Dimer states in atomic mixtures

Klaus G. Ziegler

Angaben zur Veröffentlichung / Publication details:

Ziegler, Klaus G. 2008. "Dimer states in atomic mixtures." *Physical Review A* 77 (1): 013623. https://doi.org/10.1103/physreva.77.013623.

Dimer states in atomic mixtures

K. Ziegler
Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany
(Received 21 December 2006; revised manuscript received 30 November 2007; published 30 January 2008)

A mixture of heavy atoms in a Mott state and light spin-1/2 fermionic atoms is studied in an optical lattice. Inelastic scattering processes between the two atomic species excite the heavy atoms and renormalize the tunneling rate as well as the interaction of the light atoms. An effective Hamiltonian for the latter is derived that describes tunneling of single fermions, tunneling of fermionic pairs, and an exchange of fermionic spins. Low-energy states of this Hamiltonian are a Néel state for strong effective repulsion, dimer states for moderate interaction, and a density wave of paired fermions for strong effective attraction.

DOI: 10.1103/PhysRevA.77.013623 PACS number(s): 03.75.Mn, 03.75.Ss, 05.30.Fk, 34.50.−s

I. INTRODUCTION

Recent experimental work on ultracold bosonic and fermionic atoms opened a field to study quantum states in optical lattices, like superfluid or Mott states [1,2], where the interaction between the atoms can be controlled by a magnetic field via a Feshbach resonance [3]. Spin-dependent effects [4], formation of dimers from fermionic atoms [5], and mixtures of two atomic species [6–8] provide opportunities for more complex quantum states. An interesting example of the latter is the dimer states. Such states have been discussed in solid-state systems [9] and recently also for an ultracold Bose gas with ring exchange [10]. Frustrated spin systems have been discussed for a number of atomic systems [11].

The idea of this paper is to study a system in an optical lattice that undergoes a first-order phase transition when a model parameter is changed. If this parameter is easily accessible in the experiment it can be adjusted exactly at the transition point. As a consequence, the quantum system at the transition point describes a physical situation that has a number of interesting features. First, there is the coexistence of the phases in the form of a metastable state, leading possibly to phase separation. Second, new translationally invariant quantum states can appear. A system that realizes this type of physics is an atomic mixture which is subject to inelastic scattering between the atomic species. It can be controlled by adjusting physical parameters, including the optical-lattice parameters (by choosing the frequency and amplitude of the laser field) and the fermion-fermion interaction through a Feshbach resonance. This enables us to create ground states as well as excited states of the system, and to study their dynamics.

In the specific case of this paper, an optical lattice is filled with heavy (bosonic or fermionic) atoms (HAs) (e.g., ^{87}Rb or ^{40}K), one at each lattice well, which form a Mott state. The tunneling of these HAs is neglected since the potential barriers of the optical lattice are sufficiently high. Excitations are due only to collisions with other atoms. For this purpose light fermionic atoms (LFAs) (e.g., ^{6}Li) are added to the optical lattice. These atoms can tunnel because of their low mass and can be scattered by the HAs. It is assumed that the HAs experience a harmonic potential in the optical lattice, at least at low energies. Then their excitations are harmonic-oscillator states. During the scattering process the HAs can also transfer energy to the LFAs. Moreover, we consider spin-1/2 fermions with local (on-site) repulsion. This scenario can be described by a Bose-Fermi model that is known in solid-state physics as the Holstein-Hubbard model [12]. The excitations of the HAs are local phonons. This model is quite different from models with density-density interaction, where only thermal fluctuations of the HAs and elastic scattering between the atomic species were studied [15].

II. HOLSTEIN-HUBBARD MODEL

LFAs with spin σ $(=\uparrow,\downarrow)$, defined by fermionic creation and annihilation operators $c^{\dagger}_{\mathbf{j}\sigma}$ and $c_{\mathbf{j}\sigma}$ in a well of the optical lattice with position $\mathbf{j}$, tunnel between nearest-neighbor wells. The corresponding tunneling Hamiltonian in tight-binding approximation reads

$$H_t = -J \sum_{\langle \mathbf{j},\mathbf{j}' \rangle} \sum_{\sigma=\uparrow,\downarrow} (c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{j}'\sigma} + \text{H.c.}). \tag{1}$$

The HAs, forming a Mott state, are harmonic oscillators at each well with eigenfrequency ω_0 and energies $E_N=\omega_0 N$ $(N=0,1,\ldots)$. It is assumed that a HA in one well is excited independently of the HAs in the other wells. This gives the Hamiltonian $\omega_0 \Sigma_{\mathbf{j}} b^{\dagger}_{\mathbf{j}} b_{\mathbf{j}}$, where $b^{\dagger}_{\mathbf{j}}$ and $b_{\mathbf{j}}$ are the creation and annihilation operators for the oscillator excitations at each well, respectively. They can be considered as local phonons. The LFAs are scattered by the HAs due to an exchange of excitations of the HAs (i.e., by creating or absorbing an excitation), defined by the Hamiltonian

$$H_I = \sum_{\mathbf{j}} [\omega_0 b^{\dagger}_{\mathbf{j}} b_{\mathbf{j}} + g(b^{\dagger}_{\mathbf{j}} + b_{\mathbf{j}})(n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow}) + U n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow}]. \tag{2}$$

Here a local repulsive interaction between the LFAs with strength $U \geq 0$ has been included. The phonons couple to the fermionic densities $n_{\mathbf{j}\uparrow}$ and $n_{\mathbf{j}\downarrow}$ with strength g. Thus the atomic mixture is defined by the Hamiltonian $H=H_t+H_I$, also known as the Holstein-Hubbard model [12].

For a given ensemble of LFAs, represented by integer numbers $n_{\mathbf{j}\sigma}=0,1$, the Hamiltonian H_I can be diagonalized with product states $\Pi_{\mathbf{j}}|N_{\mathbf{j}};\sigma_{\mathbf{j}}\rangle$ (for $N_{\mathbf{j}}=0,1,2,\ldots$; $\sigma_{\mathbf{j}}=0,\uparrow,\downarrow,\downarrow\uparrow$). $|N_{\mathbf{j}};0\rangle$ is an eigenstate of the phonon-number operator $b^{\dagger}_{\mathbf{j}} b_{\mathbf{j}}$ with eigenvalue $N_{\mathbf{j}}$. A lattice product of these states is an eigenstate of the Hamiltonian H_I. Other eigen-

states of H_I with fermions can be constructed from

$$|N_{\mathbf{j}};\sigma\rangle = c^{\dagger}_{\mathbf{j}\sigma} \exp\left(-\frac{g}{\omega_0}(b^{\dagger}_{\mathbf{j}} - b_{\mathbf{j}})\right)|N_{\mathbf{j}};0\rangle, \quad (\sigma = \uparrow, \downarrow), \quad (3)$$

and from a state with two fermions per well,

$$|N_{\mathbf{j}};\downarrow\uparrow\rangle = c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow} \exp\left(-2\frac{g}{\omega_0}(b^{\dagger}_{\mathbf{j}} - b_{\mathbf{j}})\right)|N_{\mathbf{j}};0\rangle. \quad (4)$$

The eigenvalue of $\Pi_{\mathbf{j}}|N_{\mathbf{j}},\sigma_{\mathbf{j}}\rangle$ with respect to H_I is

$$\sum_{\mathbf{j}} \left(\omega_0 N_{\mathbf{j}} - \frac{g^2}{\omega_0}(n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow})^2 + U n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow}\right), \quad (5)$$

where the integers $n_{\mathbf{j}\sigma}=0,1$ count the number of fermions at the well $\mathbf{j}$ with spin σ. This expression represents an effective *attractive* fermion-fermion interaction of strength g^2/ω_0, which competes with the *repulsive* fermion-fermion interaction of strength U. Thus the system is given by the transformed Hamiltonian

$$H_{\gamma} = TH_tT^{\dagger} + \omega_0 \sum_{\mathbf{j}} b^{\dagger}_{\mathbf{j}} b_{\mathbf{j}} + \gamma \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} - \frac{g^2}{\omega_0} \sum_{\mathbf{j}} (n_{\mathbf{j}\uparrow} + n_{\mathbf{j}\downarrow})^2 \quad (6)$$

with the effective coupling $\gamma = U - 2g^2/\omega_0$ and the unitary operator

$$T = \prod_{\mathbf{j}} \left(\sum_{N_{\mathbf{j}} \geq 0} \sum_{\sigma=0,\uparrow,\downarrow,\downarrow\uparrow} e^{-\alpha_n g(b^{\dagger}_{\mathbf{j}} - b_{\mathbf{j}})/\omega_0} |N_{\mathbf{j}};\sigma\rangle\langle N_{\mathbf{j}};\sigma| \right), \quad (7)$$

where $\alpha_0=0$, $\alpha_{\uparrow}=\alpha_{\downarrow}=1$, and $\alpha_{\downarrow\uparrow}=2$. The states $|N_{\mathbf{j}};\sigma\rangle$ contain phonons even for $N_{\mathbf{j}}=0$ due to the exponential factors in Eqs. (3) and (4). Therefore, $N_{\mathbf{j}}>0$ will be called phononic excitation, in contrast to $N_{\mathbf{j}}=0$, which is the phononic ground state. The ground states of H_I have $N_{\mathbf{j}}=0$ and are $\Pi|0;\downarrow\uparrow\rangle$ for $U<3g^2/\omega_0$ and $\Pi(a_1|0;\downarrow\rangle + a_2|0;\uparrow\rangle)$ for $U>3g^2/\omega_0$ with $|a_1|^2+|a_2|^2=1$. The corresponding energies are $E_0=U-4g^2/\omega_0$ and $E_0=-g^2/\omega_0$, respectively. For strong repulsive interaction there is only one fermion in each well, whereas a strong attractive interaction leads to formation of a local fermion pair (i.e., a bipolaron [12]). Both interactions are balanced for $U_c=3g^2/\omega_0$, leading to a degeneracy of the two states. The ground-state energy E_0 as a function of U has a cusp at $U=U_c$.

It is crucial that unpolarized spin-1/2 fermions are considered. In the case of spin-polarized fermions (e.g., in a magnetic trap), the only local interaction is due to Pauli's principle. This excludes multiple occupation of a well by the LFAs. Consequently, the coupling to the HAs results only in a g-dependent chemical potential $\mu' = -g^2/\omega_0$ because $n^2_{\mathbf{j}}=n_{\mathbf{j}}$ in Eq. (5). This favors the complete filling of the optical lattice with one LFA per well.

A. Half-filled states

Now it is assumed that the atomic system is prepared such that the number of LFAs is equal to the number of lattice wells (i.e., $2M$ fermions for $2M$ lattice wells). This is the case of half filling and it is of particular interest because it allows highly degenerate quantum states. The energy of $TH_IT^{\dagger}$ for a half-filled system is calculated as a state that can have $2j$ singly occupied wells with energy $E_1=-2(g^2/\omega_0)j$ and $M-j$ doubly occupied wells with energy $E_2=(U-4g^2/\omega_0)(M-j)$. The total energy then is

$$E_0 = \epsilon M - \gamma j \quad \text{with} \quad \epsilon = U - 4g^2/\omega_0. \quad (8)$$

Here γ, the effective fermion-fermion interaction of Eq. (6), is an important parameter that controls two different phases: For $\gamma>0$ the ground state has $j=M$ (i.e., $2M$ singly occupied wells), whereas for $\gamma<0$ the ground state has $j=0$ (i.e., M doubly occupied and M empty wells). The ground-state energy is $-2(g^2/\omega_0)M$ for $\gamma>0$ and ϵM for $\gamma<0$, respectively. At $\gamma=0$ the ground-state energy E_0 does not depend on the number of singly occupied wells, i.e., it is highly degenerate. This point describes a first-order phase transition in terms of $TH_IT^{\dagger}$, changing from a singly occupied lattice for $\gamma>0$ to a mixture of doubly occupied and empty wells for $\gamma<0$. Moreover, both states are highly degenerate even for $\gamma\neq 0$ because the *local* Hamiltonian H_I does not determine how the spins and the empty and doubly occupied wells are distributed in the lattice. At $U=U_c$ a pair of singly occupied wells can be replaced by a pair of a doubly occupied and an empty well without costing energy. These degeneracies are lifted by the tunneling term H_t if the more realistic Hamiltonian $H=H_t+H_I$ is considered. It is known that this leads to a staggered spin state (Néel state) if $U \gg U_c$ and to a state with alternating empty and doubly occupied wells if $U \ll U_c$ [12]. The latter is a density wave of fermion pairs. This is plausible if a nearest-neighbor pair of wells is considered: Two tunneling processes are possible in the case of a pair of singly occupied wells with opposite spin orientations, but due to Pauli's principle no tunneling occurs if the spin orientation is equal. Two tunneling processes are also possible in the case of a nearest-neighbor pair of an empty and a doubly occupied well. On the other hand, tunneling is blocked by Pauli's principle for a nearest-neighbor pair of doubly occupied wells. Since tunneling lowers the energy, the Néel state is close to the ground state for $U \gg U_c$ and the density wave is the ground state for $U \ll U_c$. In the remainder of this paper the situation of $U \approx U_c$ will be studied.

B. Partition function and resolvent

Many physical quantities of an atomic system at temperature $T=1/\beta$ can be calculated from the partition function

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int_{\Gamma} \mathrm{Tr}[(z-H)^{-1}] e^{-\beta z} \frac{dz}{2\pi i}, \quad (9)$$

which is expressed here by the resolvent $G(z)=(z-H)^{-1}$. Γ is a closed contour in the complex plane that encloses all eigenvalues of H and Tr is the trace over all quantum states of the system. At low temperatures this expression is dominated by the lowest eigenvalues of H, and one can use the approximation $Z \approx Z_0$ with

$$Z_0 = \int_\Gamma \mathrm{Tr}[P_0(z-H)^{-1}P_0]e^{-\beta z}\frac{dz}{2\pi i}, \tag{10}$$

where the trace is projected by the projector P_0 to quantum states that are energetically close to the ground state of the Hamiltonian H. In the specific case of $H=H_t+H_I$ the restriction to states without phononic excitations (i.e., $N_\mathbf{j}=0$),

$$P_0 = \prod_\mathbf{j}\left(\sum_{\sigma_\mathbf{j}} |0;\sigma_\mathbf{j}\rangle\langle 0;\sigma_\mathbf{j}|\right), \tag{11}$$

is an obvious choice for sufficiently large ω_0 (i.e., sufficiently strong amplitude of the optical lattice). However, virtual phononic excitations are possible, excited by the Hamiltonian of $e^{-\beta H}$ in the partition function.

As an example, we consider the case without tunneling ($J=0$). The projection P_0 is onto half-filled states. The poles of the projected resolvent then read $z_0=\epsilon M$ for a density-wave state and $z_0=(\epsilon-\gamma)M$ for a single-fermion state. Depending on the parameter γ, the partition function Z_0 is dominated by the lowest pole:

$$-\frac{1}{\beta M}\ln(Z_0) = \epsilon - \gamma\Theta(\gamma),$$

where $\Theta(\gamma)$ is the Heaviside function. At the transition point $\gamma=0$ this expression is continuous in γ but its first derivative jumps with respect to γ. According to the Ehrenfest classification scheme of phase transitions, this behavior characterizes a first-order phase transition.

III. RECURSIVE PROJECTION APPROACH

In order to evaluate the P_0-projected resolvent $G_0(z)=P_0(z-H)^{-1}P_0$ a recursive projection approach can be applied [13]. The main idea of this method is to control the mapping of states $|\Psi'\rangle=H|\Psi\rangle$, provided by the Hamiltonian H. For an initial state $|\Psi_0\rangle$ a sequence of linear independent states $|\Psi_k\rangle$ ($k=1,2,\ldots$) is created by a successive application of H. This idea has been used in the Lanczos method and in the doorstep approach [14]. The sequence of states is related to a sequence of projectors P_k, acting on the Hilbert space of all quantum states of the system. For an initial projector P_0 and its complement $P_1=1-P_0$, this sequence is created by the Hamiltonian H. For instance, the projector P_2 is defined by applying H to P_0 and projecting with P_1: P_2 is the projector of the space that is created by the operator P_1HP_0. This can be repeated by using P_3HP_2 to define P_4, where $P_3=P_1-P_2$, etc. It is important that the projectors with even index P_{2j} project onto separate subspaces. An advantage of the method is that for a proper choice of P_0 the spectrum of the projected Hamiltonians is shifted to higher energies at each step. In the specific case of this paper, the shift will be provided by phononic excitations. With the projections, a sequence of projected resolvents is defined as

$$G_0 = P_0(z-H)^{-1}P_0,$$

$$G_{2j+2} = P_{2j+2}[P_{2j+1}(z-H)P_{2j+1}]^{-1}P_{2j+2}$$

for $j=0,1\ldots$, which are connected by the identity (more details are given in Ref. [13])

$$G_{2j} = (z - P_{2j}HP_{2j} - P_{2j}HG_{2j+2}HP_{2j})^{-1}. \tag{12}$$

The iteration terminates at the jth level when P_{2j} projects onto a subspace whose basis consists only of eigenstates of H. Such a subspace we call the eigenspace. Moreover, when P_{2j} projects on a subspace that is close to an eigenspace (i.e., a basis of this subspace has very large overlap with eigenstates), the truncation of the iteration is a good approximation. In terms of the Hamiltonian this means that HP_{2j} and $P_{2j}H$ are small. This fact allows us to control the quality of the approximation.

Here only the lowest poles are of interest because they dominate the partition function in Eq. (10). Depending on the Hamiltonian H and the choice of the initial projection P_0, the lowest pole z_0^j of the projected resolvents $G_{2j}(z)$ can be increasing with j. If the values of z are restricted to those where $G_0(z)$ has poles but $G_2(z)$ has not, the sequence of projected resolvents can be truncated by approximating $G_2(z)$. The recursive projection method, given by Eq. (12), is now employed for the Hamiltonian H_γ of Eq. (6). This Hamiltonian describes tunneling of LFAs in the optical lattice and interaction with HAs, and direct interaction between the LFAs.

The initial projector P_0 is given in Eq. (11). This implies

$$P_1 = 1 - P_0 = \sum_{\{N_\mathbf{j}\geq 0\}}{}' \prod_\mathbf{j}\left(\sum_{\sigma_\mathbf{j}} |N_\mathbf{j};\sigma_\mathbf{j}\rangle\langle N_\mathbf{j};\sigma_\mathbf{j}|\right),$$

where Σ' restricts the summation to $\Sigma_\mathbf{j}N_\mathbf{j}\geq 1$. The P_0-projected Hamiltonian experiences a renormalization of the tunneling rate:

$$\begin{aligned} P_0H_\gamma P_0 &= P_0\Bigg(TH_tT^\dagger + \omega_0\sum_\mathbf{j} b_\mathbf{j}^\dagger b_\mathbf{j} + \gamma\sum_\mathbf{j} n_{\mathbf{j}\uparrow}n_{\mathbf{j}\downarrow} \\ &\quad - \frac{g^2}{\omega_0}\sum_\mathbf{j}(n_{\mathbf{j}\uparrow}+n_{\mathbf{j}\downarrow})^2\Bigg)P_0 \\ &= (\epsilon-\gamma)M + e^{-g^2/\omega_0^2}P_0H_tP_0 + \gamma\sum_\mathbf{j} P_0n_{\mathbf{j}\uparrow}n_{\mathbf{j}\downarrow}P_0. \end{aligned} \tag{13}$$

An important consequence of the coupling between HAs and LFAs is the renormalization of the tunneling rate as

$$J \to \tau = e^{-g^2/\omega_0^2}J, \tag{14}$$

which is the well-known polaron effect [12].

A. Effective Hamiltonian

The recursive projection will be applied to a restricted Hilbert space, where the recursion terminates at level $j=2$. This should be sufficient for small tunneling (i.e., for $J\ll\omega_0$). Then the resolvent G_0 can be written as $G_0=(z-H_0)^{-1}$ with the effective Hamiltonian

$$H_0 = P_0HP_0 + P_0HG_2HP_0, \tag{15}$$

and $G_2=(z-H_2)^{-1}$ with

$$H_2 = P_2H_IP_2 + P_2H_tP_2 + P_2HG_4HP_2. \tag{16}$$

The first term is

$$P_2 H_I P_2 = (\epsilon - \gamma) M + \omega_0 \sum_{\mathbf{j}} P_2 b_{\mathbf{j}}^\dagger b_{\mathbf{j}} P_2 + \gamma \sum_{\mathbf{j}} P_2 n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} P_2, \tag{17}$$

whereas the third term vanishes because HP_2 produces only states *outside* the restricted Hilbert space. Moreover, it is assumed that the second term vanishes because $H_t P_2$ produces only states outside the P_2-projected Hilbert space. This allows us to evaluate G_2 and subsequently the effective Hamiltonian H_0 in Eq. (15). The first part of H_0 was given in Eq. (13), and the second part $P_0 H G_2 H P_0$ must be calculated now. The latter separates into two parts, namely, a term H_s that exchanges single fermions with opposite spins and a term H_p that exchanges a fermionic pair with an empty well:

$$H_s = \tau^2 \sum_{\langle \mathbf{j},\mathbf{j}' \rangle} \sum_{\sigma,\sigma'=\uparrow,\downarrow} P_0 c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{j}'\sigma} G_2 c_{\mathbf{j}'\sigma'}^\dagger c_{\mathbf{j}\sigma'} P_0 \equiv \sum_{\langle \mathbf{j},\mathbf{j}' \rangle} h_{1,\mathbf{j},\mathbf{j}'} \tag{18}$$

describes the exchange of spins: $h_{1,\mathbf{j},\mathbf{j}'}$ gives $(\downarrow,\uparrow) \leftrightarrow (\uparrow,\downarrow)$ for $\sigma \neq \sigma'$ and is diagonal for $\sigma = \sigma'$. Moreover,

$$H_p = \tau^2 \sum_{\langle \mathbf{j},\mathbf{j}' \rangle} \sum_{\sigma,\sigma'=\uparrow,\downarrow} P_0 c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{j}'\sigma} G_2 c_{\mathbf{j}\sigma'}^\dagger c_{\mathbf{j}'\sigma'} P_0 \equiv \sum_{\langle \mathbf{j},\mathbf{j}' \rangle} h_{2,\mathbf{j},\mathbf{j}'} \tag{19}$$

describes the tunneling of two fermions as the exchange of a doubly occupied well with an empty well $(0,\downarrow\uparrow) \leftrightarrow (\downarrow\uparrow,0)$.

B. Eigenstates for two wells

Now the effective Hamiltonian H_0 for two wells is studied, where

$$H_0 = \epsilon - \gamma + h_{t,\mathbf{j},\mathbf{j}'} + h_{1,\mathbf{j},\mathbf{j}'} + h_{2,\mathbf{j},\mathbf{j}'} + \gamma(n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} + n_{\mathbf{j}'\uparrow} n_{\mathbf{j}'\downarrow}) \tag{20}$$

with the single-fermion tunneling term

$$h_{t,\mathbf{j},\mathbf{j}'} = -\tau \sum_{\sigma} (c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{j}'\sigma} + c_{\mathbf{j}'\sigma}^\dagger c_{\mathbf{j}\sigma}).$$

Eigenstates of H_0 on the P_0-projected Hilbert space can be constructed from dimer states:

$$|s_{\mathbf{j},\mathbf{j}'}\rangle = (|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle)/\sqrt{2}, \quad |d_{\mathbf{j},\mathbf{j}'}\rangle = (|\downarrow\uparrow,0\rangle + |0,\downarrow\uparrow\rangle)/\sqrt{2}. \tag{21}$$

These are eigenstates of $h_{1,\mathbf{j},\mathbf{j}'}$ with eigenvalues K_1 and 0,

$$h_{1,\mathbf{j},\mathbf{j}'}|s_{\mathbf{j},\mathbf{j}'}\rangle = K_1 |s_{\mathbf{j},\mathbf{j}'}\rangle, \quad h_{1,\mathbf{j},\mathbf{j}'}|d_{\mathbf{j},\mathbf{j}'}\rangle = 0, \tag{22}$$

and also eigenstates of $h_{2,\mathbf{j},\mathbf{j}'}$ with eigenvalues K_2 and 0,

$$h_{2,\mathbf{j},\mathbf{j}'}|d_{\mathbf{j},\mathbf{j}'}\rangle = K_2 |d_{\mathbf{j},\mathbf{j}'}\rangle, \quad h_{2,\mathbf{j},\mathbf{j}'}|s_{\mathbf{j},\mathbf{j}'}\rangle = 0. \tag{23}$$

The eigenvalues, which have been plotted in Fig. 1, are

$$K_1 = 2\tau^2 \sum_{m \geq 1} \frac{1}{m!} \frac{(2g^2/\omega_0^2)^m}{z - 2\epsilon + 2\gamma - \omega_0 m},$$

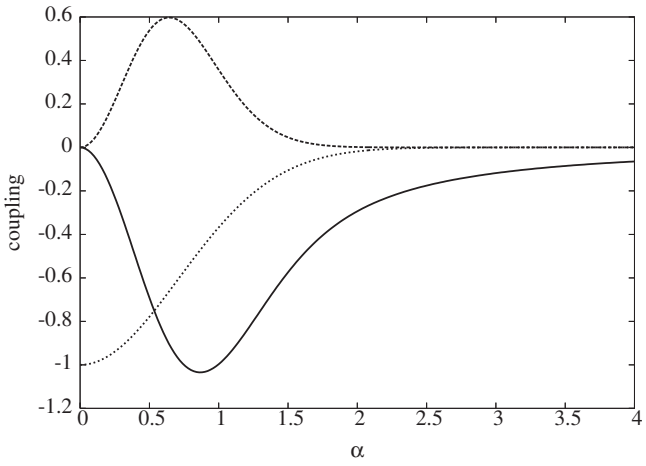

FIG. 1. Behavior of K_1 (full curve), K_2 (dashed curve), and $-\tau$ (dotted curve) vs the strength of the fermion-phonon coupling $\alpha = g/\omega_0$. The other parameters in K_1 and K_2 are $\omega_0 = J = 1$, $\gamma = 0$, and z is given by the lowest pole. All energies are measured in units of ω_0.

$$K_2 = 2\tau^2 \sum_{m \geq 1} \frac{1}{m!} \frac{(-2g^2/\omega_0^2)^m}{z - 2\epsilon - \omega_0 m}. \tag{24}$$

$h_{k,\mathbf{j},\mathbf{j}'}$ $(k=1,2)$ do not connect different dimer components:

$$h_{k,\mathbf{j},\mathbf{j}'}|\downarrow\uparrow,\sigma\rangle = h_{k,\mathbf{j},\mathbf{j}'}|\sigma,\downarrow\uparrow\rangle = h_{k,\mathbf{j},\mathbf{j}'}|0,\sigma\rangle = h_{k,\mathbf{j},\mathbf{j}'}|\sigma,0\rangle = 0$$

$$(\sigma = \downarrow,\uparrow; \ k = 1,2). \tag{25}$$

Moreover, $h_{t,\mathbf{j},\mathbf{j}'}$ switches between dimers with rate 2τ:

$$h_{t,\mathbf{j},\mathbf{j}'}|s_{\mathbf{j},\mathbf{j}'}\rangle = 2\tau|d_{\mathbf{j},\mathbf{j}'}\rangle, \quad h_{t,\mathbf{j},\mathbf{j}'}|d_{\mathbf{j},\mathbf{j}'}\rangle = 2\tau|s_{\mathbf{j},\mathbf{j}'}\rangle.$$

Since always $K_1 < K_2$ (cf. Fig. 1), the formation of dimers $|s_{\mathbf{j},\mathbf{j}'}\rangle$ is favored. However, when $\gamma < 0$, the disadvantage of the dimer $|d_{\mathbf{j},\mathbf{j}'}\rangle$ can be compensated by the local interaction term in H_0, which is diagonal and counts the number of doubly occupied wells. For the state $a|s_{\mathbf{j},\mathbf{j}'}\rangle + b|d_{\mathbf{j},\mathbf{j}'}\rangle$ we get the relation

$$H_0(a|s_{\mathbf{j},\mathbf{j}'}\rangle + b|d_{\mathbf{j},\mathbf{j}'}\rangle) = (\epsilon - \gamma + K_1 + 2\tau b/a)a|s_{\mathbf{j},\mathbf{j}'}\rangle + (\epsilon + K_2 + 2\tau a/b)b|d_{\mathbf{j},\mathbf{j}'}\rangle. \tag{26}$$

This state is an eigenstate of $h_{\mathbf{j},\mathbf{j}'}$ for $\gamma = K_1 - K_2 + 2\tau(b^2 - a^2)/ab$ with eigenvalues $\epsilon - \gamma + K_1 + 2\tau b/a$. For a given γ we can evaluate a and b and then determine the related eigenvalues. In particular, for $\gamma = K_1 - K_2$, there are solutions $a = \pm b$ with corresponding eigenvalues $\epsilon + K_2 \pm 2\tau$.

K_1 and K_2 still depend on the parameter z which has to be determined as a pole of the resolvent $G_0(z)$:

$$z = \epsilon + K_2(z) \pm 2\tau, \tag{27}$$

where the lowest pole is the most relevant contribution. Other solutions of this equation refer to excited states that are not relevant for the discussion here.

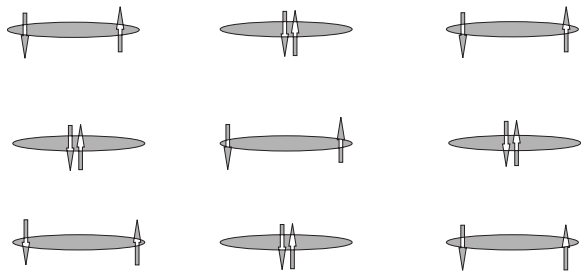

FIG. 2. The alternating dimer state of Eq. (21) on a square lattice, where the elements represent $|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle$ and $|\downarrow\uparrow,0\rangle + |0,\downarrow\uparrow\rangle$, respectively.

C. Eigenstates for the lattice

On the lattice with $2M$ wells the effective Hamiltonian H_0 can be constructed from the effective Hamiltonian in Eq. (20) by a summation over nearest neighbors. In order to study simple eigenstates of the lattice system first, the tunneling of single fermions is excluded from the discussion:

$$H_0' = H_0 - \sum_{\langle \mathbf{j},\mathbf{j}'\rangle} h_{t,\mathbf{j},\mathbf{j}'}. \tag{28}$$

Eigenstates of H_0' are product dimer states,

$$|\Psi_1\rangle = \prod_{\langle \mathbf{j},\mathbf{j}'\rangle} |s_{\mathbf{j},\mathbf{j}'}\rangle, \quad |\Psi_2\rangle = \prod_{\langle \mathbf{j},\mathbf{j}'\rangle} |d_{\mathbf{j},\mathbf{j}'}\rangle, \tag{29}$$

with eigenvalues

$$\lambda_1 = (\epsilon - \gamma)M + 2M\tau^2 \sum_{m\geq 1} \frac{1}{m!} \frac{(2g^2/\omega_0^2)^m}{z - (\epsilon-\gamma)M - \omega_0 m} \tag{30}$$

and

$$\lambda_2 = \epsilon M + 2M\tau^2 \sum_{m\geq 1} \frac{1}{m!} \frac{(-2g^2/\omega_0^2)^m}{z - \epsilon M - \omega_0 m}. \tag{31}$$

The alternating dimer state

$$|\Psi_{\mathrm{AD}}\rangle = \prod_{\langle \mathbf{j},\mathbf{j}'\rangle \in C} (a_{\mathbf{j},\mathbf{j}'}|s_{\mathbf{j},\mathbf{j}'}\rangle + b_{\mathbf{j},\mathbf{j}'}|d_{\mathbf{j},\mathbf{j}'}\rangle)$$

is also an eigenstate of H_0' with eigenvalue

$$\lambda_{\mathrm{AD}} = (\epsilon - \gamma/2)M + M\tau^2 \sum_{m\geq 1} \frac{1}{m!} \frac{(2g^2/\omega_0^2)^m}{z - (\epsilon-\gamma/2)M - \omega_0 m}$$
$$+ M\tau^2 \sum_{m\geq 1} \frac{1}{m!} \frac{(-2g^2/\omega_0^2)^m}{z - (\epsilon-\gamma/2)M - \omega_0 m}. \tag{32}$$

The coefficients $a_{\mathbf{j},\mathbf{j}'}$ and $b_{\mathbf{j},\mathbf{j}'}$ are either 0 or 1, alternating on the lattice. C covers the lattice with dimers, separated by nearest-neigbor bonds (cf. Fig. 2).

Next, the energy z must be determined by the lowest poles of the resolvent G_0. This gives, up to small corrections, for λ_1 the value $z=(\epsilon-\gamma)M$ such that

$$\lambda_1/M = \epsilon - \gamma - 2\frac{\tau^2}{\omega_0} F(g^2/\omega_0^2) \quad \text{with} \quad F(x) = \sum_{m\geq 1} \frac{(2x)^m}{m\,!\,m}. \tag{33}$$

For λ_2 the value $z=\epsilon M$ gives

$$\lambda_2/M = \epsilon - 2\frac{\tau^2}{\omega_0} F(-g^2/\omega_0^2), \tag{34}$$

and for λ_{AD} the value $z=(\epsilon-\gamma/2)M$ leads to

$$\lambda_{\mathrm{AD}}/M = \epsilon - \gamma/2 - \frac{\tau^2}{\omega_0} F(g^2/\omega_0^2) - \frac{\tau^2}{\omega_0} F(-g^2/\omega_0^2). \tag{35}$$

Dimer states in a bipartite lattice are not expected to be ground states. For instance, the Néel state gives for $z=(\epsilon-\gamma)M$

$$\langle \Psi_N|H_0|\Psi_N\rangle/M = (\epsilon-\gamma) + \langle \Psi_N| \sum_{\langle \mathbf{j},\mathbf{j}'\rangle} h_{1,\mathbf{j},\mathbf{j}'}|\Psi_N\rangle/M$$
$$= (\epsilon-\gamma) - \frac{z_L\tau^2}{\omega_0} F(g^2/\omega_0^2),$$

where z_L is the number of nearest-neighbor wells. The corresponding matrix element for a density-wave state of fermion pairs is ϵ, which is very close to the eigenvalue λ_2/M of the paired fermion dimers $|\Psi_2\rangle$.

The single-fermion tunneling has not been included, since the renormalized tunneling rate τ is very small for sufficiently large coupling g/ω_0. Therefore, its effect on the eigenvalues will be negligible, provided the system is not at a degeneracy point. Although the dimer states are not ground states, the system can stay in them for very long times, in terms of a typical experiment.

IV. DISCUSSION AND CONCLUSION

An effective Hamiltonian H_0 has been derived within a truncated recursive projection approach for a half-filled optical lattice. The truncation should be valid under the assumption that the tunneling rate J is small in comparison with the local potential of the HAs (i.e., for $J \ll \omega_0$). The properties of the effective Hamiltonian in Eq. (15) can be summarized as follows. (I) H_0 acts in a four-dimensional space at each well of the optical lattice, spanned by $\{|0\rangle,|\uparrow\rangle,|\downarrow\rangle,|\downarrow\uparrow\rangle\}$. (II) H_0 describes one- and two-fermion processes between nearest-neighbor wells. Phonons (i.e., excitations of the HAs) are created by the unitary operator T of Eq. (7) and appear in the eigenvalues of the effective Hamiltonian H_0 as excitation of m phonons. In the case of a system with two wells, the eigenstates of H_0 are superpositions of dimer states, where either the fermions are in separate wells or exist as a pair in only one well. The contribution of each of the two dimers to the eigenstate can be controlled by the parameter $\gamma = U - 2g^2/\omega_0$. This result was extended to an optical lattice with $2M$ wells. If single-fermion tunneling is neglected in H_0 (this is a good approximation for sufficiently strong fermion-phonon coupling g/ω), dimer states are eigenstates of the effective Hamiltonian. Although the dimer

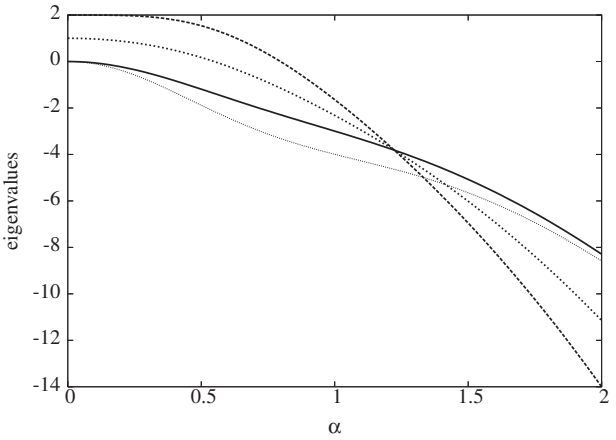

FIG. 3. Eigenvalues of H_0' of Eq. (28) for dimer states: λ_1/M (full curve) for singlets, λ_2/M (dashed curve) for paired fermion dimers, and λ_{AD}/M (dotted curve) for an alternating dimer state vs the strength of the fermion-phonon coupling $\alpha=g/\omega_0$ and fixed $J=1$ and $U=2$. For comparison, the diagonal matrix element with respect to the Néel state is shown for $z_L=4$ by the thin curve. All energies are measured in units of ω_0.

states are not ground states of the system, they can be prepared by using a modulated optical lattice, where the tunneling barrier is higher between the dimers. This is possible because we have control of the optical lattice (laser frequency and amplitude) and of the fermion-fermion interaction U through the Feshbach resonance. After the preparation of the dimer state, the modulation can be turned off without destroying the dimers, since it is (almost) an eigenstate. The main effect of the (weak) single-fermion tunneling term is to flip singlet dimers into dimers of paired fermions (and vice versa) with a rate 2τ. Therefore, single-fermion tunneling favors the formation of neighboring pairs of different dimers. Three different dimer states were studied: states with singlet dimers, states with dimers of paired fermions, and states with two dimers, placed in alternating order in the lattice. Their corresponding energies (given by their eigenvalues with respect to the effective Hamiltonian) are different. However, there is a point of degeneracy for

$$\gamma_c = 2\frac{\tau^2}{\omega_0}[F(-g^2/\omega_0^2) - F(g^2/\omega_0^2)],$$

as plotted in Fig. 3.

The interaction between LFAs and HAs in an optical lattice can be understood in a simple physical picture. Already, in the absence of tunneling, the local repulsive interaction U of the LFAs is affected by the coupling to the HAs. It results in a reduction of U to $\gamma=U-2g^2/\omega_0$. The reason is that the HAs absorb interaction energy from the LFAs by going into an excited state [cf. Eq. (5)]. In the presence of a tunneling rate J of the LFAs, kinetic energy is also taken away by the HAs, leading to a reduction of the tunneling rate to $\tau=J\exp(-g^2/\omega_0^2)$. The renormalization of the tunneling rate and the interaction strength depends on the parameter g/ω_0. This means that the effect of the HAs on the LFAs is stronger the easier it is to excite the HAs with energy ω_0. The latter can be controlled in an optical lattice by tuning the shape of the potential at the bottom of the wells. Since excitations of energy ω_0 are essential, a deviation of the potential from the assumed harmonic form at higher energies does not affect the qualitative picture. The fact that γ can be negative (attractive interaction) implies a transition from a repulsive to an attractive gas of LFAs. At half filling the ground state of the LFAs in an unfrustrated lattice is a Néel state in the case of strong repulsion and a density wave of paired fermions in the case of strong attraction. For $\gamma=0$ there is no effective interaction between the LFAs. However, this does not mean that there is a free Fermi gas because the scattering with the HAs still affects the tunneling processes. Our calculation, based on a small tunneling rate, shows that the LFAs form dimer states for $\gamma\approx 0$, where either two fermions on nearest-neighbor wells with opposite spin orientations or a locally bound pair of two fermions and an empty well are formed.

The dimer states, as well as the Néel and the density-wave states, should be observable in a Stern-Gerlach experiment [4]. For this purpose, a mixture of two atomic species, constituted of the same number of LFAs (e.g., ^{6}Li) and HAs (e.g., ^{87}Rb or ^{40}K) is brought into an optical lattice, where half filling is maintained at low temperature. Then the interaction parameter $\gamma=U-2g^2/\omega_0$ is adjusted, either by tuning U through a magnetic field near a Feshbach resonance, or by tuning the excitation energy ω_0 of the HAs (i.e., the tightness of the wells in the optical lattice). Moreover, the tunneling rate J is adjusted using the amplitude of the optical lattice. After the creation of the quantum state, the optical lattice is turned off to allow the gas to expand and to measure the spin projections in a Stern-Gerlach experiment. The Néel state, consisting of individual fermions with alternating spin orientations, would separate in the inhomogeneous magnetic field into two parts. In contrast, the density wave of paired fermions and the dimer states would not separate so easily.

In conclusion, a mixture of heavy atoms and light fermionic atoms has been investigated. Inelastic scattering processes generate an attraction between the light atoms and a strong reduction of the tunneling rate. Depending on the total interaction, there is the possibility of a Néel state, a density wave of paired fermions, and different dimer states in an optical lattice.

ACKNOWLEDGMENT

This research was supported by SFB 484.

[1] I. Bloch, Rev. Financ. Stud. **1**, 23 (2005).
[2] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).
[3] S. Inouye *et al.*, Nature (London) **392**, 151 (1998).
[4] A. Görlitz, T. L. Gustavson, A. E. Leanhardt, R. Low, A. P. Chikkatur, S. Gupta, S. Inouye, D. E. Pritchard, and W. Ketterle, Phys. Rev. Lett. **90**, 090401 (2003); O. Mandel, M. Greiner, A. Widera, T. Rom, T. W. Hansch, and I. Bloch, *ibid.* **91**, 010407 (2003); H. Schmaljohann, M. Erhard, J. Kronjager, M. Kottke, S. van Staa, L. Cacciapuoti, J. J. Arlt, K. Bongs, and K. Sengstock, *ibid.* **92**, 040402 (2004); M. Köhl, H. Moritz, T. Stoferle, K. Gunter, and T. Esslinger, *ibid.* **94**, 080403 (2005); G. B. Partridge, W. Li, Y. A. Liao, R. G. Hulet, M. Haque, and H. T. C. Stoof, *ibid.* **97**, 190407 (2006).
[5] K. E. Strecker, G. B. Partridge, and R. G. Hulet, Phys. Rev. Lett. **91**, 080406 (2003); H. Uys, T. Miyakawa, D. Meiser, and P. Meystre, Phys. Rev. A **72**, 053616 (2005).
[6] C. A. Stan, M. W. Zwierlein, C. H. Schunck, S. M. F. Raupach, and W. Ketterle, Phys. Rev. Lett. **93**, 143001 (2004).
[7] K. Günter, T. Stoferle, H. Moritz, M. Kohl, and T. Esslinger, Phys. Rev. Lett. **96**, 180402 (2006).
[8] C. Ospelkaus, S. Ospelkaus, K. Sengstock, and K. Bongs, Phys. Rev. Lett. **96**, 020401 (2006).
[9] D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1988); R. Moessner and S. L. Sondhi, Phys. Rev. B **68**, 184512 (2003).
[10] C. Xu and M. P. A. Fisher, Phys. Rev. B **75**, 104428 (2007).
[11] M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
[12] A. S. Alexandrov and N. Mott, *Polarons & Bipolarons* (World Scientific, Singapore, 1995).
[13] K. Ziegler, Phys. Rev. A **68**, 053602 (2003); K. Ziegler, Phys. Rev. B **74**, 014301 (2006).
[14] A. N. Salgueiro *et al.*, e-print arXiv:cond-mat/0510120, and references therein; Nucl. Phys. A **790**, 780 (2007).
[15] C. Ates and K. Ziegler, Phys. Rev. A **71**, 063610 (2005); K. Ziegler, Nucl. Phys. A **790**, 718 (2007).