

Chapter 2

Introduction to Optical Lattices and Excited Bands (and All That)

“And God said, “Let there be light,” and there was light. And God saw that light was good. Some time later, there were optical lattices; and then it was even better.”

—Adapted from a famous book.

This chapter provides an introduction to the physics in excited bands of optical lattices. We will start by briefly discussing general features of the physics in optical lattices in Sect. 2.1. In Sect. 2.2 we review properties of single particles in periodic potentials and introduce the p and d orbitals in excited bands. The Hamiltonians of the many-body systems are discussed in Sect. 2.3, together with symmetry properties of each case.¹ In Sect. 2.5 we present an overview about experiments with cold atoms in excited bands of optical lattices.

2.1 Optical Lattices

Optical lattices are spatially periodic potentials, created from the superposition of linearly polarized lasers, that can be used to trap neutral atoms via AC Stark shift [5].

The basic idea behind the implementation of optical lattices relies on the use of electric field with a spatial dependence for inducing a position-dependent shift on the energy levels of an atom [5, 6]. We will illustrate how this works by considering the interaction of a two-level atom with monochromatic laser light [7, 8]. For that, we

¹The presentation of the p -band case follows Refs. [1–3]. The discussion about the d -band case follows Ref. [4].

start with the Hamiltonian describing two electronic atomic levels, i.e., the ground $|g\rangle$ and excited $|e\rangle$,

$$H_a = E_g |g\rangle\langle g| + E_e |e\rangle\langle e|, \quad (2.1)$$

where E_g and E_e are the corresponding ground and excited states energies and we define $\omega_0 = E_e - E_g$.

Let us assume that the wavelength of the laser λ_L is much greater than the atomic size² and write the Hamiltonian describing the dipole coupling of the atom with the oscillating electric field

$$H_I = -e\mathbf{r} \cdot \mathbf{E}_0 \cos(\omega_L t), \quad (2.2)$$

where $-e\mathbf{r}$ is the electric dipole moment operator, $\mathbf{E}_0$ is the electric field amplitude and ω_0 the laser frequency [7]. The Hamiltonian of the atom-laser interaction then follows

$$H = H_a + H_I = \hbar \begin{pmatrix} -\omega_0/2 & \Omega \cos(\omega_L t) \\ \Omega^* \cos(\omega_L t) & \omega_0/2 \end{pmatrix}, \quad (2.3)$$

where $\Omega = \frac{E_0}{\hbar} \langle g|e\mathbf{r}|e\rangle$ is the Rabi frequency, and due to parity selection rules $\langle g|\mathbf{r}|g\rangle = \langle e|\mathbf{r}|e\rangle = 0$.

Two situations are of particular interest here [9]: (i) close to resonance, when $\omega_0 \approx \omega_L$, $|\omega_0 - \omega_L| \ll \omega_0, \omega_L$; and (ii) far off resonance, when $|\omega_0 - \omega_L| \gg \omega_0, \omega_L$. We consider them separately:

- (i) Close to resonance, the probability of transition between the $|g\rangle$ and $|e\rangle$ states is time dependent and given by

$$P(t) = \frac{\Omega^2}{|\Omega|^2 + (\omega_L - \omega_0)^2} \sin^2 \left(\frac{t}{2} \sqrt{|\Omega|^2 + (\omega_L - \omega_0)^2} \right). \quad (2.4)$$

In particular, if an initial state is given such that all the atoms are in the $|g\rangle$ state, a pulse of π duration—the so called π pulse, is capable of exciting the entire population to the $|e\rangle$ state. This is not the regime for implementation of optical lattices, but as will be discussed later, it is of relevance for manipulations in experiments with cold atoms.

- (ii) The regime of interest for creating optical lattices is far-off resonance, where one obtains the Stark shifts. In fact, in the rotating frame with respect to the light field, the effective Hamiltonian of the total system is static, and given by³

$$H = \frac{\hbar}{2} \begin{pmatrix} \Delta & 2\Omega \\ 2\Omega^* & -\Delta \end{pmatrix}, \quad (2.5)$$

²At the atomic scale, i.e., the Bohr radius, spatial variations of the electric field can be neglected. This is called the *dipole approximation* [7].

³To derive Eq. (2.5), one applies the *rotating wave approximation*, where rapidly oscillating terms are neglected.

where $\Delta = \omega_L - \omega_0$ is the detuning of the laser with respect to the atomic transition. Far from resonance, when $|\Delta| \gg |\Omega|$, the energies of the eigenstates of this effective system⁴ are then given by

$$\begin{aligned}\epsilon_g &= -\frac{\hbar\omega_0}{2} + \frac{\hbar}{4} \frac{|\Omega|^2}{(\omega_L - \omega_0)} \\ \epsilon_e &= \frac{\hbar\omega_0}{2} - \frac{\hbar}{4} \frac{|\Omega|^2}{(\omega_L - \omega_0)},\end{aligned}\tag{2.6}$$

showing that as the result of atom-light interactions, we can create a conservative potential⁵ with the shifts of the atomic energy levels. Accordingly, if the electric field has a spatial dependence,⁶ then the induced shift on the atomic levels will also depend on the position. As stated in the beginning, this is the basic principle underlying the implementation of optical lattices⁷! The potential produced is in turn proportional to the intensity of the light field,

$$V = -\frac{1}{2}\alpha(\omega_L)|E|^2 = \frac{\hbar|\Omega|^2}{4\Delta},\tag{2.7}$$

with $\alpha(\omega_L)$ the polarizability of the atom [10].

In its simplest implementation, an optical lattice can be constructed from the interference of counter-propagating laser beams [10]. This gives rise to a standing wave

$$V(\mathbf{r}) = \sum_{\sigma} \frac{V_0}{4} \sin^2(k_{\sigma}\sigma),\tag{2.8}$$

where $\sigma = \{x, y, z\}$ labels the different direction, $k_{\sigma} = 2\pi/\lambda_{\sigma}$ is the wave number of the laser in the direction σ and $V_0 = \hbar\Omega_0^2/4\Delta$. From here on, unless stated otherwise, all the periodic potentials are sinusoidal potentials, as in Eq. (2.8). In this context, any of the inverse wave vectors $l_{\sigma} = k_{\sigma}^{-1} = \lambda_{\sigma}/2\pi$ provide a natural choice for parametrizing the length scale,⁸ and any of the recoil energies $E_r^{\sigma} = \hbar^2 k_{\sigma}^2/2m$ (for an atom of mass m) provides a natural choice for fixing the energy scale.

A final disclaimer is in order: Whenever the words “dimensionless” and “position” appear together, we mean that position is scaled in terms of one of the l_{σ} . Whenever

⁴That is, the bare energies plus the Stark shifts.

⁵Dissipative processes involve spontaneous emission, that can be neglected in the large detuning case since excited states have vanishingly probability of being populated.

⁶That is, if $\Omega = \Omega(\mathbf{r})$.

⁷As a sidenote, we notice that this relies on the assumption of adiabatic motion of the atoms and therefore, outside the very low temperature regime, this derivation should include corrections.

⁸Notice that the size of each site in a 1D lattice taken in the direction σ , for example, is $\lambda_{\sigma}/2$, which is typically of the order of 400 nm. For comparison, the typical size of the cells in solid state is of the order of Ångströms.

“dimensionless” comes together with “energy”, the energies are scaled in terms of one of the E_r^σ , for the direction σ to be specified. $1D$, $2D$ and $3D$ are used to denote one, two and three dimensions, respectively.

2.2 Single Particles in Periodic Potentials

Two main properties characterize the problem of a quantum particle interacting with a periodic potential [11, 12]: (i) that the energy spectrum displays a band structure, where regions with allowed energies are separated by forbidden gaps, and (ii) that the solutions of the eigenvalue equation are given by *Bloch functions*. This is formulated in one dimension⁹ (1D) as

$$\hat{H}\Psi(x) = E\Psi(x), \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m}\partial_x^2 + V(x) \quad (2.9)$$

with m the mass of the particle and $V(x) = V(x + d)$ the periodic potential with periodicity d . The expression for the Bloch functions can be obtained from the Bloch theorem [12] and is given by

$$\Psi_{\nu,q}(x) = e^{iqx} u_{\nu,q}(x), \quad (2.10)$$

where $u_{\nu,q}$ is a periodic function satisfying $u_{\nu,q}(x) = u_{\nu,q}(x + d)$. q and ν are good quantum numbers labeling, respectively, quasi-momentum and band index, and the use of ν implicitly assumes the reduced scheme where quasi-momentum $q \in [-\pi/d, \pi/d]$ varies in the first *Brillouin zone* [12]. To each of the values of ν and q there is an associated energy, and in general the relation between the free particle momentum and the quasi-momentum q appears in the form of a complicated (transcendental) equation.¹⁰ Nevertheless, the eigenstates of Eq. (2.9) are plane waves (delocalized in the lattice) that experience a modulation due to the lattice periodicity.

As an alternative to Bloch functions, a basis that is commonly used for describing particles interacting with periodic potentials is given by the *Wannier functions* [11]. They are constructed in terms of the Bloch functions according to the prescription

$$w_{\nu,j}(x) = \sum_q e^{-iqR_j} \Psi_{\nu,q}(x), \quad (2.11)$$

⁹Extensions to other dimensions are straightforward. We use the $1D$ case here just as an illustration.

¹⁰This is already the case in the simplest example, of the Kronig–Penney problem with a repulsive potential constructed from equally spaced δ -functions (see, e.g. [12, 13] for an application in the context of many-body physics in optical lattices).

where R_j labels the coordinates of the j th site and the sum runs over the quasi-momenta in the first Brillouin zone. The Wannier basis differs from the Bloch basis in two main aspects [11]: First, the prescription given by Eq. (2.11) implies that each of the lattice sites accommodates only one Wannier function with band index ν . Second, this is a site localized basis labeled by the band index and the position in the lattice. Since Wannier functions are not the eigenstates of Eq. (2.9), quasi-momentum is not a good quantum number to be used as a label here. Nevertheless, Wannier functions at different sites satisfy the following orthonormality condition in its quantum numbers

$$\int dx w_{\nu,j}(x) w_{\nu',i}(x) = \delta_{\nu\nu'} \delta_{ij}. \quad (2.12)$$

We will illustrate further properties of these systems by considering results obtained from numerical diagonalization of the *Mathieu equation* for a particle in a sinusoidal potential, Eq. (2.9), where

$$V(x) = V_0 \sin^2(k_x x), \quad (2.13)$$

and V_0 is the lattice amplitude.

The band structure in Fig. 2.1 immediately reveals that increasing values of V_0 are associated with larger energy gaps and band energies of smaller widths. This should be the case, because the size of the energy gap is proportional to the absolute value of the reflection coefficient in the barrier [12], which is larger for larger V_0 . In the same way, the width of the band is proportional to the absolute value of the transmission

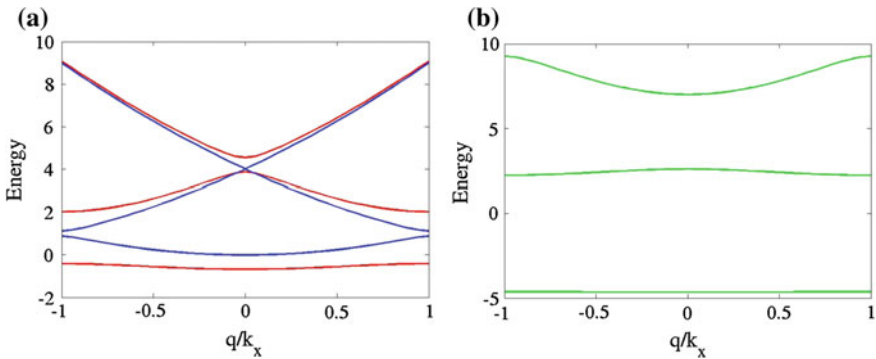


Fig. 2.1 Band structure of a system with $V_0 = 0.5E_r$ (blue), $V_0 = 5E_r$ (red) and $V_0 = 17E_r$ (green). As discussed in the text, the widths of the bands are larger for smaller values of the lattice amplitude. In addition, the energy gaps between the different bands increase for increasing values of V_0 (Color figure online)

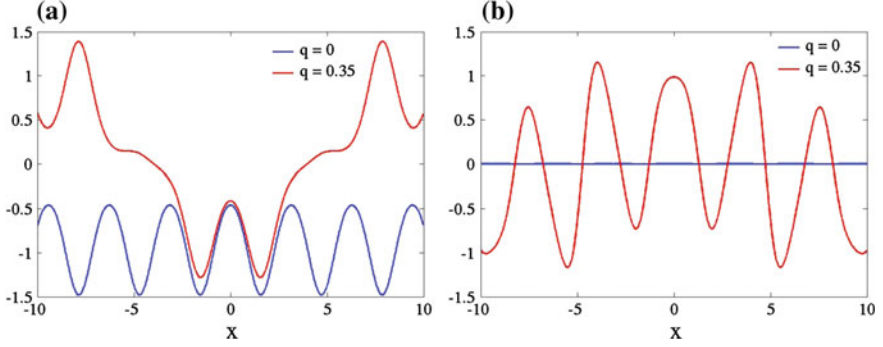


Fig. 2.2 **a** Real part of the Bloch functions of the first and **b** second bands for different values of quasi-momentum q and for $V_0 = 5E_r$. Notice here that the Bloch function of the 2nd band is strictly imaginary if $q = 0$

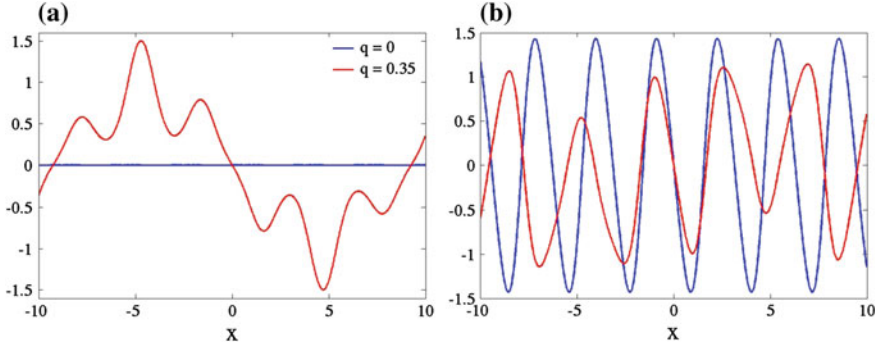


Fig. 2.3 Imaginary part of the Bloch functions of the first (in **a**) and second (in **b**) bands for different values of quasi-momentum q and for $V_0 = 5E_r$. The parameters of the color scheme in **(b)** are identical to the ones used in **(a)**. In contrast to the result of Fig. 2.2, here we notice that the 1st band Bloch function with $q = 0$ is strictly real. We point out that there is an arbitrary phase to be fixed in the definition of the Bloch functions. Once this phase is fixed, however, and say, the Bloch function of the first band with $q = 0$ is purely real, then the Bloch function in the second band with $q = 0$ will be purely imaginary

coefficient [12], which is smaller for larger values of V_0 .¹¹ Furthermore, the narrowing down of the band widths can be alternatively understood from the viewpoint of an *effective mass*, that is defined from the inverse of the band curvature. Namely, flatter bands are related to heavier effective masses and therefore reduced mobility in the lattice, whereas the contrary is valid for steeper bands [12].

We compare samples of the Bloch and Wannier functions of the first and second bands in Figs. 2.2, 2.3 and 2.4, for different values of V_0 , where the delocalized versus localized character of the Bloch versus Wannier functions can be immediately

¹¹For a more detailed discussion about how the transmission and reflection coefficients of the barrier are related to the size of the energy gaps and energy widths, see Exercise 1 (f) and (g) of Chap. 8 of Ashcroft and Mermin, Ref. [12].

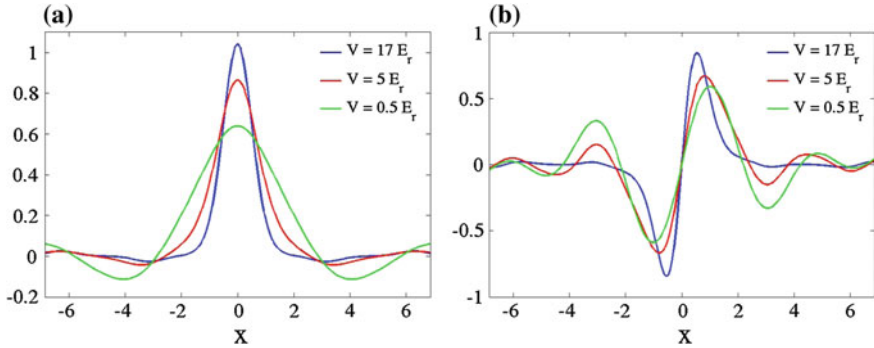


Fig. 2.4 Wannier functions of the first (a) and second (b) bands for systems with $V_0 = 0.5E_r$ (green), $V_0 = 5E_r$ (red) and $V_0 = 17E_r$ (blue). Notice that the Wannier functions are not positive definite. This is necessary in order to satisfy the orthonormality relation of Eq. (2.12) (Color figure online)

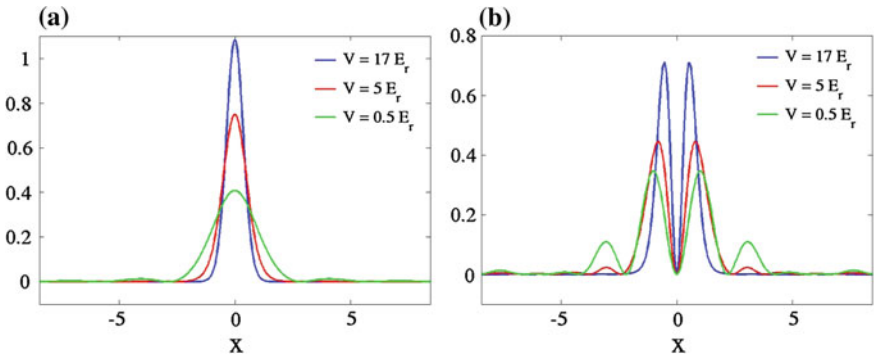


Fig. 2.5 Probability density of the first and second bands Wannier functions for systems with $V_0 = 0.5E_r$ (green), $V_0 = 5E_r$ (red) and $V_0 = 17E_r$ (blue) (Color figure online)

noticed. As for the Wannier functions, increasing values of the potential amplitude V_0 promote a faster decay from the position at the minimum of the potential, yielding Wannier functions that are more localized at each site. For completeness the probability density associated to each of these Wannier functions is given in Fig. 2.5a, b.

2.3 Meet the Orbital States!

In the context of optical lattices, *orbital states* are site-localized states in excited energy bands [1]. The first excited bands form the *p*, whereas the second excited bands form the *d* band. Accordingly, they have the associated *p* and *d* orbitals [1].

In isotropic square and cubic lattices in $2D$ and $3D$, respectively, excited bands have an intrinsic degeneracy that gives rise to a degeneracy between the orbitals [1]. In particular, orbital states are anisotropic in magnitude and in some cases also in parity [14]. In this section, we characterize the properties of the systems in the p and d bands.

2.3.1 Orbital States in the Harmonic Approximation

In order to become more familiar with the physics in excited bands, we consider the system in the *harmonic approximation*. This consists in approximating each well of the sinusoidal potential with a harmonic potential, i.e., $V(x) = \sin^2(k_x x) \approx k_x^2 x^2$, and therefore exact solutions are easily obtained and simple enough to expose properties of the physics in analytical terms. We notice, however, that the harmonic approximation is justified only in very particular cases¹² [15, 16] and that its quantitative predictions are otherwise very limited¹³ [2, 15]. Nevertheless, we use it here to construct an intuitive picture of the orbital states.

Let us then consider the eigenvalue problem in a $2D$ separable lattice,¹⁴

$$\hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\partial_x^2 + V_x \sin^2(k_x x) - \frac{\hbar^2}{2m}\partial_y^2 + V_y \sin^2(k_y y) \right) \Psi = E\Psi, \quad (2.14)$$

where V_σ and k_σ , $\sigma = \{x, y\}$ are the potential amplitude and wave vector in the direction σ . We also rescale the variables with k_y^{-1} to obtain the dimensionless positions $k_y y \rightarrow y'$ and $k_y x \rightarrow x'$, and with $E_r = \hbar^2 k_y^2 / 2m$ to obtain dimensionless energies $\tilde{V}_\sigma = V_\sigma / E_r$, and expand the potential around its minimum keeping only first order contributions. This yields,

$$\frac{\hat{H}}{E_r}\Psi = \left(-\partial_{x'}^2 + \tilde{V}_x \frac{k_x^2}{k_y^2} x'^2 - \partial_{y'^2}^2 + \tilde{V}_y y'^2 \right) \Psi. \quad (2.15)$$

Since we are dealing with the case of a separable lattice, it is possible to find the solutions in the x - and y -directions by solving each of the equations independently. We start by solving the equation for y' ,

$$\left(-\partial_{y'}^2 + \tilde{V}_y y'^2 \right) \Psi(y') = \epsilon_{y'} \Psi(y'), \quad (2.16)$$

¹²The limit of very deep potential wells is required, for example.

¹³In fact, as we discuss later in greater details, the harmonic approximation can lead to misleading conclusions in the many-body system.

¹⁴By separable lattice we mean that the dynamics of different directions is decoupled.

from where we identify the characteristic length of the oscillator $y_0^{-4} = \tilde{V}_y$. The ground, first and second excited states, with corresponding energies $\epsilon_{y'}^0$, $\epsilon_{y'}^1$ and $\epsilon_{y'}^2$, are given by

$$\phi_0(y') = \mathcal{N}_0(y_0) e^{-y'^2/2y_0^2} = \mathcal{N}_0(\tilde{V}_y^{-1/4}) e^{-\sqrt{\tilde{V}_y} y'^2/2}, \quad (2.17)$$

$$\phi_1(y') = \mathcal{N}_1(y_0) y' e^{-y'^2/2y_0^2} = \mathcal{N}_1(\tilde{V}_y^{-1/4}) y' e^{-\sqrt{\tilde{V}_y} y'^2/2}, \quad (2.18)$$

and

$$\phi_2(y') = \mathcal{N}_2(y_0) (y'^2 - 1) e^{-y'^2/2y_0^2} = \mathcal{N}_2(\tilde{V}_y^{-1/4}) (y'^2 - 1) e^{-\sqrt{\tilde{V}_y} y'^2/2}, \quad (2.19)$$

with the normalization factors

$$\mathcal{N}_0(z) = \left(\frac{1}{\pi^{1/4} z^{1/2}} \right), \quad (2.20)$$

$$\mathcal{N}_1(z) = \left(\frac{\sqrt{2}}{\pi^{1/4} z^{3/2}} \right), \quad (2.21)$$

and

$$\mathcal{N}_2(z) = \left(\frac{1}{\pi^{1/2} \left(\frac{3}{4} z^5 - z^3 + z \right)^{1/2}} \right). \quad (2.22)$$

The equations for x' are solved in the same way, but since the scaling has been taken with respect to the dynamics in the y direction, the characteristic length of the oscillator is given here by $x_0^{-4} = \tilde{V}_x k_x^2 / k_y^2$. The expression of the wave-functions of the ground and excited states, with energies $\epsilon_{x'}^0$, $\epsilon_{x'}^1$ and $\epsilon_{x'}^2$ follow as

$$\phi_0(x') = \mathcal{N}_0(x_0) e^{-x'^2/2x_0^2} = \mathcal{N}_0(\tilde{V}_x^{-1/4} (k_x/k_y)^{-1/2}) e^{-\frac{\sqrt{\tilde{V}_x k_x}}{k_y} x'^2/2}, \quad (2.23)$$

$$\phi_1(x') = \mathcal{N}_1(x_0) x' e^{-x'^2/2x_0^2} = \mathcal{N}_1(\tilde{V}_x^{-1/4} (k_x/k_y)^{-1/2}) x' e^{-\frac{\sqrt{\tilde{V}_x k_x}}{k_y} x'^2/2}, \quad (2.24)$$

and

$$\phi_2(x') = \mathcal{N}_2(x_0) (x'^2 - 1) e^{-x'^2/2x_0^2} = \mathcal{N}_2(\tilde{V}_x^{-1/4} (k_x/k_y)^{-1/2}) (x'^2 - 1) e^{-\frac{\sqrt{\tilde{V}_x k_x}}{k_y} x'^2/2}. \quad (2.25)$$

With the expressions of the eigenfunctions at hand, we can now describe the energy levels and eigenstates of the 2 dimensional system in the harmonic approximation. For simplicity we consider from now on an isotropic lattice for which $\tilde{V}_x = \tilde{V}_y$ and $k_x = k_y$. The true ground state within this approximation has energy $E_0 = (\epsilon_{x'}^0 + \epsilon_{y'}^0)$ and its eigenfunction has a Gaussian profile in both the x and y directions:

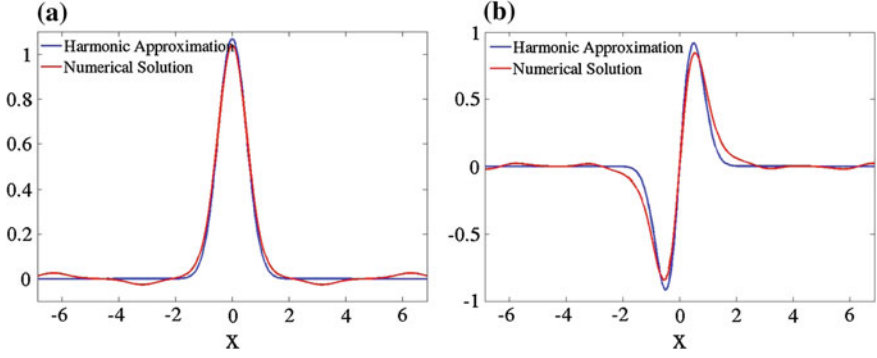


Fig. 2.6 Comparison between the numerically obtained Wannier functions and the Wannier functions in the harmonic approximation, Eqs. (2.17) and (2.19), for a 1D system with $V_0 = 17E_r$ (see discussion in the text)

$$\Psi_0(x', y') = \mathcal{N}_0(x_0)\mathcal{N}_0(y_0)e^{-x'^2/2x_0^2 - y'^2/2y_0^2}. \quad (2.26)$$

***p*-Orbital States in the Harmonic Approximation**

The first excited state is doubly degenerate. It has energy given by $E_1 = (\epsilon_x^1 + \epsilon_y^0) = (\epsilon_x^0 + \epsilon_y^1)$ and the corresponding eigenfunctions are

$$\Psi_x(x', y') = \mathcal{N}_1(x_0)\mathcal{N}_0(y_0)x' e^{-x'^2/2x_0^2 - y'^2/2y_0^2} \quad (2.27)$$

and

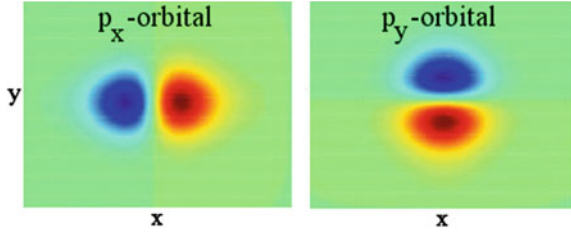
$$\Psi_y(x', y') = \mathcal{N}_0(x_0)\mathcal{N}_1(y_0)y' e^{-x'^2/2x_0^2 - y'^2/2y_0^2}, \quad (2.28)$$

respectively. These are the *p*-orbital states¹⁵! As can be verified, the different directions are characterized by different parities, i.e., the spatial profile of the different orbitals are odd in the direction of the label α , in which the wave-function has a node, and even in the perpendicular direction. From here on, we denote the orbital states in the *p* band by p_α , with α referring to a spatial direction.

In Fig. 2.6 we compare the ground and first excited Wannier functions obtained from numerical diagonalization of the Mathieu equation with the ground and first excited states obtained in the harmonic approximation. It illustrates the situation where $V_0 = 17E_r$, which represents a lattice with rather deep wells. This can be seen from the characteristic flatness of the bands in Fig. 2.1, and the harmonic approximation is expected to give a good qualitative picture of the system. In addition, in Fig. 2.7 we show the p_x and p_y orbitals obtained from diagonalization of the Math-

¹⁵These expressions are valid only in the harmonic approximation. The qualitative features, however, are still valid in the general case.

Fig. 2.7 *Left and right panels show the p_x - and the p_y -orbital states, obtained from diagonalization of the Mathieu equation*



ieu equation. Notice, however, the important difference that the energy bands are not equally spaced in sinusoidal lattices, as will always be the case in the harmonic approximation. This property has important consequences as we will discuss later in Sect. 2.6, since it helps improving the stability in experimental realizations of the many-body system in the p band [17].

d -orbital States in the Harmonic Approximation

We continue with the second excited state, which is triply degenerate in $2D$. It has energy given by $E_2 = (\epsilon_{x'}^2 + \epsilon_{y'}^0) = (\epsilon_{x'}^0 + \epsilon_{y'}^2) = (\epsilon_{x'}^1 + \epsilon_{y'}^1)$ and the corresponding eigenfunctions are given, respectively, by

$$\Psi_{x^2}(x', y') = \mathcal{N}_2(x_0)\mathcal{N}_0(y_0)(x'^2 - 1)e^{-x'^2/2x_0^2 - y'^2/2y_0^2}, \quad (2.29)$$

$$\Psi_{y^2}(x', y') = \mathcal{N}_0(x_0)\mathcal{N}_2(y_0)(y'^2 - 1)e^{-x'^2/2x_0^2 - y'^2/2y_0^2} \quad (2.30)$$

and

$$\Psi_{xy}(x', y') = \mathcal{N}_1(x_0)\mathcal{N}_1(y_0)x'y'e^{-x'^2/2x_0^2 - y'^2/2y_0^2}. \quad (2.31)$$

Now meet the d -orbitals¹⁶! In analogy to the p -orbital system, from here on we use d_{x^2} , d_{y^2} and d_{xy} to denote the states in the d band. As illustrated in Fig. 2.8, these wave-functions are also labeled after the direction of the node, and the superscript refers to the existence of two nodes. In particular, the d_{xy} orbital has one node in both directions.

As a final remark, we notice that the use of the harmonic approximation might be very dangerous when describing the system in the d band [4]. As shown in Fig. 2.9, the anharmonicity of the sinusoidal lattice is capable of breaking the three-fold degeneracy suggested in analogy with the $2D$ harmonic oscillator, such that the d_{xy} orbital has slightly higher energy. The implications for the many-body system are studied in Sect. 3.2.

¹⁶In the same way as for the p orbitals, although these expressions are only valid in the harmonic approximation, the qualitative features of the states remain valid in the general case.

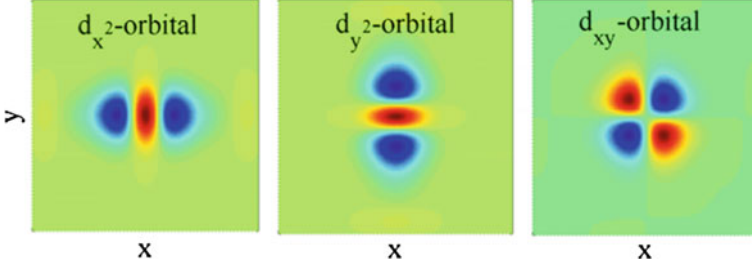
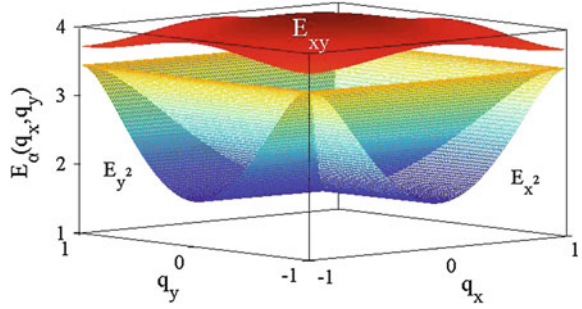


Fig. 2.8 Left, center and right panels show the d_{x^2} -, d_{y^2} - and the d_{xy} -orbital states, obtained from numerical diagonalization of the Mathieu equation

Fig. 2.9 The three d bands; $E_{x^2}(q_x, q_y)$, $E_{y^2}(q_x, q_y)$ and $E_{xy}(q_x, q_y)$ obtained from numerical diagonalization of the Mathieu equation for the potential with amplitude $V_x = V_y = 20E_r$



2.4 From One to Many: Many-Body Systems in Excited Bands

In general terms, the dynamics of a gas of N atoms of mass m can be represented by a Hamiltonian of the type

$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m} - V_{\text{ext}}(\mathbf{r}_i) \right) + V_{\text{int}}(\{\mathbf{r}_i, \mathbf{r}_j\}), \quad (2.32)$$

where the first term describes single-particle contributions including effects of an external potential V_{ext} , and the second term describes interactions between the atoms—thereby accounting for the effects of collective nature.

In the ideal scenario, V_{int} should include all interactions in the system, i.e., that appear from the result of two-body collisions, three-body collisions and so on.¹⁷ In real life, however, exact solutions for problems involving interacting many-body quantum particles are known only in very few or particular cases.¹⁸ The way out, therefore, involves the use of approximations that are capable of accounting not

¹⁷“Ambition is the last refugee of failure”—Oscar Wilde.

¹⁸When it happens, its almost like finding a unicorn.

for all, but for all the relevant interactions required for a good description of the experimental reality.

Recall that our interest is the physics of (many and also a few) interacting atoms in excited bands of optical lattices. We therefore aim at describing systems of very cold and dilute gases, where the atoms occupy the orbital states discussed in Sect. 2.4. By “very cold” we mean that the temperatures considered are close to the absolute zero.¹⁹ By “very dilute” we mean that the distance between any two atoms fixed by $n = N/V$ —where N is the total number of particles and V the volume of the system—is very large.²⁰ In the lab, for example, these systems are produced with densities²¹ of the order of 10^{15} atoms per cm^3 . Under these circumstances, it is reasonable to truncate the interaction term to the two-body part [18, 19].

Due to the characteristic low densities, the distances between the particles are always large enough to justify the use of the asymptotic expression of the wave function of the relative motion [19]. In addition, as a consequence of the low temperatures T , the relative momentum corresponding to kinetic energies $k_B T$, where k_B is the Boltzmann constant, justifies that the collisions are effectively described by s -wave scattering processes, that are completely characterized by the corresponding phase shift [20]. At very low temperatures, however, the phase shift is not the best parameter for characterizing the cross section of the scattering processes.

The reason why this is the case can be illustrated²² by considering the (differential) cross section σ of two particles in a state with relative momentum $\mathbf{k}$ and energy $\hbar^2 k^2 / 2\mu$, where μ is the reduced mass:

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2(\delta_0(k))}{k^2} \xrightarrow{k \rightarrow 0} a^2, \quad (2.33)$$

with $\delta_0(k)$ the phase shift and a a quantity with dimensions of length. Since at very low temperatures $\lim k \rightarrow 0$, the presence of k^2 in the denominator of Eq. (2.33) would require that $\sin(\delta_0(k))$ vanishes linearly for any value of the cross section [20].

The trick here is to use instead the *scattering length* a defined as

$$\lim_{k \rightarrow 0} \frac{k}{\sin(\delta_0(k))} \equiv -\frac{1}{a}, \quad (2.34)$$

that is, up to the choice of a sign, exactly the same length parameter in Eq. (2.33). Now this is a good quantity for parametrizing the low energy scattering cross section, for it can also be further interpreted as the first term of the expansion in powers of k of the effective range expansion [20],

$$k \cot(\delta_0(k)) \equiv -\frac{1}{a} + \frac{r_0}{2} k^2 + \dots, \quad (2.35)$$

¹⁹Or much less than the bandwidth. The temperature is typically of the order of ~ 1 nK.

²⁰Compared to the scattering length, as we discuss next.

²¹For comparison, the density of air at room temperature is $\sim 1.25 \times 10^{-3} \text{ g/cm}^3$, the density of water is 1 g/cm^3 and the density of a white dwarf can be estimated as $1.3 \times 10^6 \text{ g/cm}^3$ [18].

²²This argument is based on the discussion presented in Ref. [20].

where r_0 is the so called *effective range* of the potential. In these terms, low energy scattering processes can be characterized by only two parameters,²³ a and r_0 .

The values of a are determined with the standard scattering theory. Now assuming that a is a known quantity, the Hamiltonian (2.32) is implemented in terms of an effective interaction that we assume can capture the physics seen in the lab. We consider here that $V_{int}(\mathbf{r}_i, \mathbf{r}_j)$ describes short-range (contact) interactions, $V_{int} = g\delta(\mathbf{r}_i - \mathbf{r}_j)$, with coupling constant given by $g = 2\pi\hbar^2 a/\mu$, where μ is the reduced mass of the two particles [10]. Accordingly, the effective potential for two identical particles of mass m follows as

$$V_{int}(\mathbf{r}_i, \mathbf{r}_j) = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}_i - \mathbf{r}_j). \quad (2.36)$$

In the language of second quantization, this can be further re-written with the field operators $\hat{\Psi}(\mathbf{r})$ and $\hat{\Psi}^\dagger(\mathbf{r})$, that annihilate and create a particle of mass m at position $\mathbf{r}$ as

$$\hat{V}_{int} = \frac{4\pi\hbar^2 a}{m} \int d\mathbf{r}' d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}^\dagger(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}') = \frac{4\pi\hbar^2 a}{m} \int d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}'). \quad (2.37)$$

If the system is composed of bosonic atoms, the operators satisfy the commutation relations $[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$. If the atoms are fermions, then $\{\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}')$. Therefore, the full expression of the Hamiltonian describing the weakly-interacting many-body system is given by

$$\hat{H} = \int d\mathbf{r}' \left\{ \hat{\Psi}^\dagger(\mathbf{r}') \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}') \right] \hat{\Psi}(\mathbf{r}') + \frac{\tilde{U}_0}{2} \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}') \right\}, \quad (2.38)$$

where $V(\mathbf{r}')$ accounts for the effects of external potentials superimposed to the system, and the coupling constant $\tilde{U}_0 = 4\pi\hbar^2 a/m$.

We will now expand the field operators in terms of the orbital states of the p and d bands of the sinusoidal optical lattice²⁴

$$V_{latt}(\mathbf{r}) = \sum_{\sigma} \tilde{V}_{\sigma} \sin^2(\sigma') \quad (2.39)$$

in 3D and 2D, respectively, and with σ the corresponding directions. We assume for the moment that no other external potential is present in the system and therefore we take $V(\mathbf{r}') = V_{latt}(\mathbf{r}')$ in Eq. (2.32).

²³In fact, regardless of formal expressions, any two potentials that are characterized by the same s -wave scattering length a and effective range interaction r_0 will give rise to the same effective interaction.

²⁴Since we will restrict the atoms to live in the corresponding band, we are also assuming the *single-band approximation*.

In these terms, the expression of the field operators follows as

$$\begin{aligned}\hat{\Psi}^\dagger(\mathbf{r}) &= \sum_{\alpha,j} w_{\alpha,j}^*(\mathbf{r}) \hat{a}_{\alpha,j}^\dagger(\mathbf{r}) \\ \hat{\Psi}(\mathbf{r}) &= \sum_{\alpha,j} w_{\alpha,j}(\mathbf{r}) \hat{a}_{\alpha,j}(\mathbf{r}),\end{aligned}\tag{2.40}$$

where $\hat{a}_{\alpha,j}^\dagger$ and $\hat{a}_{\alpha,j}$ create and annihilate an atom in an orbital state $w_{\alpha,j}(\mathbf{r})$, taken here as the lattice Wannier function in the j th site of the lattice ($\mathbf{j} = (j_x, j_y, j_z)$, $j_x, j_y, j_z \in \mathcal{N}$). We will use $\alpha = \{x, y, z\}$ whenever studying the p -band system with the p_α -orbital states in the 3D lattice; and $\alpha = \{x^2, y^2, xy\}$ whenever studying the d -band system in 2D.

As an additional point, let us stress here that the orbital states are not eigenstates of the single-particle Hamiltonian. We illustrate this by considering the explicit expression of the p -orbital wave-functions of a separable lattice, constructed with the site-localized Wannier functions,²⁵ $w_{\nu,j}(\alpha)$, with $\nu = 1, 2$ and α a spatial direction,²⁶ that are given by

$$\begin{aligned}w_{x,j}(\mathbf{r}) &= w_{2,j_x}(x)w_{1,j_y}(y)w_{1,j_z}(z) \\ w_{y,j}(\mathbf{r}) &= w_{1,j_x}(x)w_{2,j_y}(y)w_{1,j_z}(z) \\ w_{z,j}(\mathbf{r}) &= w_{1,j_x}(x)w_{1,j_y}(y)w_{2,j_z}(z).\end{aligned}\tag{2.41}$$

Now recall that the eigenstates of the single-particle Hamiltonian are Bloch functions (see Eq. (2.10)), and that the relation between Bloch and Wannier functions is given by

$$w_{\nu,\mathbf{R}_j}(\mathbf{r}) = \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}_j} \phi_{\nu,\mathbf{q}}(\mathbf{r}),$$

where we use $\mathbf{R}_j = (x_j, y_j, z_j) = (\pi j_x, \pi j_y, \pi j_z)$ and $\mathbf{q} = (q_x, q_y, q_z)$ is the index which labels the quasi-momentum.

2.4.1 The Many-Body System in the p Band

The Bosonic Case

After inserting (2.40) in Eq. (2.38) and truncating the kinetic term to its leading contribution—the *tight-binding approximation*; and the interaction processes to happen only onsite, the Hamiltonian describing bosonic atoms in the p band of a 3D optical lattice is given by

$$\hat{H}_B = \hat{H}_0 + \hat{H}_{nn} + \hat{H}_{nn'} + \hat{H}_{OD}.\tag{2.42}$$

²⁵Which themselves are also not eigenstates of the single-particle Hamiltonian.

²⁶Our notation here assumes that ν is the index which labels the energy band from which the Wannier function is computed.

The first term is the free Hamiltonian

$$\hat{H}_0 = - \sum_{\sigma, \alpha} \sum_{\langle i, j \rangle_{\sigma}} t_{\sigma}^{\alpha} (\hat{a}_{\alpha, i}^{\dagger} \hat{a}_{\alpha, j} + \hat{a}_{\alpha, j}^{\dagger} \hat{a}_{\alpha, i}), \quad (2.43)$$

that describes the nearest neighbour tunneling of atoms in the p_{α} -orbital state, $\alpha = \{x, y, z\}$, in the direction $\sigma = \{x, y, z\}$. Notice the absence of tunneling events with change of orbital state: Such processes are excluded by parity selection rules.²⁷

The second and third terms of Eq. (2.42) describe different types of density–density interactions:

$$\hat{H}_{nn} = \sum_{\alpha} \sum_i \frac{U_{\alpha\alpha}}{2} \hat{n}_{\alpha, i} (\hat{n}_{\alpha, i} - 1), \quad (2.44)$$

between atoms in the same orbital state, with $\hat{n}_{\alpha, i} = \hat{a}_{\alpha, i}^{\dagger} \hat{a}_{\alpha, i}$; and

$$\hat{H}_{nn'} = \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i U_{\alpha\beta} \hat{n}_{\alpha, i} \hat{n}_{\beta, i}, \quad (2.45)$$

$\beta = \{x, y, z\}$, between atoms in different orbital states.

Finally, the last term

$$\hat{H}_{OD} = \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i \frac{U_{\alpha\beta}}{4} (\hat{a}_{\alpha, i}^{\dagger} \hat{a}_{\alpha, i}^{\dagger} \hat{a}_{\beta, i} \hat{a}_{\beta, i} + \hat{a}_{\beta, i}^{\dagger} \hat{a}_{\beta, i}^{\dagger} \hat{a}_{\alpha, i} \hat{a}_{\alpha, i}) \quad (2.46)$$

describes interactions that transfer atoms within different types of orbital states.

The expression for the tunneling amplitude in the direction σ is given in terms of the orbital states by

$$t_{\sigma}^{\alpha} = - \int d\mathbf{r} w_{\alpha, j}^*(\mathbf{r}) [-\nabla^2 + V(\mathbf{r})] w_{\alpha, j+1_{\sigma}}(\mathbf{r}), \quad (2.47)$$

and due the different curvatures of the excited bands in the directions perpendicular ($\perp$) and parallel ($\parallel$) to the label of the orbital wave functions, $t_{\perp} t_{\parallel} < 0$, where $t_{\perp}$ and $t_{\parallel}$ refer to the tunnelings in the corresponding directions. In the same way, the expression of the interaction coefficients is given by

$$U_{\alpha\beta} = U_0 \int d\mathbf{r} |w_{\alpha, j}(\mathbf{r})|^2 |w_{\beta, j}(\mathbf{r})|^2. \quad (2.48)$$

As a final remark we recall that in the bosonic case $[\hat{a}_{\alpha, i}, \hat{a}_{\beta, j}^{\dagger}] = \delta_{\alpha\beta} \delta_{ij}$.

²⁷In the separable lattices considered here. This needs not to be the case in different setups.

Symmetries of the Many-Body Bosonic System in the p Band

Because each term in Eq. (2.42) has the same number of creation and annihilation operators, the Hamiltonian is clearly invariant under global $U(1)$ transformations. This reflects the overall conservation of particle number in the system, and therefore

$$[\hat{H}, \sum_j (n_j^x + \hat{n}_j^y + \hat{n}_j^z)] = 0. \quad (2.49)$$

Here, however, the key ingredient that distinguishes the dynamics in the p band from the systems in the ground band, is the presence of processes that transfer atoms between different orbital states, Eq. (2.46). Although a similar term is present in the Hamiltonian describing spinor Bose–Einstein condensates, its relative strength compared to other processes is typically very small, such that these contributions can be safely neglected [3]. This is not the case for the p -band system, because the coupling constant of orbital changing processes is exactly the same as the one of mixed density–density interactions defined in Eq. (2.45). Furthermore, the presence of orbital changing processes implies that instead of a $U(1) \times U(1) \times U(1)$ global symmetry, the dynamics of bosonic atoms in the p band has a $U(1) \times Z_2 \times Z_2$ global symmetry, and therefore total population of each of the orbital states is conserved only modulo 2 [1]. This has also fundamental implications on the establishment of long-range phase coherence in the system, because the presence of Z_2 (discrete) symmetries violate the assumptions of the *Hohenberg–Mermin–Wagner theorem* [21, 22]. As a consequence, this system is not prohibited of (long-range) ordering even in low dimensions, and therefore the existence of a true condensate in the thermodynamic limit is not precluded for bosons in the p band.

We also notice that in isotropic lattices²⁸ transformations of the type

$$\hat{a}_{\alpha,j} \rightleftharpoons \pm \hat{a}_{\beta,j} \quad (2.50)$$

leave the Hamiltonian invariant for any permutation of α and β . Moreover, these lattices feature additional Z_2 symmetries, associated to the swapping of any two orbital states, followed by a change of indices in the lattice, i.e.,

$$\begin{aligned} \hat{a}_{\alpha,j} &\rightarrow \hat{a}_{\beta,j'} \\ \hat{a}_{\beta,j} &\rightarrow \hat{a}_{\alpha,j'}, \end{aligned} \quad (2.51)$$

where the $\mathbf{j} = (j_x, j_y, j_z)$ indices become $j_\alpha \rightarrow j_\beta$ and $j_\beta \rightarrow j_\alpha$ in $\mathbf{j}'$.

Let us now take a closer look at the symmetries of the $2D$ lattice by considering the isotropic case, where $U_{xx} = U_{yy}$, $U_{xy} = U_{yx}$, $t_{\parallel}^x = t_{\parallel}^y$ and $t_{\perp}^x = t_{\perp}^y$. Here the rotation

²⁸Where $t_{\parallel}^\alpha = t_{\parallel}^\beta$ and $t_{\perp}^\alpha = t_{\perp}^\beta$ for $\alpha \neq \beta$ and $U_{xx} = U_{yy} = U_{zz}$ with again all the $U_{\alpha\beta}$ equal for $\alpha \neq \beta$.

$$\begin{pmatrix} \hat{a}_{x,j'} \\ \hat{a}_{y,j'} \end{pmatrix} \rightarrow \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \hat{a}_{x,j} \\ \hat{a}_{y,j} \end{pmatrix} \quad (2.52)$$

leaves the Hamiltonian invariant for different values of $\theta = (0, \pi/2, \pi) \pm k\pi$, where $k \in \mathbb{Z}$. This is not the case in asymmetric lattices, however, where even under the condition of orbital degeneracy the tunneling coefficients $t_{\parallel}^{\alpha} \neq t_{\parallel}^{\beta}$, $t_{\perp}^{\alpha} \neq t_{\perp}^{\beta}$. As a consequence, transformations of the type $\hat{a}_{x,j} \rightarrow \hat{a}_{y,j}$, $\hat{a}_{y,j} \rightarrow \hat{a}_{x,j}$ do not leave the Hamiltonian unaltered.

For asymmetric lattices there is a particular case for which the system contains an additional $SO(2)$ symmetry [16]. This corresponds to the harmonic approximation in the limit of vanishing tunneling,²⁹ where $U_{\alpha\alpha} = 3U_{\alpha\beta} = U$. As pointed out in Ref. [16], this special case is better studied with the angular-momentum like annihilation operators $\hat{a}_{\pm,j} = (\hat{a}_{x,j} \pm i\hat{a}_{y,j})/\sqrt{2}$, in terms of which the local part of the Hamiltonian can be written as [16]

$$\begin{aligned} \hat{H}_j = & \frac{U}{2} \left[\hat{n}_j \left(\hat{n}_j - \frac{2}{3} \right) - \frac{1}{3} \right] + \delta \left[(\hat{n}_j - 1)(\hat{L}_{+j} + \hat{L}_{-j}) \right] \\ & + \lambda \left[\frac{1}{4} \hat{L}_{z,j}^2 - 3(\hat{L}_{+j} - \hat{L}_{-j})^2 - \hat{n}_j \right], \end{aligned} \quad (2.53)$$

where $U = (U_{xx} + U_{yy})/2$, $\delta = (U_{xx} - U_{yy})/2$ and $\lambda = U_{xy} - U/3$. The density operator can be expressed as $\hat{n}_j = \hat{a}_{+j}^{\dagger} \hat{a}_{+j} + \hat{a}_{-j}^{\dagger} \hat{a}_{-j}$, and the angular momentum operators are $\hat{L}_{z,j} = \hat{a}_{+j}^{\dagger} \hat{a}_{+j} - \hat{a}_{-j}^{\dagger} \hat{a}_{-j}$ and $\hat{L}_{\pm,j} = \hat{a}_{\pm,j}^{\dagger} \hat{a}_{\mp,j}/2$. It follows from the properties of the harmonic oscillator eigenstates that in the harmonic approximation $\lambda = \delta = 0$ for any lattice configuration, and therefore $[\hat{H}_j, \hat{L}_{z,j}] = 0$ [16]. This is not the case for sinusoidal optical lattices, for there $\lambda, \delta \neq 0$ destroys the axial symmetry, and consequently $[\hat{H}_j, \hat{L}_{z,j}] \neq 0$ [16]. Notice, however, that rather than being of geometric character, this dynamical enhancement [23] of the $SO(2)$ symmetry appears entirely due to the specific form in which the eigenvalue problem can be rewritten in the harmonic approximation.³⁰

The Fermionic Case

Due to the *Pauli blockade* preventing the occupation of the same orbital state by more than one particle, fermionic atoms in the p band behave according to

$$\hat{H}_F = \hat{H}_0 + \hat{H}_{nn'}, \quad (2.54)$$

with $\hat{H}_0$ and $\hat{H}_{nn'}$ defined in Eqs. (2.43) and (2.45), respectively. Here, however, $\{\hat{a}_{\alpha,i}, \hat{a}_{\beta,j}\} = \delta_{\alpha\beta} \delta_{ij}$. The expressions for the tunneling elements and the various coupling constants are the same as in the bosonic case, defined in Eqs. (2.47) and (2.48).

Symmetries of the Many-Body Fermionic System in the p Band

Since Eq. (2.54) contains only number operators, the Hamiltonian of the fermionic system in the p band has the $U(1) \times U(1) \times U(1)$ symmetry. Accordingly, in addition

²⁹This is only valid in the case of separable lattices.

³⁰This is similar to the conservation of the *Laplace–Runge–Lenz vector* in Kepler problems (see e.g. Ref. [23]).

to a global $U(1)$ transformation, associated to conservation of total number in the system, it also conserves the number of particles in each of the orbital states.

To P or not to P? (bands!)

—William Shakespeare. Adapted from the tragedy of *Hamlet*.

2.4.2 The Many-Body System in the d Band

We obtain the many-body Hamiltonian describing bosonic atoms in the d band by following the same procedure adopted for treating the p -band system: We expand the field operators, Eq. (2.40), in terms of the orbital states of the d band for $\alpha = \{x^2, y^2, xy\}$,³¹ and assume the tight-binding and single-band approximations. The result is [4]

$$\hat{H} = \hat{H}^d + \hat{H}^{xy}, \quad (2.55)$$

where the first term describes the processes involving only the d_{x^2} - and d_{y^2} -orbital states, while the second term contains all the processes that involve the d_{xy} orbital. The two parts of the Hamiltonian can be decomposed further, according to the different types of processes:

$$\hat{H}^d = \hat{H}_0^d + \hat{H}_t^d + \hat{H}_{nn}^d + \hat{H}_{da}^d + \hat{H}_{od}^d \quad (2.56)$$

and

$$\hat{H}^{xy} = \hat{H}_0^{xy} + \hat{H}_t^{xy} + \hat{H}_{nn}^{xy} + \hat{H}_{da}^{xy} + \hat{H}_{od}^{xy}. \quad (2.57)$$

The first terms in each of these equations describe the onsite energies of the different orbitals E_α and E_{xy} , with $\alpha = \{x^2, y^2\}$,

$$\hat{H}_0^d = \sum_{\alpha} \sum_i E_{\alpha} \hat{n}_{\alpha,i}, \quad (2.58)$$

and

$$\hat{H}_0^{xy} = \sum_i E_{xy} \hat{n}_{xy,i}. \quad (2.59)$$

The second terms describe the tunneling processes,

$$\hat{H}_t^d = - \sum_{\sigma, \alpha} \sum_{\langle i,j \rangle_{\sigma}} \left(t_{\sigma}^{\alpha} \hat{d}_{\alpha,i}^{\dagger} \hat{d}_{\alpha,j} + H.c. \right) \quad (2.60)$$

³¹We denote the creation and annihilation operators for the states in the d band by $\hat{d}_{\alpha}^{\dagger}$ and $\hat{d}_{\alpha}$.

and

$$\hat{H}_t^{xy} = - \sum_{\sigma} \sum_{\langle i,j \rangle_{\sigma}} t^p \hat{d}_{xy,i}^{\dagger} \hat{d}_{xy,j}. \quad (2.61)$$

Notice here that while atoms in the d_{x^2} and d_{y^2} orbitals are characterized by anisotropic tunneling in the directions parallel ($\parallel$) and perpendicular ($\perp$) to the nodes of the orbital state, the d_{xy} -orbital atoms tunnel in both directions with the same magnitude, t^p . The expressions of the tunneling amplitudes are given below:

$$\begin{aligned} t_{\sigma}^{\alpha} &= - \int d\mathbf{r} w_{\alpha,i}^*(\mathbf{r}) [-\nabla^2 + V(\mathbf{r})] w_{\alpha,i+1_{\sigma}}(\mathbf{r}) \\ t^p &= - \int d\mathbf{r} w_{xy,i}^*(\mathbf{r}) [-\nabla^2 + V(\mathbf{r})] w_{xy,i+1_{\sigma}}(\mathbf{r}). \end{aligned} \quad (2.62)$$

In addition, as opposed to the situation in the p band, the parallel and perpendicular tunnelings in the d band satisfy $t_{\parallel}^{\alpha} t_{\perp}^{\alpha} > 0$. Furthermore, $t^p < 0$.

We turn now to the interacting part of the Eq. (2.55). It contains the density-density interactions, both between atoms in the same orbital, and in different orbital states,

$$\hat{H}_{nn}^d = \sum_{\alpha} \sum_i \frac{U_{\alpha\alpha}}{2} \hat{n}_{\alpha,i} (\hat{n}_{\alpha,i} - 1) + \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i U_{\alpha\beta} \hat{n}_{\alpha,i} \hat{n}_{\beta,i} \quad (2.63)$$

and

$$\hat{H}_{nn}^{xy} = \sum_i \frac{U_{pp}}{2} \hat{n}_{xy,i} (\hat{n}_{xy,i} - 1) + \sum_{\alpha} \sum_i 2U_{p\alpha} \hat{n}_{xy,i} \hat{n}_{\alpha,i}; \quad (2.64)$$

interactions that move population between the orbital states in pairs,³²

$$\hat{H}_{od}^d = \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i \frac{U_{\alpha\beta}}{4} \left(\hat{d}_{\alpha,i}^{\dagger} \hat{d}_{\alpha,i}^{\dagger} \hat{d}_{\beta,i} \hat{d}_{\beta,i} + \hat{d}_{\beta,i}^{\dagger} \hat{d}_{\beta,i}^{\dagger} \hat{d}_{\alpha,i} \hat{d}_{\alpha,i} \right) \quad (2.65)$$

and

$$\hat{H}_{od}^{xy} = \sum_{\alpha} \sum_i \left[\frac{U_{p\alpha}}{2} \left(\hat{d}_{xy,i}^{\dagger} \hat{d}_{xy,i}^{\dagger} \hat{d}_{\alpha,i} \hat{d}_{\alpha,i} + \hat{d}_{\alpha,i}^{\dagger} \hat{d}_{\alpha,i}^{\dagger} \hat{d}_{xy,i} \hat{d}_{xy,i} \right) + \sum_{\beta \neq \alpha} U_{n_{\alpha}\alpha\beta} \hat{d}_{\alpha,i}^{\dagger} \hat{d}_{\beta,i}^{\dagger} \hat{d}_{xy,i} \hat{d}_{xy,i} \right] \quad (2.66)$$

³²These are the same orbital-changing interactions of the p -band system.

and finally, the density-assisted processes that also transfer atoms, albeit without conserving any particle number apart from the total population, between the different orbital states:

$$\hat{H}_{da}^d = \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i U_{n_p \alpha \beta} \left(\hat{d}_{\alpha, i}^\dagger \hat{n}_{\alpha, i} \hat{d}_{\beta, i} + \hat{d}_{\beta, i}^\dagger \hat{n}_{\alpha, i} \hat{d}_{\alpha, i} \right) \quad (2.67)$$

and

$$\hat{H}_{da}^{xy} = \sum_{\alpha, \beta, \alpha \neq \beta} \sum_i 2U_{n_p \alpha \beta} \hat{d}_{\alpha, i}^\dagger \hat{n}_{xy, i} \hat{d}_{\beta, i}. \quad (2.68)$$

The various coupling constants are given by

$$\begin{aligned} U_{\alpha\beta} &= \frac{U_0}{2} \int d\mathbf{r} |w_{\alpha, i}(\mathbf{r})|^2 |w_{\beta, i}(\mathbf{r})|^2, \quad \alpha = (x, y, p), \quad \text{for } (x^2, y^2, xy), \\ U_{n_\alpha \alpha \beta} &= \frac{U_0}{2} \int d\mathbf{r} |w_{\alpha, i}(\mathbf{r})|^3 |w_{\beta, i}(\mathbf{r})|, \quad \alpha = (x, y), \quad \text{for } (x^2, y^2), \\ U_{n_p \alpha \beta} &= \frac{U_0}{2} \int d\mathbf{r} |w_{xy, i}(\mathbf{r})|^2 |w_{\alpha, i}(\mathbf{r})| |w_{\beta, i}(\mathbf{r})|, \quad \alpha = (x, y), \quad \text{for } (x^2, y^2). \end{aligned} \quad (2.69)$$

Symmetries of the Many-Body Bosonic System in the d Band

Since each term in Eq. (2.55) contains the same number of operators and complex conjugates, the system is invariant under a global $U(1)$ phase transformation that is associated to the overall conservation of number in the system. As opposed to the bosonic system in the p band, however, the presence of density-assisted processes in the d band breaks the conservation of number modulo 2 in each of the orbital states. Therefore, the only symmetry left is the Z_2 symmetry associated to the swapping of the d_{x^2} and d_{y^2} orbital states, followed by the interchange of spatial indices. More explicitly, the many-body Hamiltonian (2.55) is invariant under the transformation

$$\begin{aligned} \hat{d}_{x^2, \mathbf{j}} &\rightarrow \hat{d}_{y^2, \mathbf{j}'} \\ \hat{d}_{y^2, \mathbf{j}} &\rightarrow \hat{d}_{x^2, \mathbf{j}'}, \end{aligned} \quad (2.70)$$

where $\mathbf{j} = (j_x, j_y)$ and $\mathbf{j}' = (j_y, j_x)$. In particular, since the t^p tunneling amplitude is isotropic in the different directions, $\hat{d}_{xy, \mathbf{j}} = \hat{d}_{xy, \mathbf{j}'}$.

To D or ..?

—Re-adapted.

2.5 How to Get There?

The novel features of the dynamics in excited bands, and in particular, the possibility of probing orbital selective phenomena in optical lattices [17], stimulated considerable experimental effort in recent years for exploring the physics beyond the ground band. Although nowadays we are provided with different techniques [24, 25] for loading atoms to higher bands, in this section we restrict the discussion to experiments with bosons, and to the ones of greatest relevance to the lattice configurations that are covered in this thesis.

2.6 Loading Atoms to the p Band—The Experiment of Müller et al.

As reported in the experiment of Müller et al. [17], bosonic atoms³³ can be loaded from the Mott insulator phase in the s band to the p band of optical lattices with stimulated *Raman transitions*.

The idea here is to use the interaction of a two-level atom with the laser light to couple different vibrational levels of a sinusoidal and separable 3D lattice potential. Deep in the Mott insulator phase, single sites can be approximated by harmonic potentials, and different vibrational levels in this potential correspond to the different bands of the optical lattice.

To illustrate how this happens, consider a Raman coupling between electronic atomic states of ^{87}Rb . These are two-photon processes where the two levels are coupled with an intermediate virtual state, far detuned from all the other states of the system [17]. Because of this intermediate coupling, implementation of Raman transitions requires the use of two different lasers, whose corresponding wave vectors we denote here by $\mathbf{k}_{L_1}$ and $\mathbf{k}_{L_2}$. In addition, since the photons carry momentum, this will also couple the vibrational levels that we call $|1\rangle$ and $|2\rangle$, with a matrix element given by

$$\frac{\Omega_1 \Omega_2^*}{\delta} \langle 2 | e^{i(\mathbf{k}_{L_1} - \mathbf{k}_{L_2}) \cdot \mathbf{x}} | 1 \rangle. \quad (2.71)$$

Ω_i are the Rabi frequencies between the $|i\rangle$ states, $i = 1, 2$ with another far detuned auxiliary state of this system, say $|aux\rangle$, and δ is the detuning between $|aux\rangle$ and the virtual intermediate state.

Now recall the discussion on Sect. 2.1, where in the regime far off resonance the probability of transitions between the states of the two-level system are time dependent and given by Eq. (2.4). By selecting a pulse with the appropriate time,

³³Fermionic atoms can be promoted to the p band by a different process, which is based on full occupation of the states in the s band in such a way that the next atoms are restricted to occupy the excited band.

and the laser wave vector with the appropriate configuration,³⁴ it is then possible to transfer population from the ground to the excited vibrational level in a particular direction [8]. In other words, the coupling here is between the different orbital states!

With use of these techniques, Müller et al. experimented with atoms in the p band of 1D, 2D and 3D (separable) optical lattices. The main results are summarized here:

- (i) *Long lifetimes*: Atomic population was reported to survive in a metastable state in the excited band with considerable long lifetimes, of the order of 10–100 times larger than the characteristic scale for tunneling in the lattice. The lifetimes depend mainly on two factors, namely the atomic density, and the depth of the lattice sites.
- (ii) *Decay channels*: The reason why the lifetimes in the p band are affected both by the atomic density and the depth of the lattice sites is because the main decay channel stems from atom-atom collisions. Therefore the larger the densities, the larger the probability of atomic collisions. In the same way, the increased rate of tunneling in the limit of shallower potential wells increases the probability of encounters between two atoms, and consequently, the probability of atomic collisions. In addition, we notice that the anharmonicity of the sinusoidal lattices prevents the occurrence of first order processes in which the energy of a state of two atoms in the p band is resonant with the energy of a state with one atom in the s and the other in the d band. Although this increases the stability of the system in the p band, we remark that higher order processes can still contribute to the decay of population from the excited band.
- (iii) *Establishment of coherence*: the authors found that by changing the parameters of the system, i.e., by lowering the lattice such as to reach the regime of the superfluid phase, the system exhibited a state with long-range coherence at nonzero quasi-momentum. This observation was based on time of flight experiments, where the momentum distribution in the lattice was recorded. In particular, for specific conditions of hold times it was possible to notice a π phase difference in between neighbouring sites in the directions parallel to the label of the orbital wave functions.

We will address experimental considerations about many-body systems in the p band in Sect. 5.2.2, where the techniques used in this experiment are extended for further manipulation of the orbital states.

Going Even Higher—A Brief Comment Regarding Experiments in the d Band

The possibility of preparing atoms in the d band with 99 % fidelity has been recently reported in Ref. [25]. This realization is based on the use of a *standing-wave pulse*, for instantaneously switching an optical lattice on and off. This induces transitions between states of definite quasi-momentum in different bands that are allowed by selection rules. Starting from the ground-state of the system with the lattice switched off, for example, it is possible to prepare superpositions of states at even bands

³⁴That is, a pulse that couples the two states in different directions of the optical lattice.

$s, d, g \dots$ Transitions between the states of odd bands are also possible, with use of a moving lattice.

Although this experimental scheme is not suitable for promoting atoms to the p band from the ground-state of a system without the lattice, the lifetime on the d band is quite long, of the order of μs . As we discuss further in Sect. 5.4, this opens great opportunities in the context of quantum simulations.

Appendix: p -Band Hamiltonian Parameters in the Harmonic Approximation

For further reference, we compute here the various coupling constants in the harmonic approximation. As discussed before, under this assumption the Wannier functions are taken as Hermite polynomials, and therefore (2.48) and (2.47) can be obtained from computation of simple Gaussian integrals. Here

$$\begin{aligned} U_{xx} &= U_0 \int dx \left(\frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} \right)^4 x^4 e^{-2x^2/x_0^2} \int dy \left(\frac{1}{\pi^{1/4} y_0^{1/2}} \right)^4 e^{-2y^2/y_0^2} \\ &= U_0 \left(\frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} \right)^4 \frac{3}{4} \frac{\sqrt{\pi}}{2^{5/2}} x_0^5 \left(\frac{1}{\pi^{1/4} y_0^{1/2}} \right)^4 \sqrt{\frac{\pi}{2}} y_0 = U_0 \left(\frac{3}{8\pi} \frac{1}{x_0 y_0} \right). \end{aligned} \quad (2.72)$$

Analogous calculation yields $U_{yy} = U_0 \left(\frac{3}{8\pi} \frac{1}{x_0 y_0} \right)$.

We now compute U_{xy} :

$$\begin{aligned} U_{xy} &= U_0 \int dx \left(\frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} \right)^2 x^2 e^{-x^2/x_0^2} \left(\frac{1}{\pi^{1/4} x_0^{1/2}} \right)^2 e^{-x^2/x_0^2} \times \\ &\quad \int dy \left(\frac{\sqrt{2}}{\pi^{1/4} y_0^{3/2}} \right)^2 y^2 e^{-y^2/y_0^2} \left(\frac{1}{\pi^{1/4} y_0^{1/2}} \right)^2 e^{-y^2/y_0^2} \\ &= U_0 \int dx \left(\frac{\sqrt{2}}{\pi^{1/2} x_0^2} \right)^2 x^2 e^{-2x^2/x_0^2} \int dy \left(\frac{\sqrt{2}}{\pi^{1/2} y_0^2} \right)^2 y^2 e^{-2y^2/y_0^2} \\ &= U_0 \left(\frac{1}{8\pi} \frac{1}{x_0 y_0} \right), \end{aligned} \quad (2.73)$$

from where it follows that $U_{xx} = U_{yy} = 3U_{xy}$. Notice, however, that the relation $U_{\alpha\alpha}/U_{\alpha\beta} = 3$ is only true in the harmonic approximation, and that this is the case regardless of the wave vectors of the lattice k_x and k_y . In fact, it is very surprising that the coupling constants in the harmonic approximation do not even depend on the values of the lattice vector, but only on the lattice amplitudes V_x and V_y ³⁵ [16].

³⁵In the harmonic approximation this happens because the degeneracy condition fixes the ratio k_x/k_y .

This is not the case, however, when the Hamiltonian parameters are computed with use of the lattice Wannier functions.

Now according to Eq. (2.47), we use Eqs. (2.27) and (2.28) to compute the tunneling coefficients as

$$\begin{aligned} -t_{xx} = & \left(\frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} \right)^2 V_x \int dx x(x+d) \sin^2 x e^{-x^2/2x_0^2} e^{-(x+d)^2/2x_0^2} \\ & + \left(\frac{\sqrt{2}}{\pi^{1/4} x_0^{3/2}} \right)^2 \int dx \frac{d}{dx} (x e^{-x^2/2x_0^2}) \frac{d}{dx} ((x+d) e^{(x+d)^2/2x_0^2}). \end{aligned} \quad (2.74)$$

d is used here as the lattice constant, and we have already used that the integral in the y -direction yields 1. In the same way,

$$\begin{aligned} -t_{xy} = & \left(\frac{1}{\pi^{1/4} y_0^{1/2}} \right)^2 V_y \int dy \sin^2 y e^{-y^2/2y_0^2} e^{-(y+d)^2/2y_0^2} \\ & + \left(\frac{1}{\pi^{1/4} y_0^{1/2}} \right)^2 \int dy \frac{d}{dy} e^{-y^2/2y_0^2} \frac{d}{dy} e^{-(y+d)^2/2y_0^2}. \end{aligned} \quad (2.75)$$

The expressions for t_{yx} and t_{yy} are obtained by making $x \rightarrow y$ and $y \rightarrow x$ with $x_0 \rightarrow y_0$ and $y_0 \rightarrow x_0$ (Figs. 2.10 and 2.11).

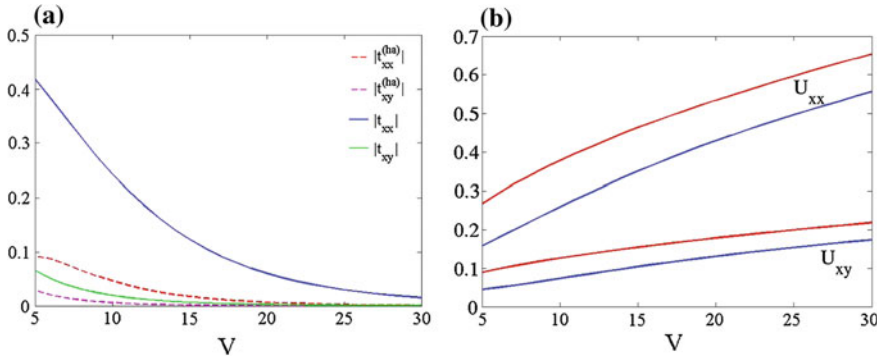
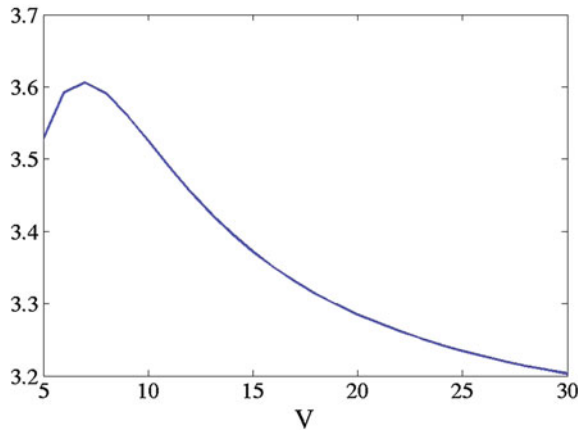


Fig. 2.10 Comparison between the values of the couplings obtained from analytical and numerical computations as a function of V . It is shown in **a** that the harmonic approximation fails to reproduce the results obtained numerically for the tunneling coefficients when tunneling occurs in the direction of the node. In **b** we show the results for the interaction coefficients. In particular the estimates obtained from the harmonic approximation are always larger than the values of the couplings computed numerically

Fig. 2.11 Ratio U_{xx}/U_{xy} for different values of the amplitude of the optical potential. Notice here that U_{xx}/U_{xy} is always larger than 3 for numerical computations with the lattice Wannier functions



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