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Numerical Computation of Wannier Functions

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Contents

1 Exact Diagonalization in Momentum Space

1.1 Calculating Bloch Functions

Consider a one-dimensional optical lattice described by the periodic potential

$$V(x) = \frac{V_0}{2}\left(1 - \cos(k_{\text{lat}}x)\right) \ , \tag{1}$$

where V_0 is the depth of the potential, and k_{lat} is the lattice-vector. *Bloch's Theorem* states that energy eigenstates of such a periodic potential are Bloch waves of the form

$$\phi_k^{(n)}(x) = e^{ikx}u_k^{(n)}(x) \ , \tag{2}$$

which is a plane wave with quasi-momentum k modulated by a function, $u_k^{(n)}(x)$, with the same periodicity as the potential. The energy eigenspace of such a potential takes the form of bands, where n denotes the band number. One can express $u_k^{(n)}(x)$ as a linear combination of plane waves with period of the reciprocal lattice

$$u_k^{(n)}(x) = \sum_l c_{l,k}^{(n)} e^{ilk_{\text{lat}}x} \ , \tag{3}$$

where $c_{l,k}^{(n)}$ are coefficients, l is the site index ranging from $-L \leq l \leq L$, where L is the number of sites. $l \cdot k_{\text{lat}} = G_l$ constitutes the reciprocal lattice vector of site l. Thus, the Bloch functions can be written as

$$\phi_k^{(n)}(x) = e^{ikx}\sum_l c_{l,k}^{(n)} e^{ilk_{\text{lat}}x} \ , \tag{4}$$

where $k \in [-k_{\text{lat}}/2 \ , \ k_{\text{lat}}/2]$ due to the periodicity of $u_k^{(n)}(x)$. Likewise, one can express the potential as a linear combination of plane waves with period of the reciprocal lattice

$$V(x) = \sum_l v_l e^{ilk_{\text{lat}}x} \ . \tag{5}$$

Hence, the eigenvalue problem of the Bloch functions reads

$$\begin{aligned} \hat{H}\phi_k^{(n)}(x) &= E_k^{(n)}\phi_k^{(n)}(x) \\ &= \sum_l c_{l,k}^{(n)} \frac{\hbar^2\tilde{k}_{l,k}^2}{2m} e^{i\tilde{k}_{l,k}x} + \sum_{l,l'} c_{l,k}^{(n)} v_{l'} e^{i\tilde{k}_{(l-l'),k}x} \ , \end{aligned} \tag{6}$$

where $\tilde{k}_{l,k} = lk_{\text{lat}} + k$. From this it is clear that the problem has a plane wave solution, thus it can be reformulated using plane wave state $|\tilde{k}_{l,k}\rangle$, such that

$$E_k^{(n)}\,|\tilde{k}_{l,k}\rangle = \sum_l c_{l,k}^{(n)} \frac{\hbar^2\tilde{k}_{l,k}^2}{2m}\,|\tilde{k}_{l,k}\rangle + \sum_{l,l'} c_{l,k}^{(n)} v_{l'}\,|\tilde{k}_{(l-l'),k}\rangle \ . \tag{7}$$

Since plane waves are orthonormal, $\langle\tilde{k}_{l,k}|\tilde{k}_{l',k}\rangle = \delta_{l,l'}$, multiplying $\langle\tilde{k}_{l,k}|$ unto the left of equation 7 leaves

$$E_k^{(n)}c_{l,k}^{(n)} = c_{l,k}^{(n)}\frac{\hbar^2\tilde{k}_{l,k}^2}{2m} + \sum_{l'} c_{(l-l'),k}^{(n)} v_{l'} \ . \tag{8}$$

Rewriting equation 1 to the form of equation 5 yields

$$V(x) = \frac{V_0}{2}\left(1 - \frac{1}{2}e^{-ik_{\text{lat}}x} - \frac{1}{2}e^{ik_{\text{lat}}x}\right) \ , \tag{9}$$

hence $v_0 = \frac{V_0}{2}$ and $v_{-1} = v_1 = -\frac{V_0}{4}$, while the remaining coefficients are zero. Finally, when performing calculations regarding optical lattices one often works in units of recoil energy, $E_{\text{r}} = \frac{\hbar^2k_{\text{r}}^2}{2m}$, where

$k_\mathrm{r} = \frac{k_\mathrm{lat}}{2}$ is the wave vector of the light constituting the optical lattice. Introducing the unit-less, rescaled quasi-momentum $q = \frac{k}{k_\mathrm{r}}$ allows expressing the Hamiltonian as

$$\hat{H}_{l,l'} = \begin{cases} (q+2l)^2 + \frac{V_0}{2}, & l = l' \\ -\frac{V_0}{4}, & |l-l'| = 1 \\ 0, & \text{otherwise} \end{cases}$$

This can be written in matrix form, which can be diagonalized in order to find the coefficients $c_{l,q}^{(n)}$.

1.2 Calculating Wannier Functions

Whereas Bloch functions are well localized in momentum space, the opposite is true for Wannier functions, which instead are well localized in real space. Hence, bases of Wannier functions are used to describe lattice systems within the tight binding limit [1]. Wannier functions are given by

$$w^{(n)}(x) = \frac{1}{\sqrt{L}} \sum_k e^{-ikR} \phi_k^{(n)}(x) \ , \tag{10}$$

where $R = \frac{2\pi}{k_\mathrm{lat}}$ is a Bravais lattice vector. Explicitly writing equation 10 using the coefficients $c_{l,q}^{(n)}$ and the unit-less quasi-momentum yields

$$w^{(n)}(x) = \frac{1}{\sqrt{L}} \sum_q \sum_l e^{i2\pi(q+2l)x} c_{l,q}^{(n)} \ . \tag{11}$$

The Wannier functions are necessary for computing the parameters

$$U = \frac{4\pi\hbar^2 a}{m} \int \mathrm{d}x \ |w(x)|^4 \ , \tag{12}$$

and

$$J = -\int \mathrm{d}x \ w^*(x - x_i) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x) \right) w(x - x_j) \ , \tag{13}$$

from the Bose-Hubbard model. Here a and m is the scattering length and the mass of the atoms within the optical lattice, and x_i is the center of the i'th cell of the lattice.

2 Numerical Results

The above calculations were one for the case of one dimension, however, such one-dimensional features can be achieved by applying two transversal lattices of large depth in the two remaining dimensions. This effectively decouples neighboring sites in the transverse directions, thus creating a lattice consisting of an array of tubes. However, this does affect the U-parameter (equation 12), as one has to integrate over the transverse directions as well. The following calculations reflects the setup described in [3]. Thus, the species of atoms used is Rubidium 87, the optical lattice is created using a wavelength of $\lambda = 1064\mathrm{nm}$, and the transverse lattice depth is $20E_r$.

Figure 1 displays Wannier functions for two neighboring sites calculated using equation 11 for various lattice depths. For $V_0 = 1E_\mathrm{r}$ the Wannier functions do not show a high degree of localization, as they extend over multiple sites. Thus, there is a large overlap between neighboring functions resulting in a large value of the J-parameter (equation 13). As the lattice becomes deeper, the Wannier functions become more localized: Within the tight binding limit the Wannier functions only overlap with their nearest neighbors. Hence, the kinetic term in the Bose-Hubbard model takes only nearest-neighbor hopping into account. At large lattice depths the Wannier functions barely overlap and are well approximated by Gaussians. As almost no interaction between sites takes place, the lattice turns into an array of decoupled harmonic oscillators. Hence, the Wannier functions tends towards Gaussians, as these are the eigenstates of the harmonic oscillator. Figure 2 displays the evolution of the Bose-Hubbard

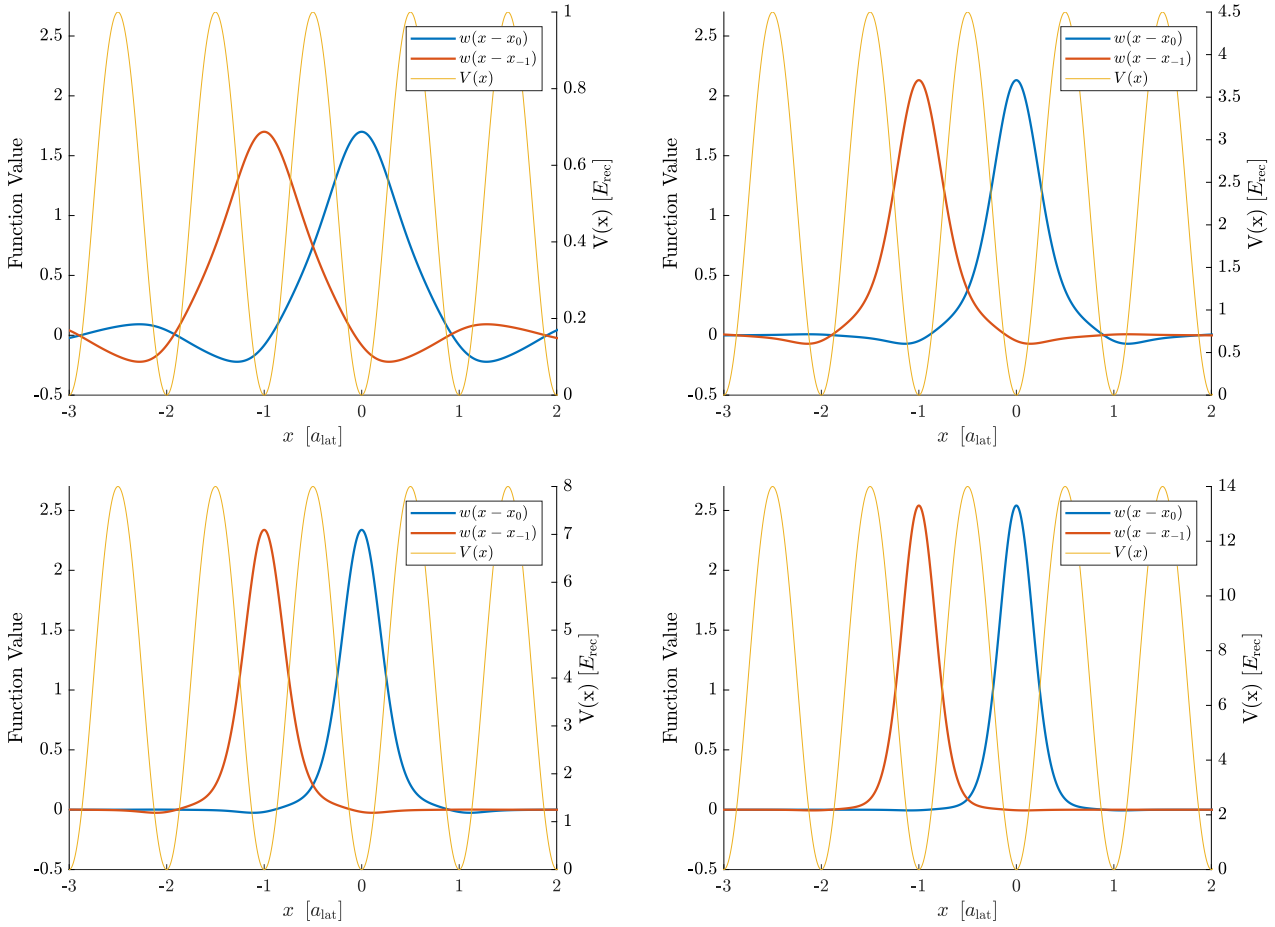

Figure 1: *Calculated Wannier functions for lattice depths* $V_0 = 1E_\mathrm{r}$, $4.5E_\mathrm{r}$, $8E_\mathrm{r}$, *and* $14E_\mathrm{r}$.

parameters as the lattice depth is increased along the final dimension. While J decreases as expected, the stronger confinement and following increase in localization of the Wannier functions results in an increase in U. In total, the fraction U/J increases rapidly with the lattice depth. The critical point of the quantum phase transition from Superfluid to Mott-Insulator for one dimension is $(U/J)_{\mathrm{crit}} = 3.37$ [2], which is marked in figure 2 by the point and the dashed line.

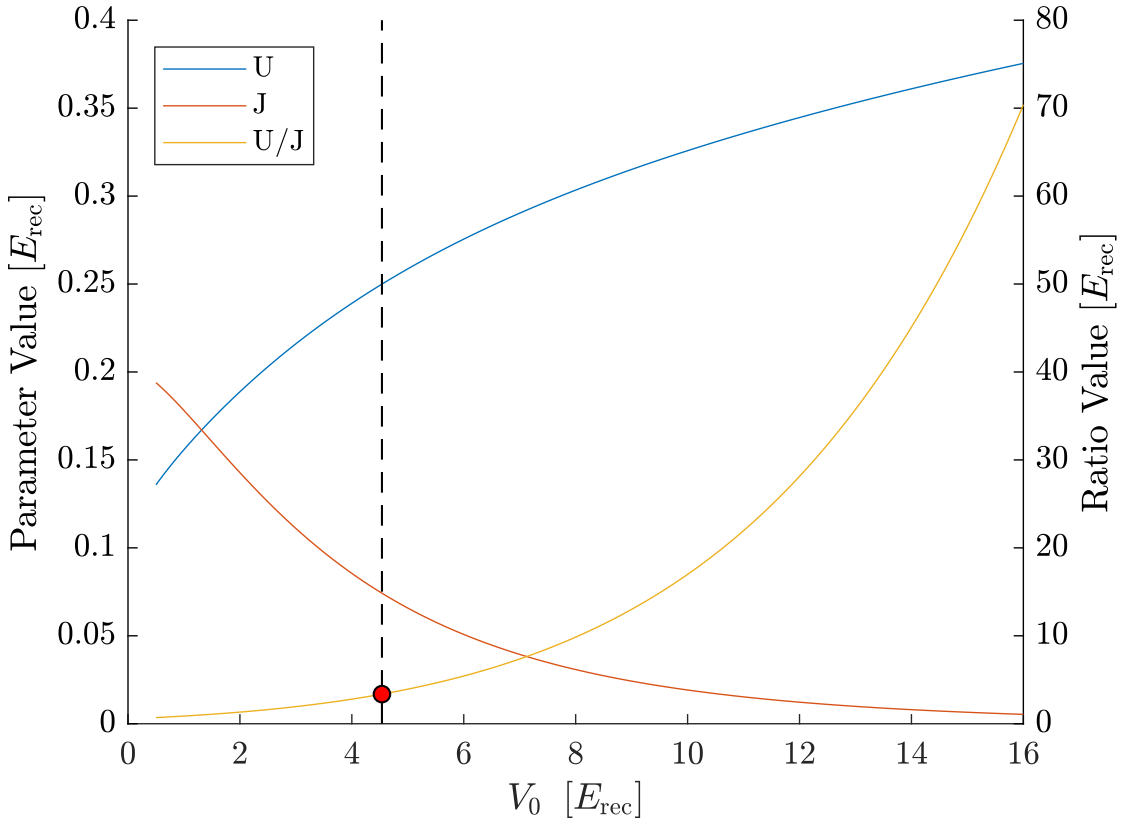

Figure 2: *Bose-Hubbard parameters calculated as function of lattice depth using a transversal confinement of* $V_{0,t} = 20E_r$. *The vertical dashed line marks the critical point of the SF-MI phase transition in 1D.*

Bibliography

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