interatomic interaction from strongly repulsive to strongly attractive in the already mentioned experiments with atoms in the optical lattices [5, 12, 13]. In general, the correct theoretical description of a MFR 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 described in [5, 12, 13] it is, however, assumed that it is possible to model the MFR in an effective two-channel picture [31]. Within this model it is straightforward to relate the applied magnetic field to a scattering-length value (see Eq. (20) below).

**E. 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 $\phi(\vec{\ell})$ as a linear combination of products of radial $B$-spline functions times spherical harmonics. The corresponding Schrödinger equations are solved numerically using the Rayleigh-Ritz-Galerkin approach [33] which leads to an algebraic eigenproblem.

In general, the lattice leads to a coupling of the angular momenta. Therefore, the spherical harmonics are no eigensolutions of the angular part. Due to the cubic trap geometry used in the experiment in [13] and also for the present calculations, the coupling of different spherical harmonics is weak. In fact, the orbitals $\psi(\vec{R})$ and $\phi(\vec{\ell})$ describing the states relevant to this work are almost converged, even if only $l = 0$ is considered. However, the coupling term $W$ in the Hamiltonian [34] 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 $\phi(\vec{\ell})$.

The required number of $B$ splines and their knot sequence depend strongly on the behavior of the wave function ($\psi(\vec{R})$ or $\phi(\vec{\ell})$) that should be described. In the context of ultracold collisions the main interest is put on..
the energetically low-lying COM orbitals $\psi(\vec{R})$ that possess a small number of nodes. For the results discussed in this work, about 70 $B$ splines were found to be sufficient to obtain convergence. Evidently, more complicated or highly anisotropic trap geometries (like double or triple wells) 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-metal atom dimers support often a large number of bound states (for example, the $^{87}\text{Rb}^{40}\text{K}$ system possesses in the $a^3\Sigma^+\rightarrow$ state 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 the orthogonality to all lower lying bound states) and a rather smooth long-range part. Correspondingly, it is practical to use 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 the interval $0 \leq r \leq 20 a_0$ are used together with about 70 $B$ splines for the remaining $r$ range. The latter 70 $B$ splines are expanded on a knot sequence in which the separation between the knot points increases in a geometric fashion.

Converged CI calculations were found, if they comprised configurations built from about 120 REL and 60 COM orbitals. After taking symmetry into account this amounts to about 1060 configurations forming the CI expansion for the states of interest in this work.

III. RESULTS

A. Energy spectrum of the $^{87}\text{Rb}^{40}\text{K}$ system

The description of an optical lattice beyond the harmonic approximation is in the present work achieved by extending the Taylor expansion of the $\sin^2$ potential beyond the harmonic (1st order and thus quadratic) term. In principle, one should seek for convergence with respect to the expansion length, but there are some practical reasons why a simple convergence study as a function of the expansion length causes problems. First of all, even-order expansions like the 2nd order one which leads to polynomials with a degree of up to 4 (quartic potential) support an infinite number of bound states with negative energy, since they tend to $-\infty$ for $x$ approaching either $+\infty$ or $-\infty$. However, these bound states with negative energies are unphysical, since they do not exist in the case of the (original) positive definite $\sin^2$ potential. The 3rd order expansion that leads to polynomials up to a degree of 6 (sextic potential) supports on the other hand (like all odd-order expansions) only bound states with positive energy values.

A comparison of this sextic potential with the $\sin^2$ potentials shows that the sextic potential reproduces extremely well a single site of the $\sin^2$ potential and thus of the optical lattice (see Fig. 1). Therefore, the sextic potential is a good choice for the investigation of the effects of anharmonicity on the bound states in a single site of an optical lattice. Evidently, the sextic potential cannot reproduce effects that are due to tunneling between neighbor potential wells. Therefore, extended (energetically higher lying) bound states in the optical lattice that are markedly affected by tunneling are not well reproduced by a sextic potential. Noteworthy, even in this case a simple convergence study will, however, not work. For example, the 5th order and thus next odd-order expansion shows a triple-well structure, but the two outer wells have a depth and width that differs pronouncedly from the correct shape (and the central well). This leads to completely wrongly described states in these outer wells and may thus show wrong tunneling behavior for the states in the middle well, especially in the case of resonant tunneling. Since the present study concentrates on the anharmonicity effects within a single site of an optical lattice, only the sextic potential and, for comparison, the harmonic one are considered. Effects that are due to tunneling between neighbor wells and thus include more than single-well potentials are investigated in a separate work.

The potential seen by the two atoms in an optical lattice contains, of course, in addition to the trap potential also the interatomic interaction potential that in the present case is described by a Born-Oppenheimer potential curve (and appears only in the REL coordinates). As is sketched in Fig. 1 the interatomic interaction dominates the short-range part of the potential and leads in the case of alkali-metal atoms to a large number of bound molecular states. Since the trap potential is compared to the variation of the BO curve almost constant in the range of the molecular bound states, especially the lower lying of these states will in practice not be influenced by the optical lattice. The largest possible effect of the optical lattice on the molecular bound states is expected to occur for the energetically highest lying one, the least bound (lb) state.

Due to the large spatial extension of the trap states of typical experimentally realized optical lattices these trap-induced states are expected to be only weakly influenced by the molecular potential. However, an immediate consequence of the existence of the molecular bound states below the trap-induced ones is the nodal structure at short distances that is imprinted on the wavefunctions and leads to the required orthogonality of the eigenstates. The energetically lowest lying and thus first trap-induced (1ti) state possesses thus exactly one more node than the lb state. In the experiments most closely related to the present work the transition energy between the lb and the 1ti state has been measured by either rf dissociation or association, respectively. This transition energy was called binding energy, but it should be kept in mind that its definition does not coincide with the standard definition of a molecular binding energy which is given by the energy difference between a molecular bound state and the (lowest) dissociation limit. In the present case
the existence of the optical lattice leads to a discretization of the dissociation continuum and thus to an additional energy shift due to the zero-point energy of the trap.

If the coupling $W$ of REL and COM coordinates is ignored, the energies $E_{\text{lb}}$ and $E_{\text{1ti}}$ of the least bound and the 1st trap-induced state, respectively, are obtained from the eigenvalues of Eq. (6) as

$$E_{\text{lb}}^{(n)} = E_{(1, \text{lb})}^{(n)} = \varepsilon_1^{(n)} + \epsilon_1^{(n)}$$

$$E_{\text{1ti}}^{(n)} = E_{(1, \text{1ti})}^{(n)} = \varepsilon_1^{(n)} + \epsilon_1^{(n)}$$

where $n$ specifies the expansion length describing the optical lattice: $n = 2$ for a harmonic and $n = 6$ for a sextic trap. In accordance with the underlying assumption of an ultracold gas, the system is assumed to be in its lowest state with respect to translational motion, i.e. in the COM ground state with energy $\varepsilon_1$. The corresponding wavefunctions are given by $\Phi_{\text{lb}}(\vec{R}, \vec{r}) = \psi_1(\vec{R})\phi_{\text{lb}}(\vec{r})$ and $\Phi_{\text{1ti}}(\vec{R}, \vec{r}) = \psi_1(\vec{R})\phi_{\text{1ti}}(\vec{r})$.

After the inclusion of the coupling of REL and COM motion the wavefunctions $\Phi$ are no longer eigenstates of the Hamiltonian, but are used as a basis for expanding the full wavefunctions $\Psi$ that are obtained together with their energies $E$ by solving the Schrödinger Eq. (7). The state $\Psi$ with a dominant contribution from $\Phi_{\text{lb}}(\Phi_{\text{1ti}})$ is then identified as least bound (1st-trap-induced) state with energy $E_{\text{lb}}^{(n)}$ ($E_{\text{1ti}}^{(n)}$), where $n$ stands again for the order of the Taylor expansion of the optical-lattice potential.

In Fig. 2 the energies of the least bound and the 1st trap-induced state are shown for $^{87}\text{Rb}-^{40}\text{K}$ dimers in a single site of an optical lattice ($\lambda = 1030 \text{ nm}$) for the potential depths (a) $V_{\text{rb}} = 27.5 \text{E}_\text{Rb}$ and (b) $V_{\text{rb}} = 40.0 \text{E}_\text{Rb}$ at different levels of approximation as a function of the trap-free scattering length (see Sec. II D for details). The energies obtained with a full CI calculation for a sextic potential ($E^{(0)}$, green chain) and a harmonic one ($E^{(2)}$, red dashes) are compared to the corresponding sextic ($E^{(0)}$, blue dots) and harmonic ($E^{(2)}$, black solid) energies that are obtained, if the coupling between COM and REL motion is neglected. (Note, the sum $\frac{3}{2}(\omega_{\text{ho}} + \Omega_{\text{ho}})$ corresponds to $E^{(2)}(a_{\text{sc}} = 0) = 100.65 \text{ kHz}$.)

FIG. 2: (Color online) Energies of the 1st trap-induced (main graph) and least bound (inset) state of $^{87}\text{Rb}-^{40}\text{K}$ dimers in a single site of an optical lattice ($\lambda = 1030 \text{ nm}$) for the potential depths (a) $V_{\text{rb}} = 27.5 \text{E}_\text{Rb}$ and (b) $V_{\text{rb}} = 40.0 \text{E}_\text{Rb}$ at different levels of approximation as a function of the trap-free scattering length (see Sec. II D for details). The energies obtained with a full CI calculation for a sextic potential ($E^{(0)}$, green chain) and a harmonic one ($E^{(2)}$, red dashes) are compared to the corresponding sextic ($E^{(0)}$, blue dots) and harmonic ($E^{(2)}$, black solid) energies that are obtained, if the coupling between COM and REL motion is neglected. (Note, the sum $\frac{3}{2}(\omega_{\text{ho}} + \Omega_{\text{ho}})$ corresponds to $E^{(2)}(a_{\text{sc}} = 0) = 100.65 \text{ kHz}$.)
TABLE I: The effect of the trapping potential on the energy spectrum of the 1st trap-induced state of $^{87}$Rb-$^{39}$K for the trapping parameters of the experiment reported in [14]. The $\Delta$ values defined by Eqs. (12)-(14) are given in units of $h^{-1}$/kHz and calculated at $a_{sc} = 6500 a_0$.

| $V_{Rb}(E_{coup}^{Rb})$ | $\Delta_{\text{geom}}$ | $\Delta_{\text{coup}}^{(2)}$ | $\Delta_{\text{coup}}^{(6)}$ | $\Delta_{\text{tot}}$ |
|-------------------------|------------------------|-----------------------------|-----------------------------|------------------|
| 27.5                    | 6.797                  | 3.022                       | 5.665                       | 12.462           |
| 40.0                    | 6.828                  | 3.689                       | 6.243                       | 13.071           |

is ignored. For the considered system the effect of anharmonicity is thus a larger correction to the separable harmonic approximation than the one caused by the coupling of COM and REL motion. A further energy reduction is found, if both effects are considered which leads to $\mathcal{E}^{(6)}$. Interestingly, the energy reduction indicated by $\mathcal{E}^{(6)}$ is larger than the sum of the energy reductions obtained separately for $\mathcal{E}^{(2)}$ and $\mathcal{E}^{(6)}$. The coupling of COM and REL motion is thus enhanced, if the more realistic sextic potential is considered instead of the harmonic one.

In order to quantitatively describe the different effects of the trapping potential the energy differences

$$\Delta_{\text{geom}} = E_i^{(2)} - E_i^{(6)}$$
$$\Delta_{\text{coup}}^{(n)} = E_i^{(n)} - E_i^{(n)}$$
$$\Delta_{\text{tot}} = E_i^{(2)} - E_i^{(6)} = \Delta_{\text{geom}} + \Delta_{\text{coup}}^{(6)}$$

may be introduced, where $i = \{1b, 1\text{ti}\}$. $\Delta_{\text{geom}}$ characterizes the effect of anharmonicity of the optical lattice based on the uncoupled solutions. $\Delta_{\text{coup}}^{(n)}$ is a measure of the coupling between COM and REL motion within the harmonic ($n=2$) or sextic ($n=6$) potential. Finally, $\Delta_{\text{tot}}$ specifies the energy difference between the simple harmonic approximation (in which the coupling of COM and REL motion is ignored) and the full solution of two atoms in a single site of an optical lattice (within the sextic approximation).

As is evident from Fig. 2, the effect is largest for the strongly repulsive regime. This is due to a rise of the energy level to the region of higher anharmonicity of the trapping potential. Moreover, the state in this point is also long-ranged due to the strong repulsive interaction. Numerical values of the differences $\Delta$ [12,14] for $^{87}$Rb-$^{40}$K, the experimental trap parameters in [13], and $a_{sc} = 6500 a_0$ are given in Table I.

For the considered system the value $\Delta_{\text{tot}}$ and thus the total energy between the uncoupled and the coupled harmonic approximation amounts to about 13 kHz for $a_{sc} = 6500 a_0$. An effect of this size should be visible in the experiment in [13] with a claimed 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 [12].

In an analysis of the influence of the interaction strength as is performed in this work it is important to stay within the restrictions of a single-site model. The parameter variation has to avoid situations in which tunneling or even over-the-barrier transfer of atoms between different sites of a physical optical lattice can occur, since this range is clearly not adequately described with a harmonic or sextic potential with infinite walls. For example, for a very large positive scattering length the large repulsive interaction shifts the lowest-lying atom-pair state (1st trap-induced state) above the barrier of a true optical lattice. While this physical lattice would not support any bound states, the harmonic or sextic potentials would still possess an infinite number of them. As is discussed in Sec. III C it was always checked that the wave functions remain well localized within the boundaries of a single site of the optical lattice for the parameters used in this study.

### B. Other systems

In order to obtain a more complete picture of the anharmonicity and the coupling effects other systems may be analyzed. Besides the already considered $^{87}$Rb-$^{40}$K pair (example of large masses and polarizabilities) other experimentally relevant alkali metal dimers like $^{6}$Li-$^{133}$Cs (small mass and polarizability of $^{6}$Li and for $^{133}$Cs both characteristics are large) and $^{6}$Li-$^{7}$Li (small masses and polarizabilities of both elements) are investigated.

Figure 3 shows the differences $\Delta$ [12,14] as a function of the scaled interaction parameter $\xi$ [see Sec. III D] for different lattice depths obtained by the laser intensity variation for the three mentioned systems. As is evident from Fig. 3 the harmonic coupling difference $\Delta_{\text{coup}}^{(2)}$ is not influenced by the lattice depth, because the coupling depends only on the polarizabilities and the masses and is of the form ($\mu_1 \alpha_1 - \mu_2 \alpha_2$). Therefore, $\Delta_{\text{coup}}^{(2)}$ is largest for $^{6}$Li-$^{133}$Cs and smallest for $^{6}$Li-$^{7}$Li as is clear from Fig. 3. Beyond the harmonic approximation the mass, polarizability, laser intensity, and $k$-vector dependence are mathematically non-trivial in the framework of the present approach. As a result, the different $\Delta$ values have a behavior which is difficult to predict a priori. For example, while the total difference $\Delta_{\text{tot}}$ decreases with the laser intensity for $^{87}$Rb-$^{40}$K and increases for the other two systems, the values $\Delta_{\text{tot}}$ and $\Delta_{\text{geom}}$ change their behavior not only with the laser intensity but also when going from one dimer to the other. Most notably, the $\Delta$ values for $^{6}$Li-$^{7}$Li are not smaller than for the other pairs although this system is almost homonuclear.

Another peculiar feature of the $^{6}$Li-$^{7}$Li dimer compared to the other considered ones is the occurrence of negative values for $\Delta_{\text{coup}}^{(6)}$ in the case of large positive values of $\xi$ and the laser intensity of 60 W cm$^{-2}$. This leads to a smaller value of $\Delta_{\text{tot}}$ compared to $\Delta_{\text{geom}}$ for these parameters. Clearly, the conclusions obtained for the generic $^{87}$Rb-$^{40}$K system are not always transferable to other alkali metal dimers.
FIG. 3: (Color online) The energy differences [see Eqs. (12-14)] \( \Delta_{\text{coup}}^{(2)} \) (blue dots), \( \Delta_{\text{coup}}^{(6)} \) (red dashes), \( \Delta_{\text{geom}} \) (green chain), \( \Delta_{\text{rot}} \) (black solid) (in multiples of \( \hbar \omega_0 \), both in atomic units) for different alkali metal dimers and intensities of the lattice laser (as specified in the graphs). The wavelength of the trap laser is 1030 nm. (The laser intensity 200 W/cm\(^2\) corresponds to a 30 \( E_\text{R}^{(1)} \) lattice depth for the \( ^{87}\text{Rb}^{-}\text{K} \) dimer.)

C. Wave-function analysis

1. Radial pair densities

An alternative analysis of the anharmonicity and COM-REL coupling effects is possible from the wave functions of the first trap induced and the least bound state. Since the probability density for finding a two-particle separation to lie in between \( r \) and \( r + dr \) is determined by the radial pair density

\[
\rho(r) = \iiint |\chi_i(\vec{R}, \vec{r})|^2 dV_{\vec{R}} v^2 d\Omega_{\vec{r}} ,
\]

it is convenient to discuss radial pair densities instead of the wave functions. In Eq. (15) the function \(|\chi_i\rangle\) stands
for $|\Psi_i\rangle$ or $|\Phi_i\rangle$ depending on the considered approximation, $dV_R$ is the COM volume element, and $\Omega_r$ is the angular part of the REL motion coordinates.

The energy spectrum of the first trap induced and the least bound states for the wide range of the interaction regimes was presented in Fig. 2. However, the three asymptotic interaction situations, namely, strong attraction ($a_{\text{sc}} \to -\infty$), the almost zero interaction ($a_{\text{sc}} \to 0$) and the strong repulsion ($a_{\text{sc}} \to +\infty$) are found sufficient for the wave function analysis. Figure 4 shows the radial pair densities at the different levels of approximation for the three interaction regimes. As is evident from Fig. 4 a large attractive interaction leads to a very confined function for the first trap-induced bound state while a large repulsive interaction does not only result in a node but also in a shift of the outermost lobe to larger interatomic distances. This shift is counteracted by the confinement of the trap. Remind, for the trap-free situation in the strongly repulsive regime the wave function crosses the internuclear axis exactly at the value of the scattering length. Evidently, the behavior of the density for almost zero interaction is only determined by the trap.

As is apparent from Fig. 4 the inclusion of the anharmonicity and the coupling leads to more extended pair densities. For all interaction regimes the following behavior is found. The effect is smallest for the harmonic coupling correction. A larger effect is found for the sextic non-coupled case which is strengthened by the sextic coupling. Effectively, the particles experience a more extended trap, if a more complete description of the problem is achieved. Such an effect is expected for the harmonic-to-sextic uncoupled description, since the harmonic trap is tighter than the sextic one as is evident from the sketch in Fig. 1. While this is expected for the inclusion of the anharmonicity, this is not immediately clear for the coupling.

The least bound state in the strongly repulsive regime is very long-ranged as the inset of Fig. 4(c) shows. This distance is almost comparable with the extension of the first trap-induced state for the strongly attractive regime. Nevertheless, the influence of the anharmonicity and the coupling on the least bound state is almost absent, because the state is energetically deeply bound and therefore does almost not probe the anharmonicity of the lattice.

In the considered parameter ranges the radial pair densities approach zero clearly before the interatomic distance reaches the boundary of a single lattice site, i.e. for $r < \lambda/2$, as can be seen from Fig. 4. Therefore, tunneling or a distribution of the dimer over more than a single lattice site does not occur and the present single-site model is applicable. Furthermore, effects of the artificial infinite walls of the harmonic or sextic potentials should not be a problem. However, the radial pair densities provide only an indication for the applicability of the single-site approximation, since it is still possible that the dimer as a whole may be distributed over more than one site. This can only be excluded form an analysis of the total wave function including the COM motion as is done in the next section.

For the present type of the coupled problem analysis the plots of the radial pair densities can be used as a good check of the validity of the pseudopotential approximation. Varying the value of the scattering length in the pseudopotential approach it is possible to match the function of the full solution at the long range distance. Such an approach is comparable to the energy-dependent concept developed for two identical particles in a harmonic trap [19] and will be discussed in a separate work. Before entering such an analysis, it may be remarked that the radial pair densities as shown in Fig. 4 are also of interest for the investigation of the validity of a pseudopotential approximation for the interatomic interaction. In fact, it may even be used in order to attempt to obtain an improved pseudopotential describing atomic pairs in an optical lattice. A corresponding study is presently underway.

2. Wave function in absolute coordinates

It is instructive to analyze the full wave function or corresponding particle density also in absolute coordinates of the laboratory space (ABS). They supply the complete information about the dimer and provide pictures of the COM and REL motion simultaneously. This is evidently not the case for the radial pair density (Fig. 4) that is averaged over the COM motion and thus does not reveal whether the pair as a whole moves through the lattice. Note, while the radial pair density provides nevertheless a rather easy to interpret picture of the underlying physics, this is far less the case for its angular part. The reason is that the anisotropic (egg-box like) shape of the (cubic) optical lattice does not trivially show up in the REL coordinate system. An analysis in the lab frame is, however, also non-trivial, since the functions depend on six spatial coordinates. Use of the cubic symmetry reduces the size of the symmetry non-equivalent space, but it is still impractical to consider the complete multidimensional function. Instead, some insight may be gained from selected cuts. Although a number of cuts was analyzed in this work, only the results for cuts along the $x$ coordinate of both atoms and thus for $y_i = z_i = 0$ (for both particles $i$) are shown and discussed.

In order to quantitatively describe the different effects of the trapping potential it is again useful to consider not the wave functions at different level of approximation itself, but their respective differences. Similarly to the energy differences defined in Eqs. 12-14, the wave-function differences

$$\Delta F_{\text{geom}}(\vec{r}_1, \vec{r}_2) = \Phi^{(2)}_i(\vec{r}_1, \vec{r}_2) - \Phi^{(6)}_i(\vec{r}_1, \vec{r}_2)$$

$$\Delta F_{\text{coup}}^{(n)}(\vec{r}_1, \vec{r}_2) = \Phi^{(n)}_i(\vec{r}_1, \vec{r}_2) - \Psi^{(n)}_i(\vec{r}_1, \vec{r}_2)$$

$$\Delta F_{\text{tot}}(\vec{r}_1, \vec{r}_2) = \Phi^{(2)}_i(\vec{r}_1, \vec{r}_2) - \Psi^{(6)}_i(\vec{r}_1, \vec{r}_2)$$

may be introduced. Cuts through these difference func-
The diagonal $x_{RB} = x_K$ defines the REL coordinate axis. The wavefunctions and therefore also their differences $\Delta F$ are strictly zero along the REL axis, since the molecular interaction potential rises exponentially to infinity for $r \rightarrow 0$. Note, even for $a_{sc} = 0$ the atoms interact in the present approach, since the scattering length characterizes only the effective long-range interaction. In the case of the often adopted $\delta$-type pseudopotential description the interaction vanishes completely for $a_{sc} = 0$ and the wavefunction does not vanish around $r = 0$. Slightly away from the REL axis the wavefunction shows rapid oscillations due to the nodal structure that is again a consequence of the realistic interatomic interaction potential used in the present work. They are, however, not resolved in Fig 5 as these oscillations occur in a very small ($\sim 10^{-3}\lambda/2$) $r$ range compared to the one displayed.

The COM axis is defined by $x_{RB} = -\mu_K/\mu_{RB} x_K$. Since $^{87}\text{Rb},^{40}\text{K}$ is heteronuclear, the COM axis is rotated from the $x_{RB} = -x_K$ diagonal and is thus for better readability explicitly indicated in the graphs. Another consequence of the heteronuclear character is the elliptical shape of the figures contours that would be circular in the case of a homonuclear system.

Figure 5(a) characterizes the geometrical effect of the anharmonicity of an optical lattice. Effectively, the sextic trap is more extended than the harmonic one. This leads to the decrease of the density at the center of the potential and an increased probability at the potential edges. Therefore, the probability to find Rb and K atoms at a larger distance from the center of the optical lattice is higher for an anharmonic trap compared with a harmonic one. Note, this probability redistribution is not homogeneous. For example, for $x_K \approx 0.3\lambda/2$ and $x_{RB} \approx -0.1\lambda/2$ a pronounced minimum of the function $\Delta F_{\text{geom}}$ exists, as is evident from Fig. 5(a). This behavior in the ABS space is a direct consequence of the different COM and REL motion trapping depths. The COM of the system is more confined. Hence, the density shift in the direction of the COM axis is larger than for the REL one, as is better seen in the inset of Fig. 5(a). In the inset one notices also that there exist small minima at the places where both atoms are close together ($r \approx 0$), but away from the center of the lattice site. In general, $\Delta F_{\text{geom}}$ is rather symmetric with respect to the COM and REL axes.

Figure 5(b) shows the effect of the coupling of COM and REL motion within the harmonic approximation. For its understanding it is important to keep in mind that the definition of coupling between the different degrees of freedom depends on the adopted coordinate system. In the present work it is defined by the Hamiltonian in Eq. 3 and thus the coupling of COM and REL coordinates. While this is a natural choice for discussions of, e.g., the radial pair density, its meaning is less transparent for a discussion of wave functions in ABS coordinates of the two atoms. An evident example is the case of two truly non-interacting atoms in a harmonic trap. Even for a heteronuclear atom pair the problem separates in ABS coordinates, as was already mentioned in Sec. II A. However, treating this system in COM and REL coordinates the coupling term $\hat{W}$ in Eq. 3 and thus also the difference $\Delta F_{\text{coup}}^{(2)}$ is non-zero, but the latter reflects the non-separability due to the adopted coordinate system.

A comparison of $\Delta F_{\text{coup}}^{(2)}$ shown in Fig. 5(b) with the one obtained from the analytically known harmonic so-
utions in either ABS or REL and COM coordinates for truly non-interacting particles (see, e. g., [34]) confirms that the structures in Fig. 5(b) for the $^{87}$Rb-$^{40}$K dimer with the long-range interaction being tuned to be almost vanishing are similar. In contrast to the case of the geometry effect visible in Fig. 5(a) the maxima and minima have a more similar magnitude (the maxima being about 16% larger in absolute value than the minima) and, clearly, they also originate from the different effects discussed above. Furthermore, they are located away from the center of the optical-lattice site. In fact, they are found, if one of the two atoms is located closely to the center and the other one is separated by about the most likely separation (about 0.2 $\lambda$/2, see Fig. 4(b)). The maxima (minima) are connected with the lighter K (heavier Rb) atom being close to the center. The anti-clockwise rotation of the maxima and minima around the origin is due to the heteronuclear character and reflects the coupling term in ABS coordinates, namely, $\Delta F_{coup}^{(2)} \sim e^{-\gamma x_K x_{Rb}}$ (where $\gamma$ is some constant). Also the different widths of the maxima and minima is a consequence of the heteronuclear character of $^{87}$Rb-$^{40}$K. While the off-centered minima of $\Delta F_{geom}$ are centered on the COM axis, the COM axis appear to separate the minima and maxima of $\Delta F_{coup}^{(2)}$, although it does not define a strict nodal plane.

The sextic coupling effect presented in Fig. 5(c) is similar to the harmonic one in Fig. 5(b). However, the two maxima are now almost connected (if there were not the strict node on the REL axis) and form more a kind of plateau. The minima are less pronounced and as a consequence, the absolute values of the maxima are now about 40% larger than the ones of the minima.

Figure 5(d) presents the complete effect of anharmonicity and coupling of the optical lattice. Compared to the previously discussed $\Delta F$ functions the shown $\Delta F_{tot}$ is in shape most similar to $\Delta F_{coup}^{(6)}$ in Fig. 5(c). However, the two maxima at the corners of the plateau appear now to be merged with the central peak due to the new scale (and are basically only separated by the node along the REL axis). As a consequence, the density of the exact sextic solution is reduced at the center of the lattice compared with the uncoupled harmonic approximation. In fact, as is evident from the equality $\Delta F_{tot} = \Delta F_{geom} + \Delta F_{coup}^{(6)}$ (compare Eq. (14)), the merging of the two maxima is simply a consequence of the superposition of the structures of $\Delta F_{coup}^{(6)}$ and $\Delta F_{geom}$. Note the correspondingly almost by a factor 2 larger amplitude of $\Delta F_{tot}$ compared to the other wavefunction differences. Since the minima of $\Delta F_{geom}$ and $\Delta F_{coup}^{(6)}$ appear at rather different places, their relative importance diminishes in comparison to the maxima. This leads to an about 66% larger absolute value of the maxima compared to the minima in the case of $\Delta F_{tot}$. However, the additivity leads to an effective broadening of the minima of $\Delta F_{tot}$ in direction of the COM axis compared to the minima found for $\Delta F_{coup}^{(6)}$.

To conclude the almost non-interacting case, the optical lattice is in the coupled sextic description effectively more extended than in the uncoupled harmonic one. As a consequence of this anharmonicity the wave-function amplitude at the center of the lattice site decreases and is redistributed to the edges of the potential. As a consequence of the coupling, the decrease of the wave-function amplitude stretches further out along a diagonal in between the COM and REL axes close to the axis defined by the Rb atom being located at the center of the lattice site ($x_{Rb} = 0$). On the other hand, the coupling leads also to minima (increased amplitude) along a diagonal between the COM and REL axes, but close to the $x_K = 0$ axis. As a consequence of the heteronuclear character of the $^{87}$Rb-$^{40}$K dimer, the two diagonals are rotated with respect to the two corresponding $x = 0$ axes.

**FIG. 6:** (Color online) Cuts through the differences $\Delta F$ as in Fig. 5 but a) $\Delta F_{geom}(x_{Rb}, x_K)$ and c) $\Delta F_{tot}(x_{Rb}, x_K)$ for strongly attractively interacting particles ($a_{sc} = -6600 a_0$); b) $\Delta F_{geom}(x_{Rb}, x_K)$ and d) $\Delta F_{tot}(x_{Rb}, x_K)$ for strongly repulsively interacting particles ($a_{sc} = +6600 a_0$).

Figure 6 characterizes the anharmonicity and coupling effect in the strongly interacting regimes. The most evident difference between the (almost) non-interacting case and the strongly interacting situations is the pronounced squeezing of the central peak along the COM axis. This
is easily seen by comparing the geometry effect characterized by $\Delta F_{\text{geom}}$ in Figs. 6(a) and (b) with Fig. 6(a). Connected with this squeezing is an increase of the maxima by a factor of almost 6 (strong repulsion) or more than 8 (strong attraction). The additional lobe occurring for strongly repulsive interaction at large distances leads to two further maxima on the COM axis (one for a positive and one for a negative value of $x_K$) for $\Delta F_{\text{geom}}$ (Fig. 6(b)), indicating a corresponding difference between the uncoupled harmonic and sextic solutions that occurs also at the outer lobes. The minima on the COM axis are in this case shifted to larger distances from the REL axis. This is not the case for a strong attractive interaction, but there the amplitude of the minimum is even smaller than in the attractive case where it is already of less relative importance compared to the central maxima than in the non-interacting case. On the other hand, the minima on the REL axis that had been very weak compared to the ones on the COM axis for the non-interacting case are in the strongly interacting cases much more pronounced, but also squeezed into a narrow regime close to the REL axis.

As for the almost non-interacting case (Fig. 6(d)), the total differences $\Delta F_{\text{tot}}$ for the strongly interacting cases (Figs. 6(c) and (d)) differ from their $\Delta F_{\text{geom}}$ counterparts by the occurrence of two minima along diagonals between the COM and REL axes for $x_K \approx 0$. While the also coupling-induced maxima for $x_{K}\approx 0$ lead for the non-interacting case to a broad central peak, they appear in the strongly interacting case as shoulders. The reason is the massive squeezing of the central peak already discussed for $\Delta F_{\text{geom}}$. The additional maxima along the COM axis in the case of strong repulsion lead to a rather structured difference surface $\Delta F_{\text{tot}}$ in this case. Another interesting effect visible from Fig. 6(d) is the enormous increase of the central maximum when comparing $\Delta F_{\text{tot}}$ with $\Delta F_{\text{geom}}$. For both the almost non-interacting and the strongly attractive case there is an approximate increase by a factor of 2, but in the strongly repulsive case there is a factor of more than 6.

Compared to the analysis of the radial pair densities in Sec. IIIA it is evident that the absolute wave-function analysis reveals much more subtle details. In the case of radial pair densities there was the clear trend that improving the level of description leads to an increasing shift of probability from the maxima towards large separations. Similarly, the energies were uniformly lowered. (Remind, however, that the energy analysis for $^6$Li$^7$Li showed that such a uniform trend is not found for all heteronuclear systems.) The cuts through the full wave functions show that the effects of coupling and anharmonicity are not as trivial. Most importantly, they indicate that there is a lot of changes of the wave functions for short internuclear separations where, e.g., a pseudopotential approach is questionable. The relative importance of this regime of interatomic separations is, however, reduced, if an average over the angles is performed; simply because it scales with the radial part of the volume element, $r^2$. This is also the reason why the energies are not very sensitive to this short-range regime and thus the pseudopotential approach may rather successfully predict also energy differences between different levels of approximation.

The wave functions (not their differences) were also used in order to assure that the parameters chosen in this work allow a discussion in terms of a single site of an optical lattice. Different cuts through the wave functions (in different directions relative to the optical lattice) never indicated a substantial wave function amplitude close to the boundaries of the single lattice site.

D. Comparison to experiment

A natural application of the present approach is to model the experimental results of C. Ospelkaus et al. [13]. In that experiment rf association was used to create molecules from fermionic $^40$K and bosonic $^{87}$Rb atoms in a 3D cubic optical lattice. The binding energy of the heteronuclear molecules was measured as a function of the strength of an applied magnetic field. Figure 7 shows the experimental data for a lattice with depth $V_{\text{Rb}} = 40 E_r^{\text{Rb}}$ and wavelength $\lambda = 1030$ nm.

Note, the binding energies measured in the experiment are not the usual ones. In free space, real molecules (RM) close to the Feshbach resonance exist only on the repulsive side of the resonance ($a_{sc} > 0$). The binding energy measured in a trap-free situation is the one relative to the threshold energy of the continuum. In the presence of an external optical lattice this continuum is discretized, and there is instead a first trap-induced state. On the attractive side of the resonance ($a_{sc} < 0$) the energy of this state is lowered relative to the field-free position. This leads to confinement-induced molecules (CIM) [12]. In the experiment reported in [13], the binding energy of the RM and CIM in a trap were measured. For $a_{sc} > 0$ the excitation energy of the repulsively interacting bound pair (RIP) [22] where repulsion between bosons and fermions shifts the two-particle ground state towards a higher energy was also measured. The corresponding RM, CIM and RIP branches are denoted in Fig. 7 in which the experimental results of [13] are reproduced for comparison.

In order to compare the experimentally measured binding energies with the theoretically calculated ones a proper mapping must be applied. Figure 8 outlines the procedure of how the binding energies were determined in the model. The scattering length $a_{bg} = -185 a_0$ is chosen as the $B$-field-free background scattering length. The energy of the first trap-induced state obtained with the full sextic solution at $a_{bg}$ is chosen as energy zero and is marked explicitly in Fig. 8. A variation of the scattering length leads to energy shifts of the least bound and the first trap-induced states relative to this energy zero. The binding energy is a function of this shift as is indicated by arrows in Fig. 8. Specifically, the binding energy as a
function of the scattering length may be obtained from the present theoretical data with help of the relation

$$E_{\text{bg}}^{(n)}(a_{\text{sc}}; i) = E_{\text{CIM}}^{(n)}(a_{\text{bg}}) - E_i^{(n)}(a_{\text{sc}})$$  \hspace{1cm} (19)

where \(i\) and \(n\) are, as before, \(i = \{\text{b}, \text{CIM} \}\) and \(n = \{2, 6\}\). Furthermore, \(E\) stands for the state energy at a given level of approximation \(E = \{E, E_{\text{bg}}, E_{\text{CIM}}\}\). This definition of a binding energy results in three different branches. While the first trap-induced state is responsible for the RIP and the CIM branch, the least bound state is responsible for the RM part. The corresponding branches are indicated in Fig. 7 and in the sketch of Fig. 8.

Experimentally, the binding energies were measured as functions of the magnetic field while theoretically calculated energies are functions of the interaction strength represented by the scattering length (see Sec. III D for details). To provide a \(B\) dependence of the theoretical data \(a_{\text{sc}}\) is mapped onto the magnetic field using a two-channel approximation \cite{31} by the aid of

$$a_{\text{sc}}(B) = a_{\text{bg}} \left( 1 - \frac{\Delta B}{B - B_0} \right)$$  \hspace{1cm} (20)

where \(\Delta B\) is the resonance width and \(B_0\) is the resonance position. Equation (20) gives in turn for the \(B\) field as a function of \(a_{\text{sc}}\)

$$B(a_{\text{sc}}) = \Delta B \left( 1 - \frac{a_{\text{sc}}}{a_{\text{bg}}} \right)^{-1} + B_0.$$  \hspace{1cm} (21)

The \(a_{\text{sc}}\) values obtained from theory are inserted into Eq. (21) to determine the \(B\) dependence of the energy.

Figure 7 shows the binding energy obtained from the full sextic solution \(E^{(6)}\) for the experimental parameters of the trap and magnetic field Feshbach resonance parameters \(\Delta B = -3 \text{ G} \) \cite{30} and \(B_0 = 546.8 \text{ G} \) \cite{30}. As is evident from Fig. 7 the model does not perfectly agree with the experiment. Some possible reasons of the disagreement are discussed in the following paragraph.

1. Possible reasons of deviation between theory and experiment

Equation (20) is derived for the lattice-free situation under the assumption that the collision between two atoms can be approximated by a two-channel scattering model. In general, as was already mentioned in Sec. III D, the correct theoretical description requires a multi-channel scattering treatment which in the present case would have to incorporate also the optical lattice. Moreover, the present model uses an "artificial" variation of the scattering length (see Sec. III D), and the \(a_{\text{sc}}\) values obtained from this variation are the ones of a single-channel approach.

Even assuming the validity of Eq. (21) there is another important factor influencing the comparison of theory and experiment. The values of the scattering length \(a_{\text{sc}}\) and \(a_{\text{bg}}\) of Eq. (20) are determined in a lattice-free situation. In the presence of a trap these values must
be revised and adjusted to the trap parameters. It was shown in [19] that the use of an energy-dependent scattering length \( a_{sc}^E \) gives almost correct energy levels for two harmonically trapped atoms. The evaluation of \( a_{sc}^E \) requires to solve the complete scattering problem and thus \( a_{sc}^E \) can only be obtained from the knowledge of the solution for the realistic atom-atom interaction potential. Eventually, the trap-free values of the scattering length \( a_{sc} \) and \( a_{bg} \) must be substituted by appropriate energy-dependent scattering length \( a_{sc}^E \) values. However, the problem is that the energy-dependent scattering length approach is so far developed only for the harmonic approximation, for s-wave collisions, and the uncoupled problem. An anharmonic, for example "sextic", energy-dependent scattering length concept as well as any other extensions of it do so far not exist to the authors' knowledge.

In view of the absence of an \( a_{sc}^E \) beyond the uncoupled harmonic approximation, the following procedure was adopted. The energy-dependent values of the scattering length are obtained using a solution for the pseudopotential energy and valid for a harmonic trap \[ \Gamma \left( \frac{1}{2} \epsilon_{11}^{(2)}/\omega_{ho} + \frac{3}{4} \right) = \frac{a_{ho}}{a_{sc}^E} \sqrt{2} \], where \( \Gamma \) is a gamma function. The energy of the REL motion obtained for the harmonic trap are imposed into Eq. (22) and the \( a_{sc}^E \) values are obtained. The new values of the scattering length obtained with this manipulation are used for the mapping of the binding energies of \( E^{(6)} \) with the help of Eq. (20). Figure 4 shows the result of this procedure. As is seen from the figure the shift of the spectral curve for the case of the energy-dependent scattering length along the \( B \)-axis is not big but the curve is shifted along itself for the RIP branch and is tilted for the other ones in immediate proximity to the resonance. This may be seen as an indication that the energy dependence of the scattering length (properly included) does not have a too big effect, but the approximate implementation is certainly not conclusive and thus cannot exclude a possible importance.

Another important reason of the mismatch between theory and experiment could be an insufficient knowledge of the resonance parameters \[ 18 \]. It turns out to be sufficient to change the center of the Feshbach resonance to the value \( B_0 = 546.66 \) G to match the experimental and the theoretical data. A variation of \( B_0 \) of this size is well within the experimental uncertainty with which the resonance parameters are known \[ 36 \]. The result obtained with this modified value of \( B_0 \) is also shown in Fig. 7. Remarkably, if both parameters \( B_0 \) and \( \Delta B \) are used together to fit the experimental curve it leads to a larger error than if only the parameter \( B_0 \) is varied (see the discussion in the following subsection, especially

![Fig. 7](image-url)

**FIG. 7:** (Color online) As Fig. 6 but using a harmonic potential, an energy-independent scattering length, and the Feshbach-resonance positions \( B_0 = 546.8 \) G (black solid) or \( B_0 = 546.66 \) G (red solid).

Finally, one may address the question whether despite the number of uncertainties the effect of the anharmonicity and coupling is visible in the experiment \[ 13 \]. Figure 9 shows the binding energies obtained from the harmonic approximation. While the harmonic approximation predicts the binding energy of the repulsively-interacting-pair of the spectrum correctly, for other parts it results in a disagreement. A variation of the MFR parameters does not lead to a simultaneous matching of all spectral branches. Therefore, it is possible to conclude that in the experiment \[ 13 \] effects of anharmonicity and coupling (and thus deviations from a simple uncoupled harmonic model) were very likely detected.

### 2. Comparison to a previous theoretical study

The effects of anharmonicity and coupling of COM and REL motion in a single site of an optical lattice were also the subject of a recent theoretical study by Deuretzbacher et al. \[ 18 \]. The approach therein differs from the present one, since (i) it does not use the full interatomic interaction potential but resorts to the pseudopotential approximation, (ii) a different partitioning of the Hamiltonian is adopted, and (iii) different basis functions (eigensolutions of the harmonic oscillator) were adopted.

The two independently developed approaches provide the possibility to further check whether theory has achieved a sufficient accuracy to investigate the small deviations from the simple uncoupled harmonic approxima-
TABLE II: Influence of different levels of approximation on the energy of the 1st trap-induced state for three heteronuclear systems. All results are obtained for $a_{\text{sc}} = 6500a_0$ (or $\xi(\text{RbK}) = 3.34$, $\xi(\text{LiCs}) = 3.76$, $\xi(\text{LiLi}) = 3.24$), lattice depths of $V_1 = V_2 = 10E_{\text{rel}}$ where $E_{\text{rel}} = k^2/(2\mu)$, and a wavelength $\lambda = 1000$ nm.

| atom pair | $E_{(2)}$ | $\Delta_2$ | $\varepsilon_{(6)}^{(2)} - \varepsilon_{(3)}^{(2)}$ | $\Delta_{\text{tot}}$ |
|-----------|-----------|-----------|----------------------------------|-----------------|
| $^{87}\text{Rb} - ^{40}\text{K}$ [present] | 3.79 | -0.12 | -0.29 | -0.41 |
| [18] | 3.74 | -0.12 | -0.27 | -0.39 |
| $^6\text{Li} - ^{133}\text{Cs}$ [present] | 2.93 | -0.38 | -0.22 | -0.60 |
| [18] | 2.88 | -0.35 | -0.22 | -0.57 |
| $^6\text{Li} - ^7\text{Li}$ [present] | 3.93 | -0.01 | -0.30 | -0.31 |
| [18] | 3.92 | -0.01 | -0.29 | -0.30 |

A consequence of difference (i) between the two approaches is furthermore the ability to investigate the adequacy of the pseudopotential adopted in [18]. As a consequence of (iii) the approach in [18] can only be applied to very deep lattices and an extension to multiple-site lattices or even to shallow lattices is not straightforward. The reason is the rather strong spatial confinement of the harmonic-oscillator solutions. As a consequence, it needs an impractical large number of basis functions in order to cover an extended spatial regime. Since anharmonicity and coupling effects are different for shallower lattices as is discussed in Sec. III A, the tunneling effects may also play an important role [32,33]. Within the present approach calculations for multiple-wells and shallow lattices are straightforward and were already recently performed [17].

The spatial compactness of the harmonic-oscillator eigenfunctions is on the other hand evident from the convergency study with respect to the Taylor expansion of the optical lattice performed in [18]. As was discussed in Sec. III A, such a study is not senseful, since, e.g., even-order expansions lead to unphysical continua. Clearly, only a basis that does not explore the corresponding regime of the configuration space does not show any signs of these unphysical continua.

Table III shows a comparison of some energies and energy differences obtained with the numerical approach in [18] and the present one for a large positive scattering length ($a_{\text{sc}} = 6500a_0$). The results obtained with the two approaches do not differ very much in the case of all three considered alkali-metal dimers. The agreement of the energy differences is overall slightly better than the one of the absolute energies. The comparison seems to confirm the proper numerical implementation of both numerical approaches. Most importantly, it demonstrates that for the calculation of energy shifts as well as anharmonic and coupling effects in a single site of an optical lattice the pseudopotential approach remains valid; at least to a very good approximation.

It is presently not possible to attribute the remaining differences to the different atomic interaction potential or some remaining numerical uncertainty. Note, the different interaction potential influences the results in two ways. First, the $\delta$-type pseudopotential does not properly account for the short-range part of the interaction. Second, the mapping of the energy to a corresponding interaction strength is different in the two approaches. In the pseudopotential approach the scattering length is simply a parameter that enters the interaction potential, while it is extracted from the resulting wave function as was described in Sec. III A. As a consequence, there is a finite range in which $a_{\text{sc}}$ can be varied within the present approach.

Compared to the present finding (see Sec. III D 1) the binding-energy spectrum of $^{87}\text{Rb} - ^{40}\text{K}$ calculated in [18] does not agree very well with the experimental one in [33], if the previously experimentally determined Feshbach-resonance parameters ($B_0 = 546.8$ G, $\Delta B = -3$ G) are used. The authors in [18] proposed that with the aid of the calculation it is in fact possible to improve on the MFR parameters. Such a fit (with the energy-independent scattering length) yielded the new resonance parameters $B_0 = 546.669$ G and $\Delta B = -2.92$ G [18]. This has to be contrasted with the present fit that yields the new resonance position $B_0 = 546.660$ G but an unchanged width ($\Delta B = -3$ G), as was discussed in Sec. III D 1. Thus there is a similar (though slightly larger) trend for $B_0$, but disagreement with the results in [18] with respect to $\Delta B$.

In view of the different fit results, it is important to investigate in more detail their sensitivity on the fit parameters. The quality of the fit depends on the agreement between the calculated binding energy ($\varepsilon^{(6)}(B)$) and the experimental one ($E_{\text{exp}}$). It is thus given by the relative error

$$\delta(B) = \left| \frac{E_{\text{exp}}(B) - \varepsilon^{(6)}(B)}{E_{\text{exp}}(B)} \right| .$$

Figure 11 shows $\delta(B)$ for three sets of MFR parameters: (i) $B_0 = 546.660$ G and $\Delta B = -3$ G (optimal fit parameters, this work), (ii) $B_0 = 546.669$ G and $\Delta B = -2.92$ G (optimal fit parameters found in [18]), and (iii) $B_0 = 546.660$ G and $\Delta B = -2.92$ G (optimal fit parameter found in this work for $B_0$, but $\Delta B$ from [18]). As is evident from Fig. 11 any variation of either $\Delta B$ or $B_0$ from their optimal values results in an increased error for all energy branches and all magnetic fields. Clearly, the fit shows a well defined minimum and thus there is no ambiguity in the fit parameters as it could occur, e.g., in the case of very shallow minima where the outcome of the fit may be determined by small numerical inaccuracies.

Provided the fit fidelity in [18] is comparable to the present one, i.e., a fit with the binding energies calculated in [18] using the optimal fit parameters of the present work would disagree with the experiment in a similarly pronounced fashion as shown in Fig. 11 it is presently impossible to conclude whether theory has already reached the level of accuracy that is required for an improved determination of MFR parameters. While both
FIG. 10: (Color online) The relative error defined in Eq. (23) for the alternative Feshbach parameters $B_0 = 546.660 \, \text{G}$, $\Delta B = -3 \, \text{G}$ (squares), $B_0 = 546.669 \, \text{G}$, $\Delta B = -2.92 \, \text{G}$ (circles), and $B_0 = 546.66 \, \text{G}$, $\Delta B = -2.92 \, \text{G}$ (triangles).

fits appear to indicate a smaller value of $B_0$ compared to the one previously extracted from experiment, the deviation between both fits is only about half as small as the improvement claimed in [18]. Clearly, such a result is from a statistical point of view inconclusive. In the case of the width $\Delta B$ the present finding agrees even fully to the previously determined value and thus disagrees with the result of the fit in [18].

In order to obtain a more conclusive result it is vital to investigate whether the differences between the results in [18] and the present ones are solely due to the use of the pseudopotential approximation or the more realistic interatomic interaction potential in the two studies. If this were the case, the fit results of the present study should be regarded as the more accurate ones. Furthermore, this would be an important example for the need to consider the interatomic interaction on a more accurate level than the one provided by the pseudopotential approximation. Since the implementation of the pseudopotential is due to the singular behavior of the $\delta$ function non-trivial in the context of the present approach, such an investigation has to be postponed to a separate work. Clearly, more experimental data (for different heteronuclear systems) would also be very important for gaining a deeper insight and it is hoped that the present work stimulates such experimental activities.

Finally, there are two further uncertainties in the determination of the MFR parameters from a fit like the one in [18] or in the present work. They are related to the way in which the mapping of the theoretical data onto the magnetic field is performed. As already mentioned, this mapping is usually based on the assumption of validity of Eq. (21) and thus on the assumption that the $B$-field mapping of the multichannel MFR can be performed based solely on a scattering-length variation. Even in this case there is, however, the problem of the proper determination of the energy-dependent scattering length in an optical lattice which is so far unknown. The use of $a_{sc}^E$ extracted from the harmonic uncoupled energies for the mapping of the the full sextic energy results effectively in a shift of the energy-independent curve, as is seen in Fig. 7. However, both the energy-dependent and energy-independent $a_{sc}$ discussed in this work utilize the same harmonic energy curve ignoring also the coupling to the COM motion. How the situation would change, if $a_{sc}^E$ for a non-harmonic solution would be used, is difficult to predict, since the other curves in Fig. 2 not only differ in shape, but are also shifted relative to each other and contain the COM part. The overall good agreement of the theoretical binding energies (with fitted MFR parameters) to the experimental data is of course very suggestive that these uncertainties have a small influence, but this may be a pure coincidence.

Both, the investigation of the appropriateness of the $B$-field mapping as well as the question of the possibility to define an energy-dependent scattering length beyond the uncoupled harmonic approximation require a theoretical approach for the treatment of two atoms in an optical lattice as the one presented in this work and is presently pursued. It should, however, be emphasized that these uncertainties only affect the analysis of dimers close to a (magnetic) Feshbach resonance or, in general, if the proper description of the atom-pair requires a multichannel treatment. The results of the previous sections are valid independently of these uncertainties. Different
IV. CONCLUSION AND OUTLOOK

An approach which allows for a full numerical description of two ultracold atoms in 3D optical lattice is developed. A detailed analysis of anharmonicity and coupling of center-of-mass and relative coordinates in terms of energy values and wave functions was performed for heteronuclear dimers in a single site of an optical lattice. It is explained, why such a single site is optimally described by a sextic potential, if a finite Taylor expansion is used. The effects of deviations from the harmonic approximation and of the coupling were quantified and analyzed for different heteronuclear systems, confinement strengths and interatomic interaction regimes. The influence of the lattice is found to be always much stronger for the first trap-induced state than for the least bound state. As a consequence, binding energies are modified by the lattice mainly by the modification of the first trap-induced state.

While the energy deviations from the harmonic uncoupled approximation is for all three considered generic heteronuclear dimers largest for strong repulsive interaction, the relative size (and even sign) of the energy change due to coupling or anharmonicity varies for the different dimers. The same is true for the influence of the trap depth. A deeper lattice can lead to smaller or larger energy differences between the harmonic uncoupled or the full coupled solution. While the analysis of the radial pair densities shows that the lattice mainly influences the maxima located at large interatomic separations, the analysis of cuts through the wave functions in absolute coordinates reveals non-negligible changes also at short interatomic distances. This may have important consequences for the validity of pseudopotential approximations.

The results of the present theoretical approach are also compared to a recent experiment in which the binding energies of $^{87}$Rb-$^{40}$K have been measured as a function of an external magnetic field tuned close to a magnetic Feshbach resonance. The assumptions necessary for such a comparison are carefully discussed. It is found that very good agreement between experiment and theory can only be reached, if the previously experimentally determined resonance parameters are modified. Since this needed modification is within the error bars with which the parameters had been determined before, this is not only reasonable, but may even indicate the possibility to more accurately determine the width and position of magnetic Feshbach resonances in ultracold atomic gases, as was proposed recently in a comparable theoretical study. However, the resonance parameters determined in the previous study based on the pseudopotential approximation differ from the ones found in the present work. If this deviation is due to the pseudopotential approximation is difficult to judge at this moment. If this were the case, the then found breakdown of the pseudopotential approximation would, of course, be a very interesting finding. A further investigation is therefore of great interest, and the present work stimulates hopefully also further experimental work in this direction. Since the influence of anharmonicity and coupling becomes more important for less deep optical lattices and for excited trap levels, corresponding experiments like the ones in [8, 40, 41] are expected to provide further tests of the approach presented in this work.

Since the present approach was rather generally formulated and implemented, it allows immediately for further investigations that have partly been started or are planned for the future. This includes the consideration of highly anisotropic, asymmetric (disordered), or multiple-well lattice geometries. First results for triple-well potentials have, e.g., recently been used for the determination of Bose-Hubbard parameters and an investigation of the validity of the Bose-Hubbard model itself [17]. The study of an interesting physical phenomena like, e.g., the trap-induced resonances [42, 43] are also planned. Further extensions of the approach 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 studies of the time-dependent dynamics of atomic pairs in time-varying lattices.

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