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RESEARCH ARTICLE

Construction of maximally localized Wannier functions

Junbo Zhu (竺俊博)[1], **Zhu Chen** (陈竹)[2], **Biao Wu** (吴飙)[1,3,4,5,†]

[1] *International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China*
[2] *Institute of Applied Physics and Computational Mathematics, Beijing 100088, China*
[3] *Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*
[4] *Wilczek Quantum Center, College of Science, Zhejiang University of Technology, Hangzhou 310014, China*
[5] *Synergetic Innovation Center for Quantum Effects and Applications (SICQEA), Hunan Normal University, Changsha 410081, China*
Corresponding author. E-mail: [†]*wubiao@pku.edu.cn*
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We present a general method for constructing maximally localized Wannier functions. It consists of three steps: (i) picking a localized trial wave function, (ii) performing a full band projection, and (iii) orthonormalizing with the Löwdin method. Our method is capable of producing maximally localized Wannier functions without further minimization, and it can be applied straightforwardly to random potentials without using supercells. The effectiveness of our method is demonstrated for both simple bands and composite bands.

Keywords Wannier function, random potential, cold atomic gases

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Wannier functions that are localized at lattice sites are a representation of electronic states in crystalline solids, alternative to Bloch waves [1]. They offer an insightful picture of chemical bonds, play a pivotal role in the modern theory of polarization [2, 3], and are the basis for efficient linear-scaling algorithms in electric-structure calculations [4, 5]. Wannier functions are also important in linking cold atom experiments in continuous light potentials with lattice Hamiltonians, such as the Bose-Hubbard model and Anderson random lattice [6–8].

Although there are explicit formulae that transform Bloch waves to Wannier functions, the construction of Wannier functions is far from trivial. The primary reason is that there are infinite Wannier functions for a given band because of the phase choices for Bloch waves, whereas in practice, the maximally localized Wannier functions (MLWFs) are sought and preferred [9]. Kohn showed a method to fix the Bloch wave phases for one-dimensional lattice to obtain these MLWFs [10]. In 1971, Teichler found a general method to construct Wannier functions, which is insensitive to the phases of Bloch waves [11]. However, this method does not guarantee maximal localization and depends on the initial trial function. A more sophisticated method involving numerical minimization of the spread of a Wannier function was developed to compute MLWFs [12]. There were also some new developments recently [13–15].

In this work, we present a general method for computing MLWFs. Our method is somewhat similar to Teichler's method as it also involves projection and the Löwdin orthonormalization method [16]. Nevertheless there is a significant difference so that our method can produce MLWFs and is insensitive to the initial trial wave functions. Compared to the method in Ref. [12], our method does not need the minimization procedure. It uses the full band projection; therefore, it can be applied straightforwardly to random potentials without using supercells. The effectiveness of our method is demonstrated for both simple and composite bands.

We consider a simple band that is isolated from the other bands. Composite bands will be discussed later. Our method of constructing MLWFs consists of three steps:

1) Guess: Choose a set of trial wave functions $|g_n\rangle$, which are localized at lattice sites.
2) Projection: $|\xi_n\rangle = P|g_n\rangle$, where $P = \sum_k |\psi_k\rangle\langle\psi_k|$ with the summation over the whole first Brillouin zone for a given band. Note that P is a full band projection and different from the projections in

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Refs. [9, 11], which are at a given k point. As a result of this crucial difference, the projected function $|\xi_n\rangle$ is localized at site n.

3) Orthonormalization: Use the Löwdin orthonormalization method [16] to transform $|\xi_n\rangle$ into a set of MLWFs $|w_n\rangle$. If one uses other methods such as Kohn's method [17] to orthonormalize $|\xi_n\rangle$, the resulting Wannier function is unlikely to be maximally localized.

Here is why our method is effective and capable of producing MLWFs. We re-write the full band projection operator in terms of Wannier functions, $P = \sum_n |w_n\rangle\langle w_n|$, where the summation is over all the lattice sites. We thus have

$$|\xi_n\rangle = \sum_m |w_m\rangle\langle w_m|g_n\rangle \approx \sum_{m=\langle n\rangle} |w_m\rangle\langle w_m|g_n\rangle, \qquad (1)$$

where $\langle n\rangle$ indicates that the summation is only over site n and its nearest neighbors. It is clear that $|\xi_n\rangle$ is localized at lattice site n. However, these projected functions $|\xi_n\rangle$'s are not orthonormal. Any orthonormalization of $|\xi_n\rangle$'s will give us a set of Wannier functions. For example, one may use Kohn's method [17]. We choose the Löwdin method [16] as it can produce MLWFs. According to Ref. [18], the Löwdin orthogonalization uniquely minimizes the functional measuring the least squares distance between the given orbitals and the orthogonalized orbitals. In our case, for the set of projected orbitals $|\xi_n\rangle$, the Löwdin method produces Wannier functions $|w_n\rangle$ that minimize

$$\sum_n \int \mathrm{d}x |\langle x|\xi_n\rangle - \langle x|w_n\rangle|^2, \qquad (2)$$

where the summation is over all the lattice sites. For a periodic potential, this is equivalent to maximizing $\langle w_n|\xi_n\rangle = \langle w_n|g_n\rangle$. Therefore, if $|g_n\rangle$ is properly chosen, the resulting Wannier function is maximally localized. No further minimization such as the one in Ref. [12] is needed.

We consider a single particle Hamiltonian with the periodic potential $V(x) = \cos(2\pi x/a)$, where a is the lattice constant, in order to illustrate our method. We construct the Wannier function for its lowest band. As each potential well is symmetric with respect to its center (the lowest point of the well), we expect that the MLWF is also symmetric with its highest peak at the center. Therefore, we choose $\langle x|g_n\rangle = \mathrm{e}^{-(x-na)^2/(2\alpha^2)}/\sqrt{2\alpha^2\pi}$. It is clear that $\langle w_n|g_n\rangle$ is the largest for the narrowest Wannier function allowed within the band or MLWF. The resulting Wannier function should be insensitive to the width of $\langle x|g_n\rangle$. This is exactly what we see in Fig. 1(a). With three Gaussians of different widths $\alpha = a, 0.5a, 0.1a$ as trial functions, the resulting Wannier functions fall right on top of each other as seen in Fig. 1(a). We have computed the spread of the Wannier functions obtained with our method; they are almost identical for Gaussian trial functions of different widths as seen in Fig. 1(b).

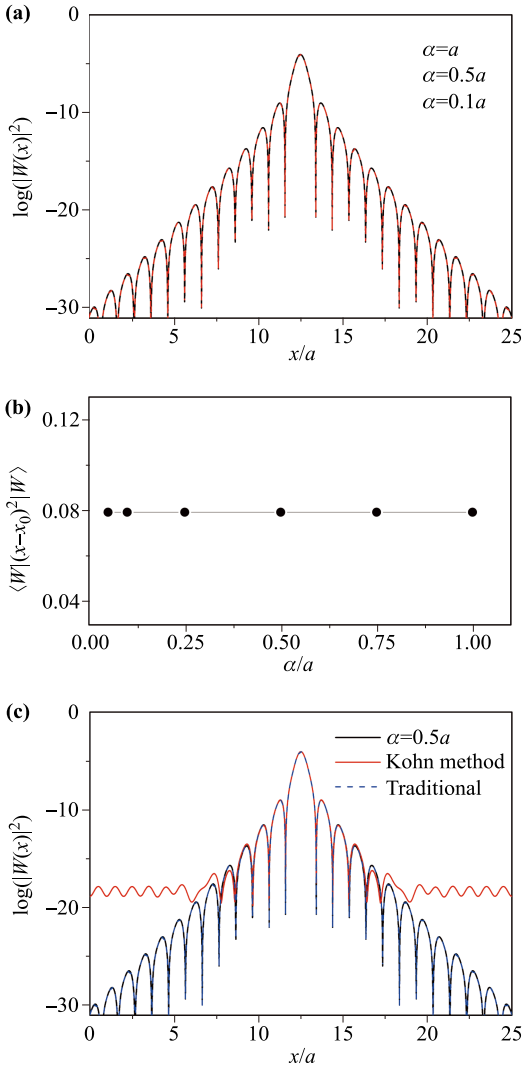

Fig. 1 Wannier functions for one dimensional periodic potential $V(x) = \cos(2\pi x/a)$. **(a)** Wannier functions obtained with our method with trial Gaussian functions of different widths α. **(b)** Spread of the Wannier function obtained with our method as a function of the width of the Gaussian function α. **(c)** Wannier functions obtained with three different methods. The black line indicates the function obtained using our method; the blue line is obtained with the traditional method, where one fixes the phases of Bloch wave according to the prescription given in Ref. [10]; the red one is obtained by orthonormalizing $|\xi_n\rangle$'s with Kohn's method [17].

We computed Wannier functions with two other methods to illustrate the effectiveness of our method further. One of them is the traditional method, where one fixes the phases of the Bloch waves according to the prescrip-

tion in Ref. [10]. The other method is to orthonormalize $|\xi_n\rangle$'s with Kohn's method [17]. The results obtained using these different methods are compared in Fig. 1(c), which shows that our result is in excellent agreement with that of the traditional method, whereas the results obtained with Kohn's method are much worse.

The Löwdin method can be implemented in different ways. However, as long as it is implemented correctly, the method transforms a given set of non-orthogonal vectors to a unique set of orthonormal vectors. Nevertheless, we explicitly demonstrate its implementation here. We impose a periodic boundary condition with N unit cells. As a result, the crystal wave vector k takes N discrete values $k_1, k_2, \cdots, k_N$. We let $|\psi_j\rangle = |\psi_{k_j}\rangle$ and $A_{nj} = \langle\psi_j|g_n\rangle$. The Löwdin orthonormalization is then implemented as

$$|w_n\rangle = \sum_{mj} (AA^\dagger)^{-1/2}_{nm} A_{mj} |\psi_j\rangle. \tag{3}$$

If the trial function $|g_n\rangle$ is translationally symmetric, $\langle x|g_n\rangle = \langle x - r_n|g_0\rangle$, we have $A_{nj} = \mathrm{e}^{-\mathrm{i}k_j r_n} A_{0j}$ and $(AA^\dagger)_{nm} = \sum_j \mathrm{e}^{\mathrm{i}k_j(r_m - r_n)} |\langle\psi_j|g_0\rangle|^2$.

Our method is applicable to composite bands. In composite bands, one or more Wannier functions have nodes. Therefore, to achieve the largest $\langle w_n|g_n\rangle$ for MLWFs, we need to choose $|g_n\rangle$'s such that they have nodes at proper positions. The node positions can be determined from the symmetries of the wells. In the worst case, we can determine these node positions by numerically computing the eigenstates of the local wells. Here we consider a two dimensional periodic potential $V(x, y) = V_0[\cos(2\pi x/a) + \cos(2\pi y/a)]$ and use its p-bands to illustrate the effectiveness of our method for composite bands. The two trial wave functions are chosen as $g_{1,2} = \sqrt{\frac{\pi}{2\alpha^4}} \eta_{1,2} \mathrm{e}^{-(x^2+y^2)/2\alpha^2}$ with $\eta_1 = x, \eta_2 = y$, which are the first two excited states of a two dimensional harmonic oscillator. The results are plotted in Fig. 2. Fig. 2(a) shows a comparison between the trial function and the resulting Wannier function. Three Wannier functions obtained from different trial functions are shown in Figs. 2(c) and (d). Our calculations show that when the width of the trial function α is sufficiently narrow, the resulting Wannier functions are almost identical to each other. When they are plotted in the figure, they fall right on top of each other. Therefore, in Figs. 2(c) and (d) only three Wannier functions are plotted. The spread of a Wannier function $\langle w|x^2+y^2|w\rangle$ is plotted as a function of α in Fig. 2(b), which shows that the Wannier function spread does not change when α is sufficiently narrow.

Our method is directly applicable to random potentials. The reason is that we use the full band projection. It can be constructed with all the energy eigenfunctions

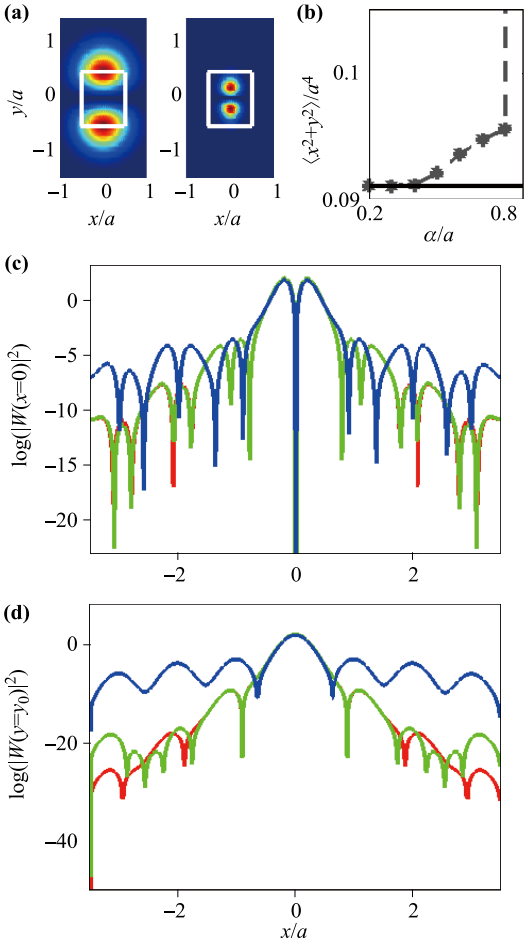

Fig. 2 Wannier functions of the composite p-bands in a two dimensional lattice $V(x, y) = V_0[\cos(2\pi x/a) + \cos(2\pi y/a)]$ with $V_0 = -30$. **(a)** trial wave function g_2 with $\alpha = 0.5a$ is shown on the left; Wannier function obtained with this trial function is shown on the right. The white dashed line marks the unit cell. **(b)** Spread $\langle w|x^2 + y^2|w\rangle$ of a Wannier function with respect to varying α. The convergence to the black line is obvious. The black line is the width of the Wannier function $w(x, y) = w_1(x)w_2(y)$, where $w_1(x)$ as the s-band Wannier function of $\cos(2\pi x/a)$ and $w_2(y)$ as the p-band Wannier function of $\cos(2\pi y/a)$ are obtained using the traditional method. **(c)** Logarithmic plot of the Wannier functions at $x = 0$ along the y-axis for different values of α: $\alpha = 0.3a$ (*red*), $0.6a$ (*green*), $0.88a$ (*blue*). Note that the latter two almost overlap. **(d)** Logarithmic plot of Wannier functions at y_0 along the x-axis for different choices of α: $\alpha = 0.3a$ (*red*), $0.6a$ (*green*), and $0.88a$ (*blue*). y_0 is the highest peak position of the Wannier functions.

in a given band regardless of whether the eigenfunctions are Bloch waves. It is well known that even in random potentials, there exist eigen-energy "bands" that are isolated from other eigen-energies by gaps that are independent of the system size. Wannier functions exist for these bands [19]. Our method can be used to com-

pute these Wannier functions by constructing the projection P using the energy eigenstates of a given random energy band. According to Eq. (2), the resulting Wannier functions maximize a sum, $\sum_n \langle w_n|g_n\rangle$. With a proper choice of $|g_n\rangle$'s, these Wannier functions can be regarded as maximally localized collectively. There are several methods to compute Wannier functions for random potentials. Our method has various advantages. The method in Ref. [20] is only applicable to cases in which the random potential is a perturbation to a periodic potential. Kivelson's method [21] has difficulty for two or three dimensional systems. Our method is clearly more efficient than the one in Ref. [8]. We recently proposed a method to compute Wannier functions for random potentials [22]. Our current method is certainly superior.

We now illustrate our method in disordered systems. We choose a disordered potential as a series of cosine-type wells of random depths, $V_n(x) = A_n[\cos(2\pi x/a) - 1]$. The well depth $A_n = A[1 + \eta \cdot \Re_n]$, where A is a constant, $\Re_n$ denotes a sequence of random numbers between -0.5 and 0.5, and η denotes the relative strength of disorder. For instance, we refer to $\eta = 0.1$ as a 10% disorder. We use $A = 5$, $a = 1$, and $\eta = 0.3$ in the example shown in Fig. 3. In our computation, we choose the same Gaussian trial functions $|g_n\rangle$ for different wells despite them being different. As shown in Fig. 3, our method successfully produces exponentially localized Wannier functions. It is clear that a narrower trial Gaussian function leads to more localized Wannier functions. Numerical results indicate that Gaussian trial functions with σ as small as $0.5a$ are sufficient to construct MLWFs.

Note that we have so far assumed that the system has time reversal symmetry. The energy eigenfunctions of these systems can always be made real. It follows that the projection P and all the matrices involved in the Löwdin method [Eq. (3)] can also be made real. Therefore, the final Wannier functions $|w_n\rangle$ are also real as long as the trial functions are real. $|w_n\rangle$ can be complex for systems in which the time reversal symmetry is broken. In this case, the Löwdin method maximizes $\mathrm{Re}\{\langle w_n|g_n\rangle\}$ and we may not obtain MLWFs. We shall leave it for future discussion.

In sum, we have presented a simple and general method for constructing MLWFs. In our method, the full band projection is used on localized trial wave functions. If the trial functions are properly chosen to respect the local potential configuration and have good node positions, the ensuing Löwdin method orthonormalizes them to MLWFs. No numerical minimization is needed. Our method can be directly applied to random potentials. The application of our method to real material is left for future.

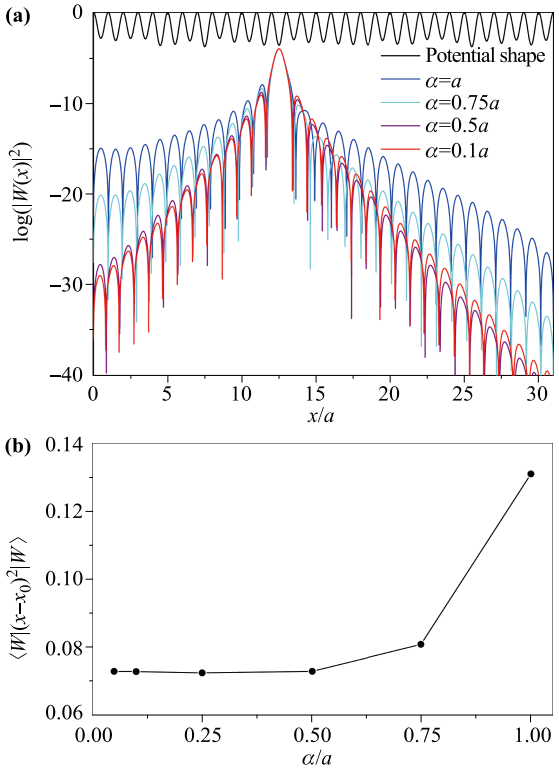

Fig. 3 Wannier functions constructed by our method for one dimensional 30% disordered potential, which is plotted as the black line at the top of (a). Initial trial Gaussian functions are the same for different wells. **(a)** Wannier functions obtained with Gaussian functions of different widths α. **(b)** Spread of the Wannier functions obtained with our method as a function of the width of the trial Gaussian function.

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