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Numerical Computation of Wannier Functions

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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, $E_{\text{rec}} = \frac{\hbar^2 k_{\text{rec}}^2}{2m}$, where

$k_{\text{rec}} = \frac{k_{\text{lat}}}{2}$ is the wave vector of the light constituting the optical lattice. Introducing the unit-less, rescaled quasi-momentum $q = \frac{k}{k_{\text{rec}}}$ 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 $R = \frac{2\pi}{k_{\text{lat}}}$ 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

Figure REF displays Wannier functions calculated using equation 11 for various lattice depths. As expected the functions become more localized for deeper lattices, thus reducing the overlap with functions at neighboring sites. This will result in a reduction of the parameter J (equation 13), as hopping to neighboring sites become decreasingly popular as the lattice depth increases. At large lattice depths the Wannier functions are well approximated by Gaussians, as the sites will be almost completely decoupled, whereby the eigenstates will be the same as for the harmonic oscillator.

The above calculation was performed in one dimension, however, when computing parameters for the Bose-Hubbard model one must take into account all three dimensions. This is due to the Wannier functions having a final extension in all dimensions even though the lattice is effectively one dimensional. Hence, for the following calculations a transverse lattice depth of $V_{0,t} = 20E_r$ was used (same as in [3]. This depth effectively decouples neighboring sites in the transverse directions, thus creating a lattice consisting of an array of tubes. Figure REF displays the evolution of the Bose-Hubbard 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 with the lattice depth, and at POINT the critical point of the quantum phase transition from Superfluid to Mott-Insulator for one dimension is reached [2].

Bibliography

[1] Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, 80:885–964, Jul 2008.

[2] Till D. Kühner, Steven R. White, and H. Monien. One-dimensional bose-hubbard model with nearest-neighbor interaction. *Phys. Rev. B*, 61:12474–12489, May 2000.

[3] S Van Frank, M Bonneau, J Schmiedmayer, Sebastian Hild, Christian Gross, Marc Cheneau, Immanuel Bloch, T Pichler, A Negretti, T Calarco, et al. Optimal control of complex atomic quantum systems. *Scientific reports*, 6, 2016.