

Interacting Wannier functions in a superlattice: An iterative method

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We present a method to compute interacting Wannier functions in an optical superlattice for cold atom gas experiments. We start from a noninteracting Wannier function obtained from the band projected position operator method and perform Trotter method to compute the interacting Wannier function. Then, we use this function to compute the on-site interaction strength in a superlattice, compare the result to a measurement, and find good agreement between simulation and data.

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I. INTRODUCTION

Local interactions fundamentally affect the behavior of quantum systems. They are the reason for phenomena such as the Mott insulating state in the Hubbard model and their interplay with the kinetic energy is believed to be one important ingredient for high-temperature superconductivity in CuO₂ layers via the superexchange mechanism [1,2]. In the two-dimensional Hubbard model, the effect of interactions has been extensively studied over the last years with cold atom quantum simulators in optical lattices [3–11]. A step beyond the two-dimensional Hubbard model is the bilayer Hubbard model with two coupled planes [12–15] that has recently been demonstrated in a quantum simulator in Refs. [16,17]. Here, the coupled planes could be realized using an optical superlattice. The calibration of the latter makes it, among other things, necessary to simulate and predict the behavior of interacting atoms in such a potential. While interacting atoms represented by interacting Wannier functions (WFs) in a monochromatic lattice have been studied in Refs. [18–20] and noninteracting WFs in a superlattice were calculated via the band projected position operator (BPPO) method in Refs. [21–23], we present a method to compute interacting WFs in a superlattice, compare our simulation to a measurement, and find good agreement between both.

The paper is structured as follows: In Sec. II A, we briefly discuss noninteracting WFs in a superlattice which we obtain from the BPPO method and recall the calculation of Hubbard parameters which are used later. In Sec. II B, we present the method to compute interacting WFs in a superlattice potential. Finally, in Sec. III, we compare our simulation to a measurement.

II. METHODS

A. Noninteracting Wannier functions in a superlattice

Maximally localized, noninteracting WFs $w(z)$ in a superlattice,

$$V_{sl}(z) = -V_l \cos^2(k_l z - \phi) + V_s \cos^2(k_s z), \quad (1)$$

can be computed via the band projected position operator (BPPO) method [21–23]. Here, V_l (V_s) is the lattice amplitude of a long, red-detuned (short, blue-detuned) monochromatic lattice with respect to the atomic transition, $k_l = \pi/a_l$ ($k_s = \pi/a_s$) is the respective lattice vector with lattice constant a_l (a_s), and ϕ is the superlattice phase. The BPPO method encompasses the summation over all Bloch bands to obtain the maximum localization of the WFs. For numerical computation, however, one needs to cut this sum. We use eight bands to calculate noninteracting WFs in the superlattice for reasonable computation time. Figure 1 exemplarily shows the ground-state WF on the left subsite of one double well of the superlattice. The lattice configuration is $V_l = 150E_{\text{rec}}^l$ and $V_s = 34E_{\text{rec}}^s$ with the recoil energy $E_{\text{rec}}^{l,s} = \hbar^2 k_{l,s}^2 / (2m)$ ($1E_{\text{rec}}^l \hat{=} 0.28$ kHz and $1E_{\text{rec}}^s \hat{=} 1.2$ kHz), $a_l = 2.12$ μm and $a_s = 1.064$ μm , and $\phi = 0.13$. We use this configuration also in the next section for better comparison.

The calculated WF can further be used to compute Hubbard parameters, namely, the kinetic energy

$$E_{\text{kin}} = \int w_{L/R}^*(z) \left[-\frac{\hbar^2}{2m} \partial_z^2 \right] w(z)_{R/L} dz, \quad (2)$$

the on-site interaction strength

$$U^{L/R} = \frac{4\pi \hbar^2 a_s}{m} \int |w_{L/R}(z)|^4 dz, \quad (3)$$

and the on-site energy

$$E_{\text{on-site}}^{L/R} = \int w_{L/R}^*(z) V_{sl}(z) w_{L/R}(z) dz, \quad (4)$$

with $\hbar$, m , and $w_{L/R}(z)$ the reduced Planck constant, the particle mass, and the WF which is centered at the left/right subsite of the double well in the superlattice. Furthermore, the scattering length a_s in Eq. (3) determines the kind of interaction,

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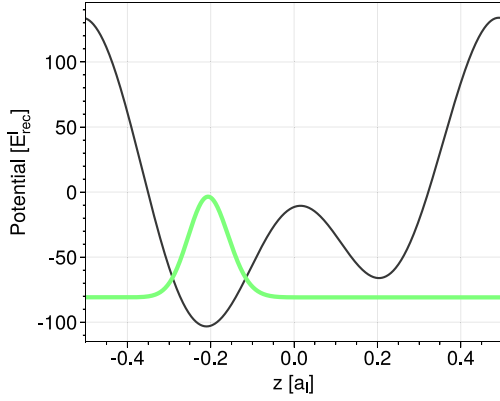


FIG. 1. Ground-state WF on the left subsite of one double well of the superlattice using eight bands for the calculation. The WF is not normalized for better illustration. The y axis is given in units of the recoil energy of the long lattice.

i.e., attractive for $a_s < 0$ and repulsive for $a_s > 0$. However, when the interaction strength U is computed via Eq. (3) using noninteracting WFs from the BPPO method as the one in Fig. 1, the result will be imprecise since the interactions alter the WF which, in turn, changes the true interaction strength.

B. Interacting Wannier functions in a superlattice

The effect of interactions on WFs in a monochromatic lattice was studied in Refs. [18–20]. Reference [19] used a self-consistent equation that was deduced from a variational approach by which the single-band ground-state energy of the WF is minimized. For the Mott-insulating regime, this equation reads

$$\sum_j \frac{\mu_j}{N_0} W(z - z_j) = H_0 W(z) + g_0(n_0 - 1)|W(z)|^2 W(z) + 2g_0 n_0 \sum_{z_j \neq 0} |W(z - z_j)|^2 W(z), \quad (5)$$

with $g_0 = 4\pi\hbar^2 a_s/m$, μ_j , n_0 , and N_0 the interaction parameter, the Lagrangian multipliers, the number of particles per site, and the total number of particles in the system, respectively. Furthermore, $H_0 = -\hbar^2/(2m)\nabla^2 + V(z)$ the lattice potential. $W(z)$ can be expressed as a sum of single-particle WFs $w_n(z - z_j)$ over n Bloch bands on site j and its nearest neighbors on site $j \pm 1$.

We modify Eq. (5) and use the superlattice potential from Eq. (1) for $V(z)$. Moreover, the superlattice has a different symmetry than the monochromatic lattice and we use the $W(z)$ that only includes contributions from $z_j = 0$. With that, the self-consistent equation (5) reads

$$\mu W(z) = H_0 W(z) + g_0(n_0 - 1)|W(z)|^2 W(z). \quad (6)$$

To solve it, we make use of the Trotter method [24]. For that, we start with an initial function $w_0(z)$ that is the noninteracting ground-state WF obtained from the BPPO method (see Fig. 1). We then iteratively perform Trotter steps in imaginary time on the k th function $W_k(z)$ to obtain $W_{k+1}(z)$ with $k \in \{0, 1, 2, \dots\}$ until the series converges to $\|W_{k+1}(z) - W_k(z)\|^2 < \Delta$ with Δ a predefined threshold. Figure 2(a)

shows the convergence of $\|W_{k+1}(z) - W_k(z)\|^2$ as a function of the iteration step k for the first twenty thousand steps for repulsive and attractive interactions. For consistency, we choose the lattice configuration and the WF from Fig. 1 as the starting function $w_0(z)$. For repulsive interactions the scattering length is $a_s = 100a_0$ and for attractive interactions $a_s = -100a_0$ with a_0 being the Bohr radius. Furthermore, we compute for each $W_k(z)$ the kinetic energy E_{kin} following Eq. (2), the interaction energy U from Eq. (3), and the on-site energy $E_{\text{on-site}}$ from Eq. (4). Figure 2(b) depicts the kinetic energy as a function of k . For repulsive interactions it decreases during iteration since the WF broadens and hence the WF's curvature decreases. For attractive interactions, the opposite is the case. The interaction strength U in Fig. 2(c) shows similar behavior. Note that for attractive interactions, U becomes negative and thus the absolute value of U increases with increasing iteration step. Finally, the on-site energy in Fig. 2(d) decreases with iteration for repulsive interactions which is because the superlattice potential outside the subsite minimum decreases in absolute value and vice versa for attractive interactions.

With that procedure, we first compute and show interacting WFs for varying scattering lengths a_s from attractive to repulsive interactions (see Fig. 3). Again, the same superlattice configuration is used as for Figs. 1 and 2 for consistency. The interacting WFs show a smooth broadening with increasing interaction strength from attractive to repulsive interactions.

Second, we compare our method to find the interacting WF in the superlattice with previous computations of interacting WFs in monochromatic lattices [19]. Figure 4(a) depicts a monochromatic lattice potential (black solid line) and the corresponding noninteracting WF (black dashed-dotted line) for a lattice depth of $V_{\text{mono}} = 150E_{\text{rec}}^1$. The superlattice approximates one potential well for an increasing superlattice phase from $\phi = 0$ to $\pi/4$ as shown in Fig. 4(a). Here, the superlattice has $V_1 = 90E_{\text{rec}}^1$, $V_s = 25E_{\text{rec}}^s$, and a phase of $\phi = 0$ (blue dotted line), $\phi = \pi/12$ (blue dashed-dotted line), and $\phi = \pi/4$ (blue solid line). We also plot the noninteracting WF from the BPPO method corresponding to the respective superlattice in Fig. 4(a) as pink dotted, dashed-dotted, and solid lines. One can see that the noninteracting WF in the superlattice approximates the WF in the monochromatic lattice with increasing phase when the potential well becomes more and more similar to the monochromatic lattice. Figure 4(b) shows the same analysis for interacting WFs where the interacting WF in the monochromatic lattice is computed according to Ref. [19] and the interacting WF in the superlattice according to the ansatz described in this work. Again, one sees that the interacting WF in the superlattice approximates the WF in the monochromatic lattice with increasing superlattice phase.

III. RESULTS AND DISCUSSION

Finally, we compute interacting WFs in the superlattice and deduce the interaction strength following Eq. (3). We then compare the results to a measurement of U between two cold atoms in an optical superlattice [17]. The measurement procedure was conducted as follows: the superlattice consisted of two vertical, monochromatic optical standing waves with long and short lattice constants $a_l = 2.12 \mu\text{m}$ and $a_s = 1.064 \mu\text{m}$, respectively. In the beginning, the atoms were

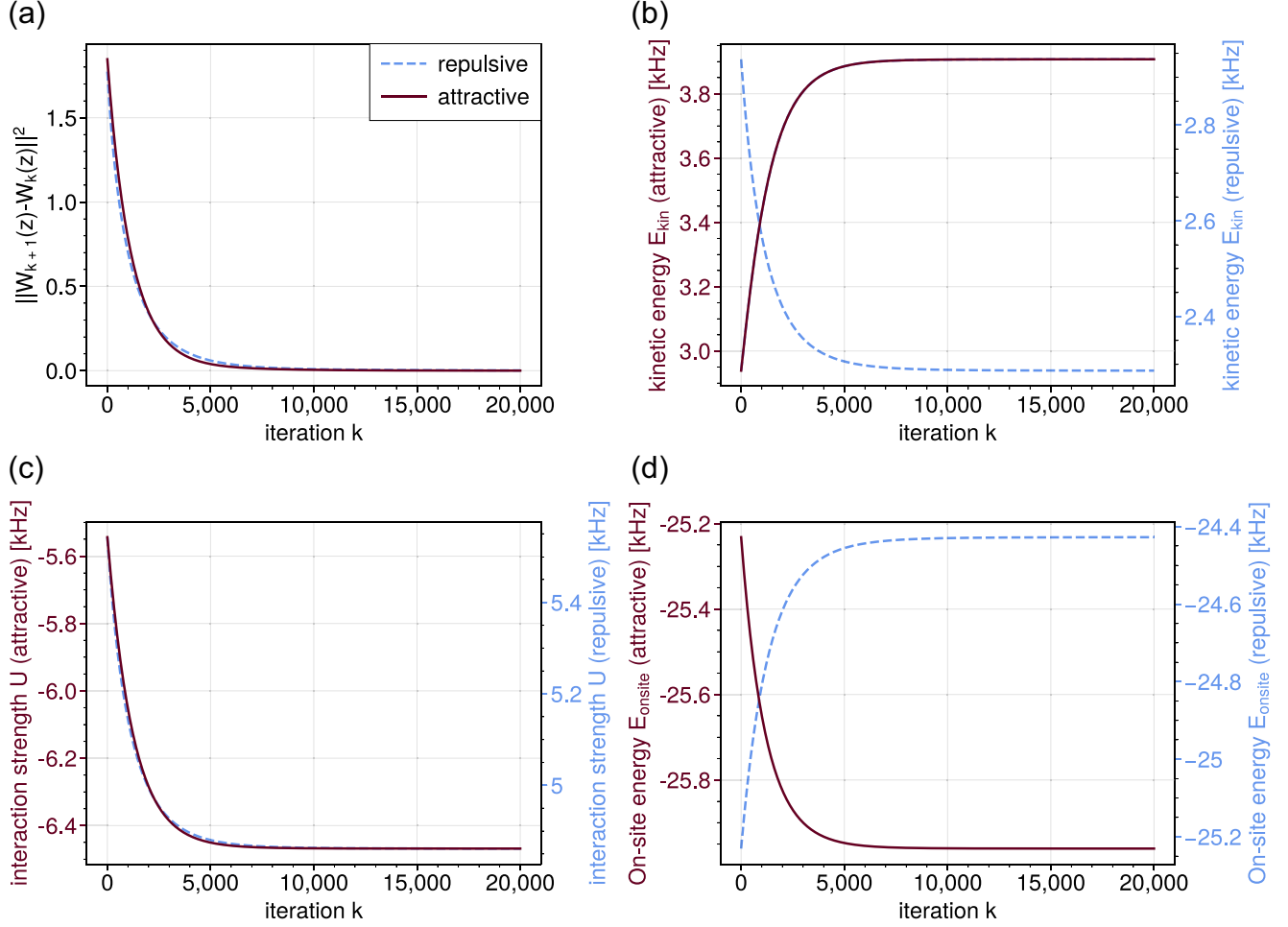


FIG. 2. (a) Convergence of $W_k(z)$ as a function of the iteration step k for attractive (red) and repulsive (blue) interactions. (b) Kinetic energy, (c) Interaction energy, and (d) On-site energy as a function of k . The left y axis refers to attractive, and the right y axis to the repulsive interactions in (a)–(c).

held in a two-dimensional, in-plane lattice at $V_{xy} = 60E_{\text{rec}}^{xy}$ with lattice constant $a_{xy} = 532$ nm and in a short vertical lattice at $V_s = 120E_{\text{rec}}^s$. The phase ϕ was stabilized by a frequency offset lock at $\phi = 0.13 \pm 0.01$. Subsequently, the vertical long lattice was increased in 50 ms to either $V_l = 150$

or $200E_{\text{rec}}^l$ and the short lattice simultaneously decreased to $V_s = 17, 25$, or $34E_{\text{rec}}^s$. In this configuration, radio-frequency spectroscopy was performed at a magnetic field of $B = 194.495$ G. This caused one of two atoms at the same superlattice site to be transferred from $|F = 9/2, m_F = -5/2\rangle$ to $|F = 9/2, m_F = -7/2\rangle$ while the second atom remained in the $|F = 9/2, m_F = -9/2\rangle$ state. Thus, we measured the relative interaction strength $\Delta U = U_{95} - U_{97}$. The data are plotted in Fig. 5 as blue and green symbols for the two long lattice amplitudes V_l . They increase in absolute value for increasing V_s due to a stronger confinement of the WFs. Moreover, the long lattice amplitude V_l has a minor impact on U .

For the simulation, the three-dimensional interaction strength is needed to compare it with the measurement. To do so, we separately integrate over WFs for each direction, i.e., $U^{3D} = g_0 \int |W(x)|^4 dx \int |W(y)|^4 dy \int |W(z)|^4 dz$. Furthermore, the scattering length of two atoms in the $|F = 9/2, m_F = -9/2\rangle$ and $|F = 9/2, m_F = -7/2\rangle$ states is $a_{97} = 322a_0$ and in the $|F = 9/2, m_F = -9/2\rangle$ and $|F = 9/2, m_F = -5/2\rangle$ states $a_{95} = 218a_0$ at a magnetic field of $B = 194.495$ G. We simulate three cases: First, we compute ΔU using WFs in a three-dimensional monochromatic

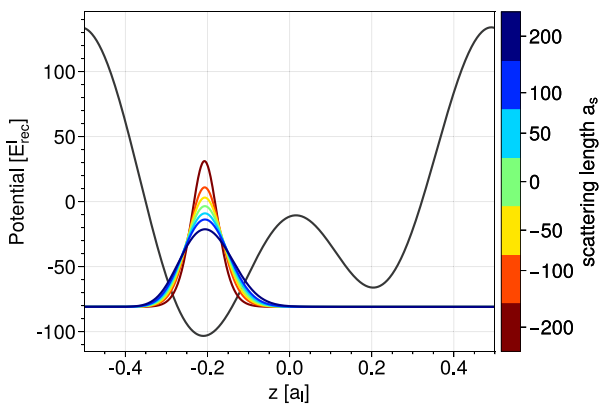


FIG. 3. Interacting WFs for different scattering lengths. The WF for $a_s = 0$ is similar to the noninteracting WF in Fig. 1.

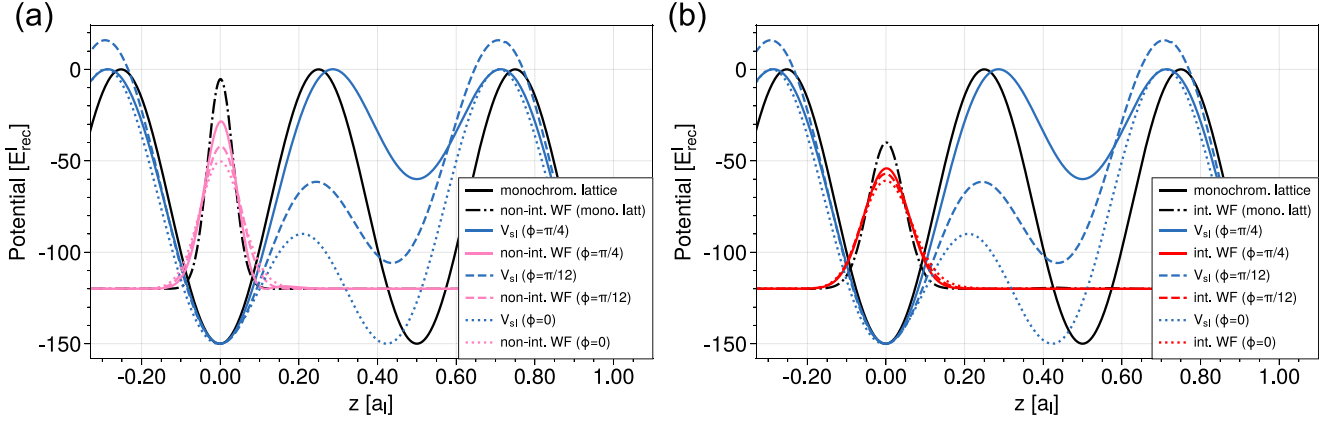


FIG. 4. Comparison of WFs in a superlattice and monochromatic lattice. (a) A monochromatic lattice potential and the corresponding noninteracting WF (black solid and dashed-dotted line). The superlattice and noninteracting WF from the BPPO method approaches the monochromatic lattice and its WF for increasing superlattice phase from $\phi = 0$ to $\pi/4$. (b) The same analysis as in (a) for an interacting WF in the monochromatic lattice computed following Ref. [19] and in the superlattice using the method in this work.

lattice with $V_x = V_y = 60E_{\text{rec}}^{xy}$ and $V_z = 120E_{\text{rec}}^l$ similar to the approximation of the superlattice in the z direction as a monochromatic lattice in Fig. 4. The result is shown in Fig. 5 for noninteracting WFs as a black dotted line and for interacting WFs as a dashed-dotted line, respectively. Second, we used a monochromatic lattice in the x and y directions with $V_x = V_y = 60E_{\text{rec}}^{xy}$ and a superlattice in the z direction with $V_l = 150$ and $200E_{\text{rec}}^l$ with noninteracting WFs in the monochromatic lattice and in the superlattice from the BPPO method (black and red squares). Finally, we use interacting WFs in the monochromatic lattice computed as in Ref. [19] and interacting WFs in the superlattice calculated with the presented method in this work (black and red solid circles). One sees that the calculation with the z superlattice and with noninteracting WFs (squares) approaches the calculated ΔU using noninteracting WFs in a three-dimensional monochromatic lattice (dotted line) for increasing V_s when the superlattice goes over into a deep monochromatic lattice. The same holds for the interacting case (solid circles and dashed-dotted line).

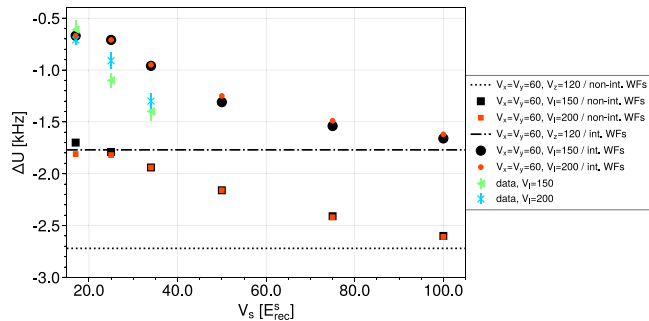


FIG. 5. Relative interaction strength measurement ΔU in an optical superlattice for two different values of the long lattice amplitude $V_l = 150, 200E_{\text{rec}}^l$ as a function of V_s . Additionally, ΔU was simulated for three cases: first, using WFs in a three-dimensional monochromatic lattice with $V_x = V_y = 60E_{\text{rec}}^{xy}$ and $V_z = 120E_{\text{rec}}^l$; Second, in a two-dimensional, in-plane lattice with $V_x = V_y = 60E_{\text{rec}}^{xy}$ and in a vertical z superlattice with $V_l = 150$ and $200E_{\text{rec}}^l$ using noninteracting WFs; and Third, using interacting WFs.

Moreover, ΔU calculated with noninteracting and interacting WFs show a similar behavior as a function of V_s as the data, i.e., it increases in absolute value for increasing V_s . However, the discrepancy in the noninteracting case is rather large with up to about 70% deviation at $V_s = 17E_{\text{rec}}^s$. In contrast, the calculation using interacting WF (solid circles) matches the data at $V_s = 17E_{\text{rec}}^s$ within the error bars. For higher V_s , we find a stronger increase in $|\Delta U|$ with V_s in the measurement than predicted by simulation. Finally, we find that the slope of $|\Delta U|$ as a function of V_s decreases, meaning it is only $\Delta U \approx -0.1$ kHz between $V_s = 75$ and $100E_{\text{rec}}^s$ in the interacting case. This underlines that interactions strongly alter the WFs in shallow lattices while, for deep lattices, the strong confinement counteracts the broadening of the WFs due to the repulsive interactions.

IV. CONCLUSION

In conclusion, we have shown a method to compute interacting Wannier functions in a superlattice. Starting from noninteracting Wannier functions obtained from the band projected position operator method, we made use of the Trotter method to iteratively modify the starting function and obtained the interacting Wannier function. We then used these interacting WFs to compute the relative interaction strength, compared it to a measurement, and find good agreement between simulation and data.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [25], embargo periods may apply.

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