Ab initio calculation of Hubbard parameters for Rydberg-dressed atoms in a one-dimensional optical lattice

Yashwant Chougale and Rejish Nath

Indian Institute of Science Education and Research, Pune 411 008, India

E-mail: rejish@iiserpune.ac.in

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Abstract

We obtain ab initio the Hubbard parameters for Rydberg-dressed atoms in a one-dimensional (1D) sinusoidal optical lattice on the basis of maximally-localized Wannier states. Finite range, soft-core interatomic interactions become the trait of Rydberg admixed atoms, which can be extended over many neighboring lattice sites. In contrast to dipolar gases, where the interactions follow an inverse cubic law, the key feature of Rydberg-dressed interactions is the possibility of making neighboring couplings to the same magnitude as that of the onsite ones. The maximally-localized Wannier functions (MLWFs) are typically calculated via a spread-minimization procedure (Marzari N and Vanderbilt D 1997 Phys. Rev. B 56 12847) and are always found to be real functions apart from a trivial global phase when an isolated set of Bloch bands are considered. For an isolated single Bloch band, the above procedure reduces to a simple quasi-momentum-dependent unitary phase transformation. Here, instead of minimizing the spread, we employ a diagonal phase transformation which eliminates the imaginary part of the Wannier functions. The resulting Wannier states are found to be maximally localized and in exact agreement with those obtained via a spread-minimization procedure. Using these findings, we calculate the Hubbard couplings from the Rydberg admixed interactions, including dominant density-assisted tunneling (DAT) coefficients. Finally, we provide realistic lattice parameters for the state-of-the-art experimental Rydberg-dressed rubidium setup.

Keywords: Rydberg atoms, Hubbard model, optical lattice

(Some figures may appear in colour only in the online journal)

1. Introduction

A new wave of study has emerged in the cold Rydberg atom community focusing on so-called Rydberg-dressed atoms [1–7]. They are mostly ground-state atoms with a very tiny fraction of Rydberg excited ones, represented by state vectors of the form \( |g\rangle + \alpha |r\rangle \) with \( |\alpha| \ll 1 \), where \( |g\rangle \) and \( |r\rangle \) are respectively the ground and Rydberg states. Rydberg excited atoms are known to exhibit prodigious interatomic interactions [9] that can suppress further excitations within a finite volume, called the Rydberg blockade [10–12]. Though the excitations are short-lived, the huge interactions made it feasible to study certain interesting many-body effects, within the frozen gas limit [13–19]. Later, Rydberg admixing proved a remedy to overcome the lifetime constraint of Rydberg excited atoms, especially augmenting their effective lifetime by a factor of \( 1/|\alpha|^2 \). Interatomic interactions with a soft-core potential barrier [5] become a trait of Rydberg-dressed atoms, as is verified in two recent experiments. In one of them, the effective interactions in the strong dressing limit are demonstrated with two individual atoms trapped in optical tweezers [20]; in contrast, the second experiment involves a two-dimensional lattice setup [21]. In a short amount of time, a variety of exciting studies have developed in such areas as quantum many-body physics [5, 22–28] including frustrated quantum magnets [29, 30], quantum computing [31–33] and spin squeezing for metrology [34, 35]. As has been recently proposed, an electromagnetically-induced transparency-based Rydberg-dressing scheme utilizing metastable states of alkaline earth atoms may help to achieve enhanced atomic interactions even with longer coherence times [36].
The quantum simulation of many-body physics predominantly relies on ultra-cold atoms loaded in optical lattices [37, 38] described by local Hubbard models [39]. The Bose–Hubbard model (BHM) with contact interactions and nearest-neighbor hoppings forms the paradigmatic example of a system exhibiting quantum phase transition, dating back to the prediction of a superfluid-mott insulator transition by Fisher et al [40]; for the first time it has been observed in a cold-atom lattice setup [41]. Due to tremendous progress in experimental techniques, in particular the ability to address a single atom in a lattice site [42–44] as well as to describe experimental results quantitatively accurately, it is necessary to calculate Hubbard parameters on the basis of highly-localized single-particle states. An example is that of maximally localized Wannier states, which can be obtained by unitary mixing of the Bloch states [45, 46]. In a seminal work by Marzari and Vanderbilt [47], the authors showed how to calculate the maximally-localized Wannier functions (MLWFs) by minimizing the spread of generalized Wannier states. Their approach has been employed successfully in the study of complex solid-state materials [48] and has recently been used for cold atoms in optical lattices [49]. When lattice depths are sufficiently large, tight binding together with harmonic approximation are in good agreement with MLWF calculations for lowest-isolated bands.

The acclaimed BHM is then generalized to systems with long-range interactions (e.g. magnetic atoms, polar molecules or atoms with laser-induced interactions); this is termed the extended BHM (EBHM) [50, 51] in which the interactions between neighboring sites are included. The EBHM is predicted to be abundant with exotic quantum phases such as stripes, checkerboard phases, supersolids, Haldane insulators, etc [52–57]; lately, it has been experimentally demonstrated using magnetic erbium atoms trapped in a three-dimensional optical lattice [58]. Here, we derive the EBHM in a one-dimensional (1D) lattice of Rydberg admixed atoms from first principles and as we show, it has certain advantages over dipolar systems. Among them, the most striking property is the possibility of engineering the strengths of onsite couplings to the same magnitude as that of onsite ones, hence being position independent. This may have far-reaching consequences in the context of quantum many-body physics [60] especially in frustrated magnetism [29, 30] to impose local constraints or conservation laws.

An additional correlated feature of interacting lattice gases is density-assisted intersite or interband tunneling, in which the former has been observed in atoms with both contact interactions [59] and long-range dipolar interactions [58]. Termed ‘bond-charge interaction’ in the context of fermions, the density-assisted tunneling (DAT) strongly influences the Mott insulator-superfluid transition points in bosonic and Bose–Fermi mixtures [61] and also leads to novel quantum phases for polar molecules in optical lattices [62].

Here, we calculate ab initio the Hubbard parameters on the basis of MLWFs for an extended Hubbard model implemented using Rydberg-dressed atoms in a 1D sinusoidal optical lattice. Motivated by the hypothesis that MLWFs are real functions apart from a trivial global phase, we implement a diagonal U(1) phase transformation for the Bloch states which eliminates the imaginary part of the Wannier states. The resulting Wannier states are found to be maximally localized and in exact agreement with those obtained via a spread-minimization procedure. We estimate the Hubbard parameters including the DAT coefficients and discuss their properties within the two lowest Bloch bands and up to second nearest-neighbor couplings for Rydberg admixed interaction potential.

The paper is structured as follows. In section 2 we discuss the Rydberg-lattice setup, the governing many-body Hamiltonian and derive ab initio the extended Hubbard model in the maximally-localized Wannier basis. In section 3 we discuss how MLWFs are calculated using a unitary diagonal phase transformation in the isolated Bloch bands for a sinusoidal 1D optical lattice potential. The results for the Hubbard parameters are discussed in section 4 and we also provide realistic numbers for the state-of-the-art experimental rubidium lattice setup in 4.4. Finally, we outline our conclusions in section 5.

2. Rydberg-dressed atoms in a 1D optical lattice

2.1. The atom lattice setup and Rydberg–Rydberg interactions

We consider bosonic atoms loaded in a 1D optical lattice of potential \( V_{\text{OL}}(x) = V_0 \sin^2(k_0 x) \), where \( V_0 \) is the lattice depth and wavenumber \( k_0 = \pi/d \) with \( d \) being the lattice spacing. The ground state \( |g\rangle \) of the atoms is weakly admixed to an excited Rydberg state \( |e\rangle \) using an optical field with a large detuning \( \Delta \) compared to Rabi frequency \( \Omega \) such that \( \Omega/|\Delta| \ll 1 \), see figure 1. We assume that both ground and...
Rydberg state atoms are trapped in a magic wavelength optical lattice (MWOL) such that atoms occupying both states experience identical lattice potentials [63–66]. Large wavelength infrared MWOLs due to effective landscape polarizability and which are suitable for high-lying alkali atom Rydberg states are also proposed [67]. If the Rydberg state trapping is neglected an additional time constraint arises due to the expansion of the atomic wave packet (see 2.3 for details) when atoms occupy the Rydberg state. Two atoms with an interatomic separation, away from the Förster regime, occupying the state $|e\rangle$ experience an interaction potential of the form $C_6/r^6$, where the van der Waals (vdW) dispersion coefficient $C_6(xn^{-1})$ can be either spatially isotropic or anisotropic [26, 29] depending on different angular momentum quantum numbers $(l, j, m_j)$ of the Rydberg state $|e\rangle \equiv [n, l, j, m_j]$, where $n$ is the principal quantum number.

The above vdw interactions between the Rydberg excited atoms lead to a tunable soft-core potential for the atoms in the admixed ground state (see figure 1c):

$$W(r_{ij}) = \frac{\Omega (2/\Delta)^4}{\Omega^4 + R_y^6},$$

(1)

The parameter, $R_y = [C_6/(2/\Delta)]^{1/6}$ denotes the Condon radius which determines the range of the interactions and $r_{ij}$ is the spatial separation between the $i$th and $j$th atoms. The Rydberg blockade effect is apparent at distances $r_{ij} \leq R_y$, where the interaction potential is saturated to a constant value provided by the light shift of the blockaded atoms [5, 20]. For large values of $r_{ij} > R_y$, we retrieve the vdw-type interactions, $W(r_{ij}) \sim C_6/r^6$ with a reduced vdw coefficient $C_6 = (\Omega/2/\Delta)^4C_6$. Notably, the range of the interactions $\sim R_y$ can be extended over several lattice sites by regulating the detuning $\Delta$ or the interaction coefficient $C_6$, fabricating a scenario identical to that of long-range interacting systems such as magnetic atoms or polar molecules [51, 58, 62].

### 2.2. Many-body Hamiltonian and the extended Hubbard model

Our starting point is the second quantization many-body Hamiltonian for a gas of interacting bosons in an external potential $V_{OL}(r)$:

$$\hat{H} = \int dr \bar{\psi}^\dagger(\mathbf{r}) \hat{h}_0 \bar{\psi}(\mathbf{r}) + \frac{1}{2} \int dr \bar{\psi}^\dagger(\mathbf{r}) \hat{U}(\mathbf{r} - \mathbf{r}') \bar{\psi}(\mathbf{r}) \bar{\psi}(\mathbf{r}'),$$

(2)

where the field operator $\bar{\psi}(\mathbf{r}) [\bar{\psi}^\dagger(\mathbf{r})]$ annihilates [creates] a boson at the position $\mathbf{r}$. The term $\hat{h}_0 = -\hbar^2\nabla^2/2m + V_{OL}(\mathbf{r})$ corresponds to the single-particle Hamiltonian. The two-particle interactions are, $\hat{U}(\mathbf{r} - \mathbf{r}') = \hat{U}(\mathbf{r} - \mathbf{r}') + W(\mathbf{r} - \mathbf{r}')$ with the first term being the typical contact interactions: $\hat{U}(\mathbf{r} - \mathbf{r}') = g^2(\mathbf{r} - \mathbf{r}')$ characterized by the parameter, $g = 4\pi\hbar^2a/m$ where $a$ is the s-wave scattering length; the second term is the interaction potential among the Rydberg adixed atoms. Next, we expand the field operators on the basis of maximally-localized single-particle Wannier functions $w_n(\mathbf{r} - \mathbf{R}_j)$ (see section 3) centered around each lattice site at $\mathbf{R}_j = j\mathbf{R}$; we find that the lattice vector $\mathbf{R}$ is such that $V_{OL}(\mathbf{r} + \mathbf{R}) = V_{OL}(\mathbf{r})$.

Hence, the field operator

$$\bar{\psi}(\mathbf{r}) = \sum_j w_n(\mathbf{r} - \mathbf{R}_j) \hat{a}_j,$$

(3)

where $\hat{a}_j (\hat{a}^\dagger_j)$ annihilates (creates) a boson in the mode represented by the Wannier function $w_n(\mathbf{r} - \mathbf{R}_j)$ at the $j$th lattice site. They satisfy the commutation relation $[\hat{a}_j, \hat{a}^\dagger_k] = \delta_{jk}$. Inserting the above expression for the field operator in equation (2), we arrive at a general extended Hubbard model:

$$\hat{H} = -\sum_{i,j,n,m} \int dr \bar{\psi}^\dagger(\mathbf{r} - \mathbf{R}_i) \bar{\psi}(\mathbf{r} - \mathbf{R}_j) \hat{h}_0(\mathbf{r} - \mathbf{R}_i) \hat{h}_0(\mathbf{r} - \mathbf{R}_j) + \frac{1}{2} \sum_{i,j,l,m} \sum_{n,m'} (U_{ij} \delta_{nm'} \hat{a}^\dagger_{ji} \hat{a}^\dagger_{jl}) \hat{a}_{ji} \hat{a}_{jl} \hat{a}_{jm} \hat{a}_{jm}$$

(4)

where the hopping and the interaction matrix elements are respectively:

$$J_{ij}^{nm} = -\int dr w_n(\mathbf{r} - \mathbf{R}_i)[-\hbar^2\nabla^2/2m + V_{OL}(\mathbf{r})]w_m(\mathbf{r} - \mathbf{R}_j)$$

(5)

$$U_{ij}^{nm} = \int d\mathbf{r} d\mathbf{r}' w_n(\mathbf{r} - \mathbf{R}_i)w_m(\mathbf{r}' - \mathbf{R}_j) \times U_l(\mathbf{r} - \mathbf{r}')w_{nm'}(\mathbf{r}' - \mathbf{R}_j)w_{nm'}(\mathbf{r} - \mathbf{R}_i).$$

(6)

The subscripts and superscripts in $J$ and $U_l$ represent the lattice site and band indices respectively. In cold atoms, it can be the case that interaction and kinetic energies are smaller than the lattice depth $V_{OL}$; in this situation the summation over the band indices is truncated beyond the few lowest Bloch bands. Below we calculate the microscopic parameters for the EBHM (equation (4)) up to the next nearest-neighbor couplings within the two lowest Bloch bands for the 1D lattice setup.

### 2.3. Validity of our model

**Rydberg state trapping.** As mentioned before, our calculations detailed below are based on the assumption that both ground and Rydberg state atoms experience the same lattice potential which requires a MWOL. If this is not the case, motional heating can occur during ground–Rydberg state transitions, which may lead to severe decoherence [68]. The Rydberg–Rydberg interactions can also induce mechanical effects at short distances; such effects can be safely neglected for Rydberg-dressed atoms [6]. In this section, we discuss the criteria in which the effective interactions calculated using equation (6) are valid when no-trapping is provided for Rydberg atoms. It depends crucially on the timescale at which the free expansion of the atomic wave packet results in a considerable change of the Wannier state. It has to be shorter compared to the lifetime of Rydberg atoms and the timescales set by effective interaction strengths in the lattice.

Assuming harmonic oscillator (HO) states for the two lowest Wannier states (valid in the tight-binding case), we estimate the duration at which the wave-packets remain intact after being excited to a trap-free Rydberg state. The time evolution of the standard deviation for the widths in the $nl^b$
state of the HO is given by

$$
\Delta X_0(t) / \Delta X_0(0) = \left[ 1 + \frac{\hbar^2 \tau^2}{m^2 \hbar_0^2} \right],
$$

(7)

where $\hbar_0 = \sqrt{\hbar / m \omega}$. The frequency $\omega$ of the HO in terms of the lattice depth $V_0$ and lattice spacing $d$ is $\omega = (\pi / d) \sqrt{\frac{m}{\hbar}}$. Note that we are interested in a duration of time $\tau$ such that the wave packet hardly undergoes any expansion, i.e. when the criteria:

$$
\frac{\hbar^2 \tau^2}{2m^2 \hbar_0^2} \ll 1 \quad \text{or} \quad \frac{\tau^2 V_0 \pi^2}{md^2} \ll 1
$$

(8)

is satisfied. For a given $V_0$, equation (8) can be satisfied by sufficiently large values of $d$ and it is also highly desirable for us since we want to access the vdW regime for the interactions between the Rydberg atoms. The large lattice spacings in the order of micrometers can be accessed by adjusting the angle $\theta$ between the co-propagating lattice beams [69], given as $d = \lambda / [2 \sin(\theta / 2)]$. In section 4.4, we discuss the criteria in equation (8) for the case of a rubidium lattice setup.

**Rydberg–Rydberg interactions.** For two atoms occupying the same Rydberg state $|\alpha\rangle$ and far away from Förster resonance, the second-order level shifts due to the dipole–dipole interactions to the pair state $|\alpha\alpha\rangle$; this provides us with the vdW interactions between the atoms. The Förster resonance is characterized by the Förster defect: $\delta_F = E_m - E_p$, where the atomic states $|\beta\rangle$ and $|\gamma\rangle$ are dipole-coupled to the state $|\alpha\rangle$. This introduces a crossover between the Förster regime at short distances and the vdW regime at large separations between the atoms. The transition point $R_F$ can be calculated as

$$
R_F^3 = \sum_{|\beta\gamma\rangle} \left| \frac{\langle \beta|V_d(R)|\alpha\alpha\rangle}{\delta_F} \right|^2,
$$

(9)

where $V_d(R)$ is the dipole–dipole interaction and hence, the lattice spacing has to be greater than $R_F$ for our calculations to be valid. We estimate the $R_F$ for rubidium $nS_{1/2}$ states in section 4.4.

### 3. MLWFs

The generalized Wannier functions are calculated by the unitary mixing of $N$ degenerate or closely spaced Bloch eigenstates; in 1D they are written as

$$
w_n(x - X) = \frac{d}{2\pi} \int_{BZ} dq \ e^{-i q x} \sum_{m=1}^{N} U_{nm}(q) \psi^m_q(x),
$$

(10)

where $\psi^m_q(x)$ is the Bloch function for the $m$th Bloch band for a quasi-momentum $q$. The operator $U_{nm}(q) \in U(N)$ is a unitary matrix satisfying the periodic boundary condition in the momentum space: $U_{nm}(q + 2q_B) = U_{nm}(q)$ with $q_B = \pi / d$ and $N$ corresponds to the number of lattice sites in the unit cell. BZ indicates that the integration is carried over the first Brillouin zone. As proposed in a seminal paper, the MLWFs can be obtained from generalized Wannier functions by obtaining $U_{nm}(q)$ which minimizes the spread functional [46]:

$$
\Omega_w = \sum_{n=1}^{N} \left[ \langle 0n|x|^2|0n \rangle - \langle 0n|x|0n \rangle^2 \right].
$$

(11)

where $\langle x|m \rangle = w_{nm}(x - X)$. MLWFs are shown to be exponentially localized [45, 70] and they provide the best optimal basis for estimating Hubbard parameters. For an isolated single Bloch band ($N = 1$), the unitary transformation is an abelian $U(1)$ gauge transformation and is nothing but an update for the phase of Bloch functions i.e. $\psi^m_q \to e^{i\phi_q^m} \psi^m_q$. This is also the case for the setup we considered here. Thus, once the Bloch spectrum (see appendix A) is found, the problem for calculating MLWFs reduces to finding the phases $\phi_q^m$ which minimize the spread $\Omega$. It has been shown that the results obtained by minimizing the Wannier spread for isolated Bloch bands are same as the exponentially-localized Wannier functions discussed by Kohn [45]. Writing the Wannier spread as the sum of gauge-independent and dependent terms, $\Omega_w = \Omega_d + \Omega_{ad}$, with a subsequent division of gauge-dependent one-diagonal and off-diagonal terms, $\Omega_d = \Omega_{dd} + \Omega_{ad}$. For an isolated band $\Omega_{ad}$ vanishes and the question reduces to finding the unitary transformation which eliminates $\Omega_d$ [46]. Note that there also exist other localization procedures for Wannier states e.g. maximizing the sum of Coulomb self-energies [71].

Here we do not employ the minimization of the Wannier spread, rather we make use of the conjecture that MLWFs are real functions up to a global phase factor. In our case ($N = 1$) the generalized Wannier functions are

$$
w_n(x - X) = \frac{d}{2\pi} \int_{BZ} dq \ e^{-i q x} \psi^m_q(x).
$$

(12)

The periodic Bloch functions $\psi_q^m(x)$ are calculated as prescribed in appendix A. The phase $\phi_q^m$ for the unitary transformation is obtained by minimizing the absolute value of the imaginary part of the Wannier function in equation (12); this leads to

$$
\phi_q^m = \arctan \left( \frac{\Im[u_q^m(x_0)]}{\Re[u_q^m(x_0)]} \right) - qx_0.
$$

(13)

In our numerics, for the symmetric $u_q^m(x)$ we took $x_0 = 0$ and for the anti-symmetric $u_q^m(x)$ we took the point at which the imaginary part of $u_q^m(x)$ is maximum. The resulting Wannier functions match perfectly with those obtained via a spread-minimization procedure [72]. As an example, MLWFs for the two lowest bands ($n = 1, 2$) in a 1D sinusoidal lattice are shown in figure 2(a) for $V_0 = 10E_R$ and their exponential localization is conspicuous in the log-scale plot of the vertical axis.

### 4. Hubbard parameters

#### 4.1. Hopping and short-range interaction parameters

We briefly summarize the behavior of hopping ($J$) and contact interaction ($U$) matrix elements as a function of the lattice depth $V_0$ calculated using MLWFs (see figure 2). The spatial spread of Wannier functions $w_n(x)$ gets larger and larger as we go higher
in bands \((n)\) and for a given \(n\) it decreases with increasing \(V_0\). The localization properties of \(w_n(x)\) are critical in determining the behavior of \(J\) and \(U\). For instance, the nearest-neighbor hopping \((J_n^0 = J_{nn}^0)\) is larger in the second band compared to that in the first one. Also for both bands, it decreases exponentially with increasing \(V_0\) (figure 2(b)). The next nearest-neighbor hopping is two orders of magnitude less than \(J_n\) and is safely disregarded in the (E)BHM. Note that there is no inter-band hopping due to the orthogonality property of Wannier functions. The results from WKB approximation \([72]\) for the lowest band are shown on the dotted line. (d) Shows the scaled (units of \(g\)) DAT amplitudes as a function of \(V_0\), which include DAT within bands to the nearest-neighbor site (solid lines) and those between bands to the nearest-neighbor site (dashed lines). The different DAT processes are shown in (e) and the corresponding amplitudes are indicated by the same numbers in (d).

Since \(w_n(x)\) gets more and more localized with larger values of \(V_0\), the onsite interactions \((U_n^0 = U_{nn}^{000})\) for any \(n\) increases as a function of \(V_0\) (figure 2(c)). As expected, the behavior for the nearest-neighbor interactions \((U_n^n = U_{nn}^{nnn})\) is just opposite and also a few orders of magnitude lower than that of the onsite ones, which may hardly affect the many-body phase diagram of the BHM. On the other hand, regarding the different DAT matrix elements shown in figure 2(d), though their magnitudes are relatively small (compared with hopping amplitudes \(J_n\) some of them may significantly modify the dynamics in the BHM \([59]\), even in sufficiently strong optical lattices. In particular, if restricted to the lowest band the dominant offsite contribution in the BHM comes from a DAT term (first processes in figure 2(e)) in the form \(\sim \sum \hat{a}_i \hat{n}_{i+1} \hat{a}_{i+1}\) and is explicitly occupation dependent. The signatures of this term in a deep MOT state are probed in a recent experiment using tilted optical lattices \([59]\). In figure 2(d) only the dominant DAT coefficients are shown and the corresponding processes are depicted in figure 2(e). Note that onsite interband tunnelings are prohibited by the orthogonality property of MLWFs. With the inclusion of DAT terms in the discrete lattice Hamiltonian, the model is now generally termed as a non-standard BHM \([61]\).
4.2. Rydberg admixed potential: density–density interactions

We rewrite the binary interaction (equation (1)) between the Rydberg admixed atoms as

$$W(r_{ij}) = \frac{W_{\text{eff}}}{[r_{ij}/R_c]^6 + 1], \quad (14)$$

with $W_{\text{eff}} = \hbar \Omega / (8|\Delta|^3)$ being an effective interaction strength given by the light shift due to the Rydberg laser and $R_c = [C_0/2\hbar|\Delta|^3]^{1/6}$ providing the interaction range. Among the two parameters, $R_c$ can be controlled independently of $W_{\text{eff}}$ by changing the Rydberg state through $C_0$, but any variation in $\Delta$ and $\Omega$ affects both simultaneously. The possibility of tuning the interaction range without affecting the effective strength can be pointed out as an elite feature of Rydberg admixed atoms compared to other existing long-range systems. See section 4.4 for the values of $R_c$ as a function of $C_0(n)$ (or simply $n$) for rubidium atoms.

With this, we estimate the Hubbard parameters for Rydberg-dressed interaction ($W_{\text{eff}}^\text{Ry}$) using MLWFs, as a function of both the lattice depth $V_0$ and $R_c$. The results for the case in which two atoms occupy the lowest band ($W_{\text{Ry}}^{l11i} = W_{\text{Ry}}^{l00i}/W_{\text{eff}}$) are shown in figure 3. For any value of $R_c$, the onsite interaction ($i = 0$) increases with increasing $V_0$ but it saturates rather quickly compared to that of short-range interactions for sufficiently large values of $R_c$. This is attributed to the flat nature of the soft-core potential. The behavior of onsite matrix elements with $V_0$ depends crucially on the value of $R_c$. For instance, for $R_c = d/2$ all of them decrease with $V_0$ and become negligible for sufficiently large $V_0$ (figure 3(a)). When $R_c \sim d$, the character of the nearest-neighbor ($i = 1$) coupling changes and it increases with $V_0$ (figure 3(b)). For $R_c \sim 2d$ it becomes almost identical to that of the onsite interaction (figure 3(c)) and in addition, the next nearest-neighbor coupling becomes significantly large; it becomes half of the onsite and first nearest-neighbor interactions. As shown in figure 3(d) for $R_c = 5d$ all the three are almost same in magnitude. Hence, as $R_c$ increases the offsite matrix elements become as relevant as onsite interactions. The same results as detailed above for the first excited band are shown in the figure 4; the results from one atom occupying the lowest band and the second in the first excited band are shown in figure 5. For all cases, the tight-binding results are shown by the dotted lines and they agree very well with the exact calculations when $V_0$ is sufficiently large. For $V_0 \gg E_R$, the Wannier states can be approximated to the Dirac delta functions and in this limit the interactions ($W_i^1$ and $W_i^2$) are just given by the bare potential $W(x)$.

The important properties to be noted are as follows. The first point is that due to the flattened nature of the Rydberg potential at short distances, the dominant matrix elements for the density–density interactions saturate quickly to $W_{\text{eff}}$ as a function of $V_0$ when $R_c > d$. This can be seen again as a unique feature of Rydberg-dressed interactions compared to other interatomic potentials. This is because the potential $W(x - x')$ changes hardly at all over an interparticle distance of $x - x' \sim R_c$, hence it can be approximated to a constant such that

$$W_{\text{eff}}^{\text{Ry}} \approx \frac{W(x - x')}{\int dx |w^\text{Ry}(x)|^2} \int dx' |w^\text{Ry}(x' - X_i)|^2 = W_{\text{eff}}. \quad (15)$$

Figure 3. The Rydberg admixed interaction parameters $\tilde{W}_i^l = \tilde{W}_{\text{Ry}}^{l11i}/W_{\text{eff}}$ in the lowest band ($n = m = 1$) as a function of the lattice depth $V_0$ with (a) $R_c = d/2$, (b) $R_c = d$, (c) $R_c = 2d$ and (d) $R_c = 5d$. The onsite ($i = 0$), nearest-neighbor ($i = 1$) and next nearest-neighbor ($i = 2$) interaction couplings are shown, as indicated by the numbers in the plot. As $R_c$ increases, the offsite matrix elements become as significant as those of the onsite ones. This arises from the flattened nature of the soft-core barrier of the Rydberg-induced potential. In addition, they all saturate to the same value independent of the separation between the atoms as $R_c$ becomes larger and larger. The results from the tight-binding approximation are shown by the dotted lines.
As we go higher in the bands, the saturation behavior with \( V_0 \) slows down. It can also be seen as that the saturation occurs when the MLWFs are fully accommodated inside the soft-core barrier of the potential or when \( W < W_{Rc} \); further, it delays the saturation as a function of \( V_0 \) for higher bands. The second point is that nearest-neighboring interactions can be made to the same strength as those of onsite interactions by adjusting the value of \( R_c \), i.e. they become position independent. This may have far-reaching consequences in the context of many-body physics [60], and in particular on frustrated magnetism [29, 30], to impose local constraints. Since \( R_c \) is varied through the vdW coefficient \( C_6 \), the different many-body quantum phases arising from the long-range nature of the interactions can be accessed simply as a function of the value of \( R_c \), i.e. they become position independent. This may have far-reaching consequences in the context of many-body physics [60], and in particular on frustrated magnetism [29, 30], to impose local constraints. Since \( R_c \) is varied through the vdW coefficient \( C_6 \), the different many-body quantum phases arising from the long-range nature of the interactions can be accessed simply as a function of the

Figure 4. The same as in figure 3, but for the first excited band \( (\tilde{W}^2 = W_{000}^{222}/W_{\text{eff}}) \). The results from tight-binding approximation are shown by the dotted lines. The value of \( i \) is used in labeling the plots.

Figure 5. The interband matrix elements \( (\tilde{W}^1_{12} = W_{000}^{1212}/W_{\text{eff}}) \) for the Rydberg admixed interaction as a function of the lattice depth \( V_0 \) for (a) \( R_c = d/2 \), (b) \( R_c = d \), (c) \( R_c = 2d \) and (d) \( R_c = 5d \). The results from the tight-binding approximation are shown by the dotted lines. The value of \( i \) is used in labeling the plots.
principal quantum number $n$ without changing other parameters in the system. The quantitative details for a rubidium lattice setup are worked out in section 4.4.

We summarize this section by showing the interaction parameters up to second nearest neighbors in the first two bands as a function of $R_c$ for a fixed $V_0$ (figure 6). The saturation of matrix elements are clearly visible here as well, and can be explained the same way as we have detailed above. Another feature we have seen is that the offsite matrix elements for the lowest and the first excited bands cross each other. At small $R_c$, it is the overlap between the MLWFs which determines the offsite couplings and they are larger for the first excited band compared to the lowest one. In contrast, at sufficiently large $R_c$ the offsite coupling strength depends on how well it is accommodated inside the soft-core barrier and in that case the lowest band dominates, resulting in a crossing between them as a function of $R_c$. We also noticed that these crossings are even more prominent at small values of $V_0$.

4.3. Rydberg admixed potential: DATs

We look at the DAT processes induced by the Rydberg admixed interactions. Here, we only discuss the two dominant processes (schematically depicted in figure 7(a)) within the two lowest Bloch bands and they both are found to be DAT interband tunnelings, with an explicit dependence on $R_c$. For a given $R_c$ and $V_0$, the amplitudes of these processes as a function of interparticle separation exhibit a sharp peak at $R_c$. This means that if $R_c = d$ only for the nearest-neighbor atoms these processes take place, and similarly when $R_c = 2d$ it happens between the next nearest-neighbor atoms.

Let us now focus on the case of nearest neighbors (depicted in figure 7(a)). For large $R_c$, the Rydberg admixed potential can be taken as a constant and it results in $\sim \int W_0(x)w_m^*(x)dx \approx 0$, hence, you observe a rapid decay for $R_c > d$. For $R_c < d$, the interactions between the sites are weak enough to trigger this process and hence result in a hump-like behavior as a function of $R_c$. The same matrix elements as a function of $V_0$ for a given $R_c (= d)$ are shown in figure 7(c). If we consider the same processes between the next nearest neighbors, the above-mentioned peak appears at $R_c = 2d$ but with a lesser magnitude and so on. Hence, we calculated the maximum of the peak as a function of interparticle separation ($R_c$) and it has changed accordingly for $V_0 = 10E_R$ (see figure 7(d)). Note that the amplitudes for all other DAT events are at least one order of magnitude lower than those shown in figure 7(a). The above processes introduce the following type of terms: $\sim \sum_{i,j} \hat{a}_{i2}^\dagger \hat{n}_{i1} \hat{a}_j$ (process 1 in figure 7(a)) and $\sim \sum_{i,j} \hat{a}_{i2}^\dagger \hat{n}_{j2} \hat{a}_j$ (process 2 in figure 7(a)) within the two lowest-band EBM for the Rydberg admixed atoms in a 1D optical lattice.

4.4. An example: rubidium atoms

In this section we consider the state-of-the-art rubidium ($^{87}$Rb) lattice setup. If the Rydberg state atoms are confined, as discussed in section 2.3, the initial atomic (Wannier) wave packet for the ground-state atoms undergoes free expansion resulting in the de-localization of the particle. This disturbs the picture of the localized Hubbard model. In order to preserve that, the experimental process has to be restricted within the timescale at which the spatial extension of the initial wave packet remains unchanged. The latter is determined by equation (8) and in figure 8(a) we plot the time taken in which the width of the wave packet is incremented by 10% from the initial value as a function of $V_0$, for rubidium atoms with a lattice spacing of $d = 4 \mu m$. The lattice spacing of $4 \mu m$ can be achieved with co-propagating laser beams, of wavelength $\lambda = 1064$ nm, forming an angle of $\theta = 13.3$ degrees between them. As $V_0$ increases the initial width gets lesser and lesser and the wave packet carries more kinetic energy, hence it takes less time to expand. This definitely restricts the study of the Hubbard-like model with un-trapped Rydberg states with large principal quantum numbers in deep-optical lattices. For $V_0 = 10E_R$ the maximum value of $n$ one can attain is $\sim 35$. Therefore MWOLs are strongly recommended to explore the physics in the tight-binding regimes using Rydberg-dressed atoms involving large principal quantum numbers.

On the other hand for any given Rydberg state $nS_{1/2}$, the validity of the vdW picture in our lattice model necessitates that the lattice separation must be larger than $R_0$ (see equation (9)), the crossover point between the Förster regime and the vdW regime. In figure 8(b), we show the numerical results of $R_F$ as a function of $n$ for $nS_{1/2}$ rubidium states. Though the main contributions from the dipole coupling are coming from the nearest $nP_{1/2}$, we also included $nP_{3/2}$. It shows that in order to access the vdW regime the lattice spacings are at least of about $2 \mu m$ for $n > 60$.

As we have pointed out earlier in section 4.2, any change in detuning $\Delta$ or $\Omega$ affect $R_c$ and $W_{\text{eff}}$ simultaneously, but the interaction range $R_c$ can be varied independently by changing the Rydberg states. Below we estimate realistic values for $R_c$ as a function of $C_6(n)$ for rubidium atoms weakly coupled to $nS_{1/2}$ states, in a 1D optical lattice (figure 9(a)). We consider a
lattice spacing of $d = 2 \mu m$. It can be seen that the range of interactions can be extended over as many as two sites when considering a Rydberg state $60S_{1/2}$ with $\Delta = 100$ MHz. Note that for fixed $C_6$, the variation of $R_c$ against $\Delta$ is relatively slow. With $\Omega/\Delta = 0.1$ and $\Delta = 100$ MHz, we can attain an effective interaction strength of $W_{\text{eff}} = 10$ kHz.

5. Conclusion

In conclusion, we have estimated ab initio the Hubbard parameters for Rydberg-dressed atoms in a 1D sinusoidal optical lattice on the basis of maximally-localized Wannier states. The finite range, soft-core nature of the Rydberg-induced vdW interactions strongly modifies the nature of the Hubbard parameters. In particular, in controlling the spatial extension of the soft-core barrier one can engineer the offsite interactions and make them the same magnitude as that of the onsite ones, hence making them position independent. This may influence the many-body dynamics a great deal. In addition to the typical density--density interactions, we provide the information for the DAT coefficients in this system. Two dominant processes which depend crucially on the soft core have been identified and discussed which will be highly relevant when studying non-standard multi-band Hubbard models. Finally, we have discussed realistic parameters for...
the state-of-the-art experimental Rydberg-dressed rubidium lattice setup.

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Appendix. Single-particle energy bands and Bloch states in a 1D optical lattice

The Hamiltonian for a single particle in the presence of a 1D optical lattice potential $V_{OL}(x)$ is

$$\hat{H}_0 = -\frac{h^2}{2m}\frac{d^2}{dx^2} + V_{OL}(x), \quad (A.1)$$

where $V_{OL}(x) = V_0 \sin^2(k_0 x)$ and the wavenumber $k_0 = \pi/d$ with $d$ denoting the lattice spacing. The single-particle energy band structure is obtained by solving the eigenvalue equation $\hat{H}_0 \psi_n^q(x) = E_n^q \psi_n^q(x)$ for a given quasi-momentum $q \in [-\pi/d, \pi/d]$ and $n$ is the band index. According to the Bloch theorem, we have Bloch solutions $\psi_n^q(x) = e^{i\mathbf{K} \cdot \mathbf{r}} u_n^q(x)$ and $u_n^q(x)$ has the same periodicity as that of the lattice potential. The above eigenvalue equation is best tackled in the Fourier space, and by introducing the Fourier expansion for the lattice potential $V_{OL}(x) = (1/\sqrt{d}) \sum_k v_k e^{i\mathbf{k} \cdot \mathbf{r}}$ and for $u_n^q(x) = (1/\sqrt{d}) \sum_k c_{n,k} e^{i\mathbf{k} \cdot \mathbf{r}}$. With Fourier coefficients $c_{n,k}$ satisfying the normalization condition $\sum_k (c_{n,k}^* e^{i\mathbf{k} \cdot \mathbf{r}}) c_{n,k} = \delta_{n,n}$, the periodic functions $u_n^q(x)$ are normalized over the primitive unit cell of the lattice in the real space. Finally we arrive at

$$\frac{h^2}{2m} (G_k + q)^2 c_{n,k}^* c_{n,k} + \frac{1}{\sqrt{d}} \sum_k v_{k-k'} c_{q,k'}^* c_{q,k} = E_n^q c_{n,k}. \quad (A.2)$$

We can write the above equation in a matrix form as $\hat{H}_q c_n^q = E_n^q c_n^q$ with eigenvectors $c_n^q$ and eigenvalues $E_n^q$. The matrix elements of $\hat{H}_q$:

$$(H_q)_{ij} = \frac{h^2}{2m} (G_i + q)^2 \delta_{ij} + \frac{1}{\sqrt{d}} v_{i,j}.$$ 

Diagonalizing $H_q$ provides us with the Fourier coefficients $c_{n,k}$ and they possess certain properties based on various symmetries. If inversion symmetry exists and together with time-reversal symmetry, they guarantee that $c_{n,k}$ are real apart from a common-phase factor and also satisfies $c_{n,k}^* = (c_{n,-k})^*$. This property can considerably reduce the numerical cost in calculating the Bloch functions $\psi_n^q(x)$. We employ a LAPACK routine to obtain the eigenstates and eigenvalues of the Hamiltonian matrix given in equation (A.3) for $q \in [-\pi/d, \pi/d]$. The eigenvectors $c_n^q$ are real-valued and the periodic Bloch function $u_n^q(x)$ is then obtained by its Fourier transform.

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