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Dipolar–Induced Resonance for Ultracold Bosons in a Quasi–1D Optical Lattice

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We study the role of the dipolar interaction, correctly accounting for the Dipolar–Induced Resonance (DIR), in a quasi–one–dimensional system of ultracold bosons. We first show how the DIR affects the lowest–energy states of two particles in a harmonic trap. Then, we consider a deep optical lattice loaded with ultracold dipolar bosons. We describe this many–body system using an atom–dimer extended Bose–Hubbard model. We analyze the impact of the DIR on the phase diagram at $T = 0$ by exact diagonalization of a small–sized system. In particular, the resonance strongly modifies the range of parameters for which a mass density wave should occur.

Introduction. The recent experimental developments in the field of ultracold dipolar gases have opened up fascinating prospects for the study of systems exhibiting Dipole–Dipole Interaction (DDI) [1, 2]. Bose–Einstein Condensates (BECs) of magnetic atoms have been realized using Chromium [3], Erbium [4], and Dysprosium [5]. However, the magnetic moments carried by single atoms are small ($\lesssim 10\,\mu_{\mathrm{B}}$, where μ_{B} is the Bohr magneton), and therefore the effects of the DDI observed with these systems have remained perturbative up to now [6]. The recent realization of the ultracold heteronuclear molecules RbK [7] and NaK [8], which both carry electric dipole moments of the order of one Debye, offer a promising route towards stronger DDI effects, but quantum degeneracy still remains to be achieved with these systems. Rydberg atoms boast much larger dipole moments and will provide an alternative way to explore the DDI, but yield challenging experimental problems associated with time and length scales [9].

The DDI is both anisotropic and long–ranged, and dipolar gases thus allow for the quantum simulation of more general Hamiltonians than the ones accessible with non–dipolar neutral particles, whose interaction is described by the standard s–wave interaction [10]. Furthermore, the trapping techniques available for ultracold atoms makes it possible to control the effective dimensionality. The use of a lower dimensionality stabilizes the system with respect to two–body and many–body instabilities caused by the attractive part of the three–dimensional DDI. This has prompted detailed studies of dipolar systems in 2D and quasi–2D [11–15], bilayer [16–18], and quasi–1D [19–21] geometries.

Experiments involving dipolar bosons in optical lattices have recently been performed both with atomic BECs [22] and non–condensed dipolar molecules [23]. The simplest theoretical description of such dipolar systems in a lattice is provided by an Extended Bose–Hubbard Model (EBHM) accounting for nearest–neighbour interactions [1]. The 1D EBHM has already been explored theoretically for generic values of the model parameters, revealing the occurrence, beyond the standard Mott–Insulator (MI) and superfluid (SF) phases, of a Mass Density Wave (MDW) phase [21, 24] and a Haldane Insulator phase [25, 26] .

In this Letter, we study ultracold bosonic dipoles in an optical lattice, in the quasi–1D tight–binding regime [27, 28]. In order to obtain accurate predictions corresponding to our specific system, our model should include the effect of the Dipolar Induced Resonance (DIR) [29, 30]. The DIR is a low–energy scattering resonance which occurs when the dipole strength is varied. Accounting for it requires going beyond the single–band EBHM [31]. We develop an atom–dimer EBHM, which is the simplest possible lattice model reproducing the DIR.

The scattering and bound–state properties of the DDI have been studied numerically for free–space models [32] as well as systems trapped in 3D and 2D optical lattices [33]. In our quasi–1D geometry, we describe the interaction using an effective potential obtained by averaging the transverse degrees of freedom into the corresponding harmonic oscillator ground state [19, 20]:

$$V_{1\mathrm{D}}(x) = \left(g_{1D} - \frac{\hbar^2}{m}\frac{2\,r^*}{3\,l_\perp^2}\right)\delta(x) + \frac{\hbar^2}{m}\frac{r^*}{l_\perp^3}\left[\sqrt{\frac{\pi}{8}}\,e^{\frac{1}{2}\frac{x^2}{l_\perp^2}}\left(\frac{x^2}{l_\perp^2}+1\right)\mathrm{Erfc}\left(\frac{|x|}{\sqrt{2}l_\perp}\right) - \frac{|x|}{2\,l_\perp}\right], \tag{1}$$

where $r^* = mD^2/\hbar^2$ is the dipolar length, with D being the dipolar strength. The range of this potential is determined by the oscillator length $l_\perp = (\hbar/m\omega_\perp)^{1/2}$ in the strongly–confined directions y and z. The term $g_{1D} = 2\hbar^2 a_{3\mathrm{D}}/ml_\perp^2$ is the strength of the standard s–wave contact interaction for a 3D scattering length $a_{3\mathrm{D}}$ [34], which can be manipulated using a Feshbach resonance [35]. It competes with the DDI to determine the stability and the phase of the system [36]. For simplicity, we assume $g_{1\mathrm{D}} = 0$ unless otherwise specified. Note that, under this assumption, the potential defined by Eq. (1) still contains a contact term proportional to r^*.

Two–body physics. The basic building block of our many–body lattice Hamiltonian (see Eq. (4) below) is provided by the solution of the two–body problem in a