Creation on demand of higher orbital states in a vibrating optical lattice

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Abstract

It is shown that the extended Hubbard Hamiltonian describing atoms confined in an optical lattice always contains commonly neglected terms which can significantly change the dynamical properties of the system. Particularly for bosonic systems, they can be exploited for creating orbital states on demand via the parametric resonance phenomenon. This indicates an additional application for optical lattices, namely the study and emulation of interactions between particles and lattice vibrations.

Introduction

Recent theoretical works and the first experiments considering higher bands in optical lattices have opened a new, promising area of ultra cold atom research – **orbital physics**. Typically, such systems are described with Hubbard-like Hamiltonians extended by additional inter-orbital interaction terms. In previous analyses, some of these additional terms, due to their non resonant character, have always been treated as unimportant and therefore omitted. I give a simple counter-example that shows that in the case of oscillating optical lattices they can efficiently transfer atoms to higher bands in a fully controlled way.

The Model

The General Hamiltonian

I consider spinless bosons interacting via two body δ-like contact interactions confined in a 2D optical lattice.

$$\mathscr{H} = \int \mathrm{d}^3\boldsymbol{r} \left[\Psi^\dagger(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\boldsymbol{r}) \right) \Psi(\boldsymbol{r}) + \frac{g}{2} \Psi^\dagger(\boldsymbol{r})\Psi^\dagger(\boldsymbol{r})\Psi(\boldsymbol{r})\Psi(\boldsymbol{r}) \right]$$

$\Psi(\boldsymbol{r})$ is a bosonic field operator; g is the strength of interactions. The lattice potential reads

$$V_{\mathrm{ext}}(\boldsymbol{r}) = q_x \sin^2(kx) + q_y \sin^2(ky) + \frac{m\omega_z^2}{2} z^2$$

where $k = 2\pi/\lambda$ is the wave vector of the laser field and ω_z is the frequency of the trapping harmonic potential in the z direction.

Dimensionless parameters

It is convenient to measure lengths in units of the laser wavelength λ, and all energies in units of the recoil energy $E_R = \frac{(2\pi\hbar)^2}{2m\lambda^2}$. The trapping potential in the z direction is characterized by the dimensionless quantity $\kappa = \hbar\omega_z/2E_R$. The dimensionless coupling constant is $g = 16\pi^2 a_0/\lambda$, where a_0 is the s-wave scattering length. In typical experiments with ^{87}Rb or ^{52}Cr confined in an optical lattice, far from the Feshbach resonance, $g \sim 1$. The lattice geometry is defined by the dimensionless algebraic vector

$$\boldsymbol{Q} = \left(\frac{q_x}{E_R}, \frac{q_y}{E_R}, \kappa \right).$$

Field operator decomposition

I expand the field operator in the ground and first excited Bloch bands as follows

$$\Psi(\boldsymbol{r}) \approx \sum_i \hat{a}_i \phi_i^0(\boldsymbol{r}) + \hat{b}_i \phi_i^x(\boldsymbol{r}) + \hat{c}_i \phi_i^y(\boldsymbol{r}), \qquad (1)$$

$$\phi_i^s(\boldsymbol{r}) = \mathscr{X}_i^0(x)\mathscr{Y}_i^0(y)\mathscr{Z}(z),$$
$$\phi_i^x(\boldsymbol{r}) = \mathscr{X}_i^1(x)\mathscr{Y}_i^0(y)\mathscr{Z}(z),$$
$$\phi_i^y(\boldsymbol{r}) = \mathscr{X}_i^0(x)\mathscr{Y}_i^1(y)\mathscr{Z}(z).$$

$\mathscr{X}_i^\alpha(x)$ and $\mathscr{Y}_i^\alpha(y)$ – one dimensional Wannier functions
$\mathscr{Z}(z)$ – ground state of harmonic oscillator
$\hat{a}_i$, $\hat{b}_i$, and $\hat{c}_i$ – bosonic operators annihilating particles at site i in the s, p_x, and p_y orbitals respectively
$\hat{n}_s^{(i)} = a_i^\dagger a_i$
$\hat{n}_x^{(i)} = b_i^\dagger b_i$ – particle number operators in given orbitals
$\hat{n}_y^{(i)} = c_i^\dagger c_i$

The Hubbard-like Hamiltonian

$$\mathscr{H} = \sum_i H_i - \sum_{\{i \xrightarrow{x} j\}} J_0^x (a_i^\dagger a_j + c_i^\dagger c_j) + J_1^x b_i^\dagger b_j - \sum_{\{i \xrightarrow{y} j\}} J_0^y (a_i^\dagger a_j + b_i^\dagger b_j) + J_1^y c_i^\dagger c_j, \qquad (2a)$$

where J_α^d is nearest neighbor hopping in the direction d for band α. The on-site Hamiltonian H_i has the form:

$$H_i = \sum_\sigma \left[E_\sigma \hat{n}_i^\sigma + \frac{U_{\sigma\sigma}}{2} \hat{n}_i^\sigma (\hat{n}_i^\sigma - 1) \right] + \sum_{\sigma \neq \sigma'} U_{\sigma\sigma'} \hat{n}_i^\sigma \hat{n}_i^{\sigma'} + \left[\frac{U_{sx}}{2} \hat{a}_i^{\dagger 2} \hat{b}_i^2 + \frac{U_{sy}}{2} \hat{a}_i^{\dagger 2} \hat{c}_i^2 + \frac{U_{xy}}{2} \hat{b}_i^{\dagger 2} \hat{c}_i^2 \right] + h.c. \qquad (2b)$$

These summations run over orbital index $\sigma \in \{s, x, y\}$. The single particle energies E_σ depend only on the lattice geometry while all the parameters U depend additionally on the dimensionless coupling g. They can be calculated directly:

$$E_\sigma(\boldsymbol{Q}) = \int \mathrm{d}^3\boldsymbol{r}\, \phi_i^\sigma(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\boldsymbol{r}) \right] \phi_i^\sigma(\boldsymbol{r}),$$
$$U_{\sigma\sigma'}(\boldsymbol{Q}, g) = g \int \mathrm{d}^3\boldsymbol{r} \left[\phi_i^\sigma(\boldsymbol{r}) \phi_i^{\sigma'}(\boldsymbol{r}) \right]^2. \qquad (3)$$

The values of these parameters for the example lattice are presented in **Figure 1**.

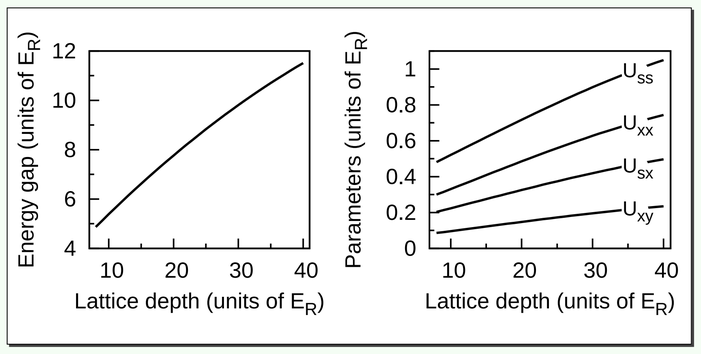

Figure 1: Parameters of the Hamiltonian (2) as functions of lattice depth for the symmetric case $\boldsymbol{Q} = (q, q, 8)$ and $g = 1$. Parameters originating in contact interactions are at least ten times smaller than the energy gap between the s and p-bands.

The Key Observation

For experimentally available systems

all contact energies U are at least ten times smaller than single-particle excitation energies $\Delta E_\sigma = E_\sigma - E_s$ where $\sigma \in \{x, y\}$.

Therefore,

due to the energy conservation, one can neglect red terms in the Hamiltonian (2b).

However,

in a scenario when the lattice parameters vary in time they can dramatically change the dynamical properties of the system.

In this paper we utilize these commonly neglected terms and propose a mechanism for creating orbital states *on demand*. To show that this scenario is realistic in present day experiments, numerical simulations are shown for ^{52}Cr atoms confined in an optical lattice with $\lambda = 523\,\mathrm{nm}$. The contact interaction coupling is $g \approx 1.8$.

The Vibrating Lattice

The Initial moment

- **two bosons** per site on average
- lattice geometry $\boldsymbol{Q}_0 = (32, 20, 8)$
- many-body state: **Mott-Insulator** in **s**-orbital

The Dynamics

- time-dependent optical lattice: $\boldsymbol{Q}(t) = \boldsymbol{Q}_0 + \delta\boldsymbol{Q}(t)$
- harmonic vibrations of the lattice: $\delta\boldsymbol{Q}(t) = (A, 0, 0)\sin(\omega t)$
- deep lattice – we neglect tunneling processes
- the dynamics takes place in the subspace spanned by:
  $|200\rangle = \frac{1}{\sqrt{2}} a^{\dagger 2}|\mathrm{vac}\rangle$, $|020\rangle = \frac{1}{\sqrt{2}} b^{\dagger 2}|\mathrm{vac}\rangle$, and $|002\rangle = \frac{1}{\sqrt{2}} c^{\dagger 2}|\mathrm{vac}\rangle$
- the Hamiltonian takes the form

$$\hat{H}(\boldsymbol{Q}(t)) = \begin{pmatrix} 2E_s + U_{ss} & U_{sx} & U_{sy} \\ U_{sx} & 2E_x + U_{xx} & U_{xy} \\ U_{sy} & U_{xy} & 2E_y + U_{yy} \end{pmatrix}. \qquad (4)$$

The results

We define **the transfer efficiency** as the highest depletion of the initial state for a given frequency ω and amplitude A (see **Figure 2a**). For two characteristic frequencies ω_1 and ω_2, the initial state can be totally depleted.

Figure 2b presents the time dependence of occupations for the corresponding two frequencies. The characteristic frequencies almost do not depend on the amplitude A and they are approximately equal to the energy difference between the appropriate eigenstates of the matrix $\hat{H}(\boldsymbol{Q}_0)$.

Testing the model

To show that the predictions described are almost insensitive to the approximations in the model, two additional tests were performed.

1. The influence of the approximation (1) was checked. The expansion was generalized and all d-orbital states and their possible interactions were taken into account (dashed line in **Figure 2a**).

2. The influence of tunneling was checked. The full many-body dynamics in a 1D optical lattice was studied. Due to computational complexity, calculations were performed for **eight atoms** in a lattice with **four sites**, and with periodic boundary conditions. Vibrations $\boldsymbol{Q} = (32 + 4\sin(\omega t), 20, 8)$ with a frequency close to ω_2 were considered. **Figure 2c** shows the resulting transfer efficiency compared to single-site predictions as well as the variance of the on-site number operator.

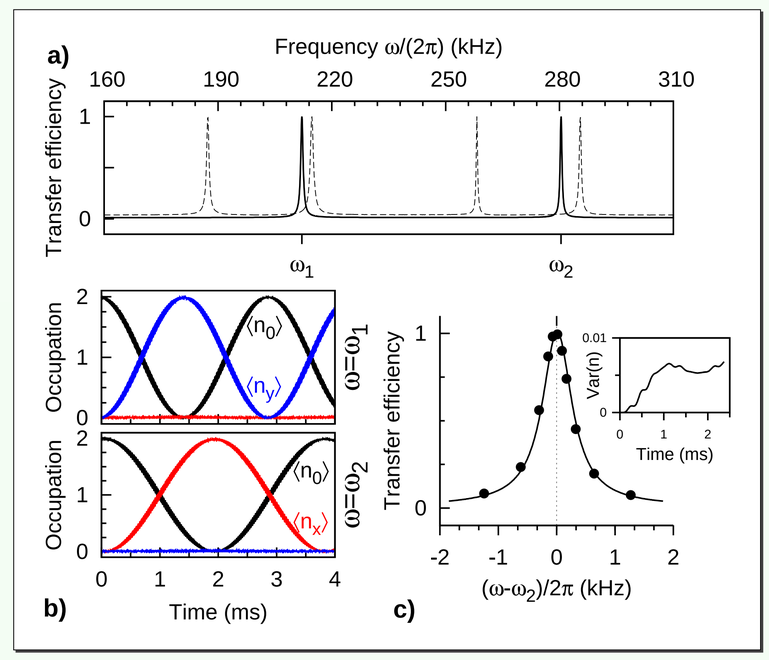

Figure 2: Creation of the p-band states by a vibrating optical lattice with $\boldsymbol{Q} = (32 + 4\sin(\omega t), 20, 8)$. **Plot (a)** presents the transfer efficiency as a function of vibration frequency ω. Two distinct peaks are visible. For these particular frequencies, p-band states become highly occupied. The dashed line comes from a generalized model that also takes into account d-band orbitals. Additional peaks correspond to resonant frequencies in which one of interacting atoms can be promoted to the d_x or d_y band, respectively. Moreover, resonant frequencies ω_1 and ω_2 are shifted. **Plot (b)** presents the occupation of basis states as a function of time for the resonant frequencies. At frequency ω_1 (ω_2) the p_y (p_x) orbital is populated. **Plot (c)** shows a comparison between the situation when tunneling is totally neglected (solid line) and when it is taken into account (filled circles). The inset shows the variance of the on-site number operator as a function of time for $\omega = \omega_2$.

Playing with orbital states

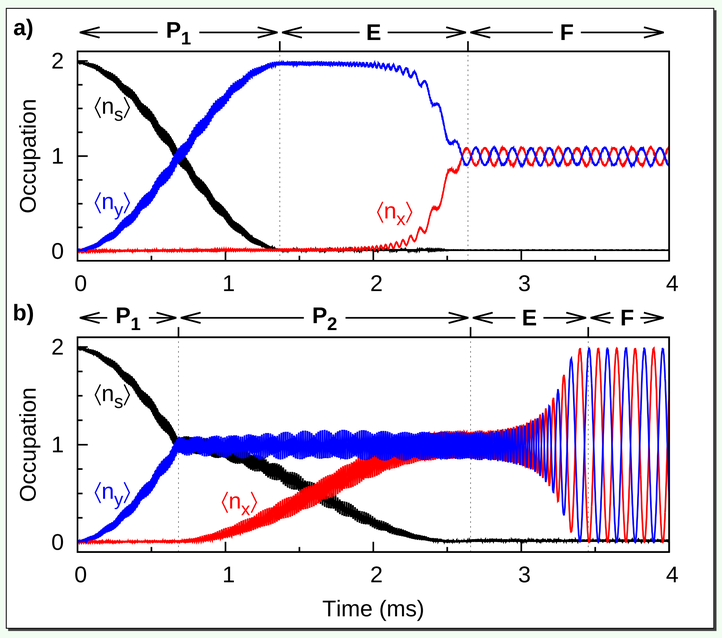

Figure 3: Two experimental scenarios for the creation of a two particle superposition in excited band states. Initially the system is prepared in the ground state of a highly non symmetric lattice $\mathbf{Q}_0 = (32, 20, 8)$. **Plot (a)**: In the first scenario, two particles are transfered to the p_y state by applying appropriate vibrations ($\mathbf{P}_1$) and then lattice depths in both directions are equilibrated (**E**). If this process is slow enough, then the final state of the system is in the superposition $(|020\rangle - |002\rangle)/\sqrt{2}$. **Plot (b)**: In the second case, two particles are transfered to the p_y state by applying appropriate vibrations ($\mathbf{P}_1$). When the initial state is half-depleted the vibration frequency is changed to the other resonance, and the p_x state is filled ($\mathbf{P}_2$). Then similarly to the previous scenario, lattice depths are equilibrated (**E**). The final state is in a complex superposition of basis states and the occupation of each basis state varies in time (**F**). At the moments when the occupation of p_x and p_y orbitals are equal, the system is in one of the vortex states $(|020\rangle \pm i|002\rangle)/\sqrt{2}$.

Summary

The results presented show that lattice vibrations can effectively couple the ground Wannier state to chosen orbital states. The mechanism described is very general since it originates from the fundamental Hubbard Hamiltonian by taking into account interactions between particles. In general, for each term describing a non vanishing interaction energy between particles in different single-particle states there always exist corresponding term describing a transfer of particles between them. In the static case these terms usually violate energy conservation and can therefore be neglected. However, when one considers time dependent Hamiltonians they should be always taken into account because they can significantly change the dynamics of the system.