Construction of localized wave functions for a disordered optical lattice and analysis of the resulting Hubbard model parameters

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We propose a method to construct localized single particle wave functions using imaginary time projection and thereby determine lattice Hamiltonian parameters. We apply the method to a specific disordered potential generated by an optical lattice experiment and calculate for each instance of disorder, the equivalent lattice model parameters. The probability distributions of the Hubbard parameters are then determined. Tests of localization and eigen-energy convergence are examined.

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I. INTRODUCTION

Understanding the properties of disordered materials has a fundamental significance in condensed matter physics. Various kinds of disorder exist in real materials, but their disorder is difficult to characterize and control experimentally. Recently developed optical lattice techniques \[\text{[1]}\] have enabled the construction of a nearly perfectly controlled disordered potential and the measurement of properties of strongly correlated atoms in that potential provides an opportunity to compare quantitatively experimental results with parameter-free theoretical calculations. Bosonic atoms are particularly interesting because then Monte Carlo simulation is efficient.

In this paper, we consider the problem of mapping a disordered single body potential to a lattice model. By removing the high energy states associated with the continuum, the Monte Carlo simulation becomes more efficient. Particularly, efficient algorithms have been developed \[\text{[2]}\text{[3]}\] for lattice models. Consider the continuum Hamiltonian of \(N\) atoms with mass \(m\) moving in an external potential \(U(r)\) and interacting with the pairwise potential energy \(V(r_\alpha - r_\beta)\)

\[
\hat{H}_N = \sum_{\alpha=1}^{N} \left( \frac{p _\alpha^2}{2m} + U(r_\alpha) \right) + \sum_{\alpha<\beta} V(r_\alpha - r_\beta) \quad (1)
\]

where indices \(\alpha, \beta\) label the atoms. On the other hand, the quantum mechanics of particles moving in a lattice is conveniently described in a basis of localized wave functions, such as the Wannier functions associated with a periodic potential. Using these localized functions, we can define an effective lattice Hubbard Hamiltonian. Written in second quantized notation it has the form:

\[
\hat{h} = -\sum_{\langle ij \rangle} t_{ij} a_\dagger_i a_j + \sum_i \epsilon_i n_i + \frac{1}{2} \sum_i u_i n_i (n_i - 1) - \frac{1}{2} \sum_{\langle ij \rangle} \tilde{t}_{ij} a_\dagger_i a_j + \frac{1}{2} \sum_{\langle ij \rangle} \tilde{u}_{ij} n_i n_j + \cdots \quad (2)
\]

where \(i\) labels the single particle states (lattice sites), \(\langle ij \rangle\) denotes a nearest neighbor pair and \(\{ ij \}\) a next-nearest neighbor pair, \(t_{ij}\) and \(\tilde{t}_{ij}\) are hopping coefficients, \(\epsilon_i\) is the on-site energy, \(u_i\) is the on-site interaction and \(\tilde{u}_{ij}\) is the nearest neighbor off-site interaction. (Terms such as next-nearest neighbor hopping and offsite interaction are often neglected.) Note that \(\hat{H}_N\) refers to the \(N\)-body Hamiltonian in continuous space and \(\hat{h}\) to its equivalent on a lattice.

In a periodic potential, Wannier functions of a given band are related to the Bloch functions \(\psi_{nk}\) of the same band \(n\) by the unitary transformation

\[
w_{ni}(r) = w_n(r - R_i) = \frac{1}{\sqrt{N}} \sum_k \psi_{nk}(r)e^{-ik \cdot R_i}. \quad (3)
\]

\(w_{ni}\) is localized around the lattice site \(R_i\) \[\text{[4]}\]. However, in the absence of periodicity, the concept of Wannier functions needs to be generalized. Two main types of generalizations exist in literature. The perturbative approach \[\text{[5]}\] assumes the existence of the band structure and thus is applicable to nearly periodic potentials. The variational approach \[\text{[6]}\text{[7]}\text{[8]}\] emphasizes the minimization of the spatial spread with respect to unitary transformations of a starting basis set, for example the Wannier functions of a periodic potential.

In order to be useful, we would like the generalized Wannier functions to have the following properties. First, localization is required by the physical picture of particles hopping in the lattice. Second, a correct description of the low energy density of states is necessary to capture the low temperature physics. Third, for convenience, the orthogonality of the basis set is required to use commutation relations of creation and annihilation operators in the second quantized Hamiltonian. Finally, we would like the lattice Hamiltonian to be free of the sign problem so that quantum Monte Carlo calculations are efficient. This requires the off-diagonal elements to be non-positive (i.e. \(t_{ij} \geq 0\)). Note that the original Hamiltonian \(\hat{H}_N\) has this property.

In section II, we propose a method of constructing localized single particle basis functions based on imaginary time evolution of localized basis functions: \(w_i(0)\) where
\( \hat{H}_1 \) denotes the one particle Hamiltonian. This has the effect of suppressing the high energy components but also spreading out the basis states. In section III, results of the method are presented for the specific disorder probed experimentally.

II. METHOD

In constructing a lattice model, our goal is to coarse grain the description of the continuum system, so that instead of recording the precise position of an atom, we only record which lattice site it occupies. We match up the lattice and continuum models using the density matrix; we require that the low temperature density matrix of the lattice model to be identical to the reduced density matrix of the continuum system when high energy degrees of freedoms are traced out. Use of the density matrix:

\[ \rho(\mathbf{r}, \mathbf{r}'; \tau) = \left\langle \mathbf{r} | e^{-\tau \hat{H}_1} | \mathbf{r}' \right\rangle. \]  

Let \( w_i(\mathbf{r}; 0) \) be a localized basis which assigns atoms to lattice sites, e.g. \( w_i(\mathbf{r}; 0) = 1 \) if \( |\mathbf{r} - \mathbf{R}_i| \) is minimized with respect to \( i \), i.e. in the \( i^{th} \) Wigner-Seitz cell. Then a course-grained density matrix is defined as

\[ S_{ij}(\tau) = \left\langle w_i(0) | e^{-\tau \hat{H}_1} | w_j(0) \right\rangle \]

\[ = \int d\mathbf{r} d\mathbf{r}' w_i(\mathbf{r}; 0) \rho(\mathbf{r}, \mathbf{r}' ; \tau) w_j(\mathbf{r}' ; 0) \]  

Note that if \( w_i(\mathbf{r}; 0) \)'s are chosen to be everywhere positive, all elements of the lattice density matrix \( S_{ij} \) are also positive and can be used in a lattice QMC calculation directly. We now want to construct a single-particle Hamiltonian which when solved gives \( S_{ij}(\tau) \) for large \( \tau \), or in matrix notation to determine \( \hat{h} \) such that

\[ \hat{S}(\tau) = e^{-\tau \hat{h}}. \]  

Formally, the solution \( \hat{h} = -\tau^{-1} \log \hat{S}(\tau) \) may have some \( \tau \) dependence and not necessarily have the other properties mentioned above. Differentiating Eq. (7) with respect to \( \tau \) and multiply on the right and left by \( \hat{S}^{-1/2} \), we find an expression for \( \hat{h} \) in terms of \( \hat{S} \):

\[ \hat{h} = -\hat{S}^{-1/2} \frac{d\hat{S}}{d\tau} \hat{S}^{-1/2} = -\int_0^\tau e^{(\lambda - \hat{z})} \hat{h} \left( \frac{dh}{d\tau} \right) e^{(\lambda - \hat{z})} d\lambda. \]  

If we assume that \( h \) becomes \( \tau \)-independent as \( \tau \to \infty \), we can neglect the second term on the right hand side and find:

\[ \hat{h} = -\hat{S}^{-1/2} \frac{d\hat{S}}{d\tau} \hat{S}^{-1/2}. \]  

Consider the eigenfunction expansion of the continuum density matrix:

\[ \rho(\mathbf{r}, \mathbf{r}'; \tau) = \sum_{\alpha} \phi^*_\alpha(\mathbf{r}) \phi_\alpha(\mathbf{r}') e^{-\tau E_\alpha} \]  

where \( E_\alpha \) and \( \phi_\alpha \) are the 1-particle eigenvalues and eigenfunctions of the continuum Hamiltonian. For a sufficiently large \( \tau \), and for a system with a gap, only states below the gap will survive. If there are \( N \) such states, it is clear that we will capture the density of states with exactly \( N \) basis functions \( w_i \). Now let us define the orthonormalized basis by splitting up the density operator

\[ \exp \left( -\tau \hat{H}_1 \right) = \exp \left( -\frac{1}{2} \tau \hat{H}_1 \right) \exp \left( -\frac{1}{2} \tau \hat{H}_1 \right) \]  

and having it act partially to the left and right in Eq. (4). Combining Eq. (4) and Eq. (9) we obtain the expression for the model Hamiltonian:

\[ h_{ij} = \sum_{kl} S^{-1/2}_{ikj}(\tau) \left\langle w_k(\tau/2) | \hat{H}_1 | w_i(\tau/2) \right\rangle S^{-1/2}_{jl}(\tau) \]

\[ = \left\langle \tilde{w}_i(\tau/2) | \hat{H}_1 | \tilde{w}_j(\tau/2) \right\rangle \]  

where \( \tilde{w}_i(\tau) = e^{-\tau \hat{H}_1} w_i(0) \) are the non-orthonormalized basis functions at time \( \tau \) and \( \tilde{w}_i(\tau/2) = \hat{S}^{-1/2}(\tau/2) w_i(\tau/2) \) are the orthonormalized basis functions because

\[ S_{ij}(\tau) = \langle w_i(\tau/2) | w_j(\tau/2) \rangle \]  

is the overlap matrix. This is known as Löwdin orthogonalization.

The imaginary time evolution is equivalent to a diffusion process with sinks or sources determined by the potential \( U(\mathbf{r}) \). Without a potential present, an initially localized distribution will spread out as \( \sqrt{\tau} \) as a function of imaginary time. When the wavepacket (or basis function) \( |w_i(\tau)\rangle \equiv e^{-\tau \hat{H}_1} |w_i(0)\rangle \) encounters the regions of high potential energy separating the lattice sites, its diffusion will stop, until it tunnels through to the next site. If the assumption of temperature-independence

\[ \lim_{\tau \to \infty} \left( \frac{dh}{d\tau} \right) = 0 \]  

is correct, according to Eq. (12), the orthogonalized basis \( \hat{S}^{-1/2} (2\tau) |w_i(\tau)\rangle \) converges at large \( \tau \). Instead of taking the logarithm of the reduced density matrix Eq. (7), we choose to construct the lattice Hamiltonian from Eq. (9) for two reasons. Firstly, numerical tests show that Eq. (9) converges faster than \(-\frac{1}{\beta} \log \hat{S}\) as \( \tau \) increases. Secondly, the explicit construction of basis functions enables us to calculate the interaction terms in the second quantized many body Hamiltonian. Finally, use of Eq. (9) instead of Eq. (7) gives a spectrum as upper bounds to the continuum spectrum.

The choice of the initial basis function \( w_i(r;0) \) is to some extent arbitrary, as long as it is non-negative and localized within a lattice cell, and there is one basis function for each lattice site. We choose to set \( w_i(r;0) = 1 \) inside a cube of side \( \sigma \) centered on \( R_i \).

**A. Algorithm for imaginary time projection and orthogonalization**

To apply the imaginary time evolution to the construction of localized wave functions and thereby to extract microscopic parameters of the corresponding lattice model, we then start with \( N \) initial trial wave functions, each of which is well localized in one lattice cell. Each wave function is independently evolved over a sufficiently long imaginary time. The set of \( N \) wave functions are then transformed into an orthonormal basis.

To perform the imaginary time evolution, consider the Trotter formula

\[
e^{-\beta \hat{H}} = \lim_{n \to \infty} \left( e^{-\frac{\beta}{n} \hat{H}} e^{-\frac{\beta}{n} \hat{U}} \right)^n.
\]

In a coordinate representation, a single step of imaginary time \( \tau \) can be written as:

\[
w(r; t + \tau) = \int d^3r' \langle r' | e^{-\tau \hat{H}} | r' \rangle w(r', t) = \left( \frac{m}{2\pi \hbar \tau} \right)^{3/2} \times \int d^3r' e^{-\frac{m}{2\pi \hbar \tau} \left( \frac{r'^2}{2m} - \mathbf{k} \cdot \mathbf{r}' \right)^2} e^{-\frac{\tau \mathbf{k} \cdot \mathbf{r}}{\hbar}} w(r', t).
\]

This integral is a convolution, and can be efficiently evaluated by Fast Fourier Transform

\[
w(r; t + \tau) = \text{FFT} \left[ e^{-\frac{2\pi i}{m} \mathbf{k} \cdot \mathbf{r}} f_k \right]
\]

where \( f_k \) is defined as an inverse-Fourier transform

\[
f_k = \text{FFT}^{-1} \left[ e^{-\frac{2\pi i}{m} \mathbf{k} \cdot \mathbf{r}} w(r, t) \right].
\]

We can also take advantage of the localization of \( w(r) \): it is vanishingly small away from its initial site, so that we only store its values in a cube enclosing the region in which the wave function is non-zero. When doing the second FFT, Eq. (17), we add a buffer layer outside the cube with thickness chosen so that the localization region of the evolved function over one imaginary time step does not exceed the cube in which FFT is performed; the thickness is proportional to \( \sqrt{\tau / m} \). We periodically examine the evolved basis set, to determine if the cube can be made smaller. A common normalization factor is required for all basis functions every several steps to avoid numerical overflow or underflow.

Eq. (9) demands orthogonalization of the basis set. Löwdin orthogonalization preserves, as much as possible, the localization and symmetry of the original non-orthogonal basis states. In terms of the overlap matrix, we construct a set of orthogonalized states

\[
|\tilde{w}_i\rangle = \sum_j (S^{-1/2})_{ij} |w_j\rangle.
\]

No other set of orthonormal states generated from the space spanned by the original non-orthogonal set of states resemble the original set more closely, in the sense of least square, than do Löwdin set of states [15]. Explicitly, Löwdin orthogonalization minimizes the expression

\[
\phi(T) = \sum_{i=1}^N \| \hat{T} w_i - w_i \|^2
\]

over all linear transformations \( \hat{T} \) which transform the original non-orthonormal set of states \( |w_i\rangle \) into an orthonormal set of states \( |\tilde{w}_i\rangle \)

\[
\langle \tilde{w}_i, \tilde{w}_j \rangle \equiv \langle \hat{T} w_i, \hat{T} w_j \rangle = \delta_{ij}.
\]

For efficiency, this procedure can be done in an iterative fashion. Because the original non-orthogonal set of wave functions are localized, the overlap matrix \( S_{mn} \) has the form of the identity matrix plus a small off-diagonal part

\[
S_{ij} = \delta_{ij} + A_{ij}
\]

where the diagonal elements of \( A \) are zero and the off-diagonal elements \( |A_{mn}| \ll 1 \). This enables us to perform Löwdin orthogonalization iteratively by repeated application of the approximate inverse square root of the overlap matrix

\[
(\hat{S}^{-1/2})_{ij} \approx \delta_{ij} - \frac{1}{2} A_{ij}
\]

to the non-orthogonal basis set by updating the overlap matrix at each step [12]. Hence the basis set is iterated as:

\[
\tilde{w} \leftarrow \left( 1 - \frac{1}{2} \hat{A} \right) \tilde{w}
\]

until convergence is reached, \( |\tilde{A}| \sim 0 \). The convergence of the overlap matrix to identity matrix is geometric.
The iterative scheme is efficient for large systems because the basis sets are sparse. The computation time of this algorithm is linear in the number of lattice sites, i.e., the complexity is proportional to

$$\text{(\# of steps)} \cdot M \cdot n \log n$$

(25)

where M is the number of lattice sites and n is the number of pixels for each basis function.

**B. Hubbard parameters**

Once the orthogonalized basis set has been constructed, the effective lattice Hamiltonian is obtained. For convenience we drop the \(\tau\) dependance. According to Eq. (12), the single particle Hubbard parameters are calculated as detailed in Eq. (26)-(27): the on-site energies

$$\epsilon_i = \int \tilde{u}_i^+(r) \hat{H}_1 \tilde{u}_i(r) d^3r,$$

(26)

and the hopping coefficients

$$t_{ij} = -\int \tilde{u}_i^+(r) \hat{H}_1 \tilde{u}_j(r) d^3r.$$

(27)

The interaction term is computed from first-order perturbation theory in \(V\). In the case of a contact interaction with the scattering length \(a_s\) we find for \(u\):

$$u_i = \frac{4\pi a_s \hbar^2}{m} \int |\tilde{w}_i(r)|^4 d^3r,$$

(28)

and the off-site interaction

$$\tilde{u}_{ij} = \frac{4\pi a_s \hbar^2}{m} \int |\tilde{w}_i(r)|^2 |\tilde{w}_j(r)|^2 d^3r.$$

(29)

The problem of a single particle moving in a periodic potential of the form \(\cos x + \cos y + \cos z\) can be solved analytically [14]. We compared the imaginary time projected states with the results from exact diagonalization; this is shown in Fig. 1 and Fig. 2. We used a spatial grid with \(8^3\) pixels per lattice cell and an imaginary time step \(\Delta\tau = 10^{-4}E_R^{-1}\). We find the error vanishes linearly as the time step goes to zero.

**C. Measures of localization and energy**

Several quantities can be used to characterize the localization and accuracy of the basis set. The spatial spread \(\Omega_w = \langle r^2 \rangle_w - \langle r \rangle_w^2\) quantifies the localization of a wave function.

The off-site integral \(\tilde{u}_{ij}\) measures the spatial overlap between a pair of basis states. If it is small relative to \(t_{ij}\) and the Hubbard \(U\), the approximation of keeping only the on-site interaction in the lattice model is appropriate.

![FIG. 1: Hubbard U as a function of the potential depth of lattice field; the line is obtained from exact diagonalization, and the open circles are obtained using the method in this paper.](image1)

![FIG. 2: Log-scale hopping coefficient as a function of the potential depth of lattice field; the line is obtained from exact diagonalization, and the open circles are obtained using the method in this paper.](image2)

Its rms value over all nearest neighbor pairs measures the whole basis set.

The convergence rate of the \(N \times N\) matrix of the single particle lattice Hamiltonian is measured by the time derivatives of its \(N\) eigenvalues \(E^{(i)}_\text{lattice}\)’s,

$$\Gamma = \frac{1}{N} \sum_i \left| \frac{d}{d\tau} E^{(i)}_\text{lattice} \right|.$$  

(30)

To determine the accuracy of the basis set we compare \(E^{(i)}_\text{lattice}\)’s with the lowest \(N\) eigenvalues \(E^{(i)}_\text{exact}\) of the original continuum Hamiltonian \(\hat{H}_1\) estimated from

$$E^{(i)}_\text{exact} = E^{(i)}_\text{lattice}(\tau \to \infty).$$  

(31)
The worst case error is defined as

$$
\epsilon_{\text{lattice}} \equiv \max_i \left| E^{(i)}_{\text{lattice}} - E^{(i)}_{\text{exact}} \right|.
$$

We did the same estimate for the lattice Hamiltonian that has only nearest neighbor hopping terms: we denote this $\epsilon_{\text{nn}}$.

**III. RESULTS FOR A DISORDERED LATTICE**

We now apply our method to the disordered lattice potential created in the White et al. experiment [1], $^{87}$Rb atoms are trapped in a background cubic lattice potential created by red lasers with wave vector $k = \frac{2\pi}{a}$. The periodic potential is:

$$
U_L(r) = -S_L \times \sum_{i=1}^{3} \cos \left( \frac{2\pi n_i \cdot r}{a} \right)
$$

where $n_i, i = 1, 2, 3$ are three mutually orthogonal unit vectors. A disordered speckle field $U_D(r)$ is produced by a laser beam with phases randomized by a diffuser. The speckle field is everywhere positive, characterized by a speckle strength $S_D$:

$$
U_D(r) > 0, \ \forall r
$$

$$
\langle U_D(r) \rangle \approx 0.75S_D
$$

$$
\langle U_D^2(r) \rangle \approx S_D^2
$$

and a spatial auto-correlation $\langle U_D(r)U_D(r') \rangle$ with correlation length $\sim 1.29a$, i.e. slightly larger than the lattice spacing.

The total external potential is a superposition of the periodic lattice potential and the speckle potential $U(r) = U_L(r) + U_D(r)$. The single particle Hamiltonian in units of the recoil energy $E_R = \frac{\hbar^2 k^2}{2m}$ is:

$$
\mathcal{H}_1 = -\frac{\nabla^2}{\pi^2} + U(r).
$$

We constructed our potential to match the experiment as closely as possible; see the reference [1] for more details.

To investigate the evolution of lattice Hamiltonian Eq. (5), at every step of the imaginary time, the basis set is orthonormalized before constructing the Hamiltonian matrix and calculating the energies $E^{(i)}_{\text{lattice}}$. Then the basis set is evolved using the previous basis set before orthonormalization; this means each basis function is evolved independently.

To illustrate the convergence of the matrix elements of the lattice Hamiltonian, the evolution diagram of an on-site energy on one particular site and a nearest neighbor hopping coefficient on one particular bond for $S_L = 14$ and $S_D = 1$ are shown in Fig. 6. We characterize the localization of the basis functions by the average nearest neighbor off-site integral $u_{ij}$, which measures the spatial overlap between a pair of nearest neighbor basis functions. Figs. 4 shows the evolution diagrams of the average on-site interaction $u_i$ and the average off-site interaction $u_{ij}$, which are also converging at large imaginary time. The limiting value of the off-site interaction is $4 \sim 5$ orders of magnitude smaller than that of the on-site interaction, which means that the basis functions are still localized at large imaginary time. Note that although the imaginary time projection operator $e^{-\tau \mathcal{H}_1}$ spreads out the basis states, Löwdin orthogonalization operator $\hat{S}^{-1/2}$ restores their localization form.

To illustrate the effect of Löwdin orthogonalization on the localization property of the basis set, the evolution diagram for $S_L = 14$ and $S_D = 1$ is shown in Fig. 5 by including the off-site integral of the set before orthogonalization. It can be seen from the graph that Löwdin procedure helps to localize the basis functions $w(\tau)$.

The localization characterized by the spatial spread $\Omega_w$ and drift $D_w$ is shown in Fig. 5. The maximum value among all basis functions is chosen to measure the whole basis set. As shown in the graph, the values that these two quantities asymptote to at large time are small compared to the lattice constant, which signifies that the basis functions are localized.

The convergence rate $\Gamma$ of eigen-energies of the lattice Hamiltonian is shown in Figs. 4. It can be seen from the graph that the effective lattice Hamiltonian becomes temperature-independent at low temperature. It is also illuminating to look at the evolution diagram of the worst case error Eq. (32), as shown in Figs. 5 where the exact eigen-energies are estimated by

$$
E^{(i)}_{\text{exact}} = E^{(i)}_{\text{lattice}}(\tau = 4E_R^{-1}).
$$

We compared the worst case error in energy for the nearest neighbor model ($i = 0$) versus the full lattice model.
FIG. 4: Evolution diagram of the average on-site interaction $u$ (left scale) and the average nearest neighbor off-site interaction $\bar{u}$ (right scale) for $S_L = 14$ and $S_D = 1$. Note that $\bar{u}$ measures the localization of a pair of basis functions. The diagram shows that limiting value of $\bar{u}$ is $4 \sim 5$ orders of magnitude smaller than that of $u$, which indicates that the basis functions at large imaginary time are still localized.

FIG. 5: The effect of Löwdin orthogonalization on the offsite integral for $S_L = 14$ and $S_D = 1.0$. It can be seen from the graph that the imaginary time evolution spreads out the wave packets, but Löwdin orthogonalization restores the localization.

The spatial overlap between basis functions remain negligible at the early stage so that the nearest neighbor model has almost the same spectrum as the full lattice model; the error in energy is reduced as imaginary time evolves. A finite error persists in the eigen-energy of the nearest neighbor model because the next nearest neighbor hopping terms are neglected. Note that this error is less than $10^{-4}E_R$.

To explain how it is possible to suppress the energy

FIG. 6: Evolution diagram of the maximum spatial spread and drift (average deviation from the initial position) in units of the lattice constant for $S_L = 14$ and $S_D = 1$. The values that these two quantities approach at large imaginary time are small compared to the lattice constant $a$, which means that the localization the basis functions is preserved.

FIG. 7: Convergence rate $\Gamma$ of eigen-energies for $S_L = 14$ and $S_D = 1$ shown in log-scale.

FIG. 8: Imaginary time evolution of the worst case error in energy for $S_L = 14$ and $S_D = 1$, shown in log-scale.
of the original localized basis set before causing significant delocalization, it is useful to look at the single particle density of states. In particular, we are interested in whether the gap between bands persists in the presence of disorder. Fig. 9 shows the density of states of a single particle in the disordered lattice with $S_L = 14$ and $S_D = 1, 2, 3$. Energy intervals with low density of states still exist in the presence of disorder.

IV. STATISTICS OF HUBBARD PARAMETERS

We now discuss the statistical properties of the calculated Hubbard parameters. These are shown in Figs. 10 - 14 for $S_L = 14$ and $S_D = 1$. About 1000 samples of $6^3$ sites are used to construct the probability distributions of Hubbard parameters.

Fig. 10 shows the probability distribution of the on-site energy $\epsilon_i$ for $S_D = 1$ and $S_L = 14$. The distribution is skewed with a steep onset at low energy and a tail at high energy. We fit the distribution to an exponential decay function

$$P(\epsilon) \sim \exp(-\epsilon/\Gamma)$$

for $\epsilon > -10.5E_R$ finding $\Gamma \approx 0.97E_R$ for $S_D = 1$ and $S_L = 14$. Note that the disorder potential is always positive, so that the on site energy is greater than its value for the periodic lattice which is $-10.58E_R$ for this value of $S_L$.

Hopping coefficients $t_{ij}$ characterize the mobility of the atoms. Recall that negative values of $t$ will cause difficulty in quantum Monte Carlo calculations. Fig. 11 shows the probability distribution of nearest neighbor hopping coefficients. This distribution is asymmetrically centered around its value $8 \times 10^{-3}E_R$ for the periodic potential with a width

$$\frac{\delta t}{\langle t \rangle} = 0.15$$

In $10^6$ sampled bonds, only positive $t_{(ij)}$ were found. For $S_L = 14$ and for $0.05 \leq S_D \leq 1$, $\delta t/\langle t \rangle$ ranges from $10^{-2}$ to $10^{-1}$.

Fig. 12 shows the probability distribution of next-nearest neighbor hopping coefficients. This distribution is symmetrically centered around zero with a width $w = 1.25 \times 10^{-5}E_R$ and about 2 orders of magnitude smaller than nearest neighbor hopping. Note that in the clean limit, the next nearest neighbor hopping coefficient
is exactly zero for the simple cubic lattice by symmetry. As shown in Fig. 3, setting \( t = 0 \) changes the resulting single particle energies by a maximum of \( 2 \times 10^{-5} E_R \).

Fig. 12 shows the probability distribution of the Hubbard \( U \), which is characterized by its narrow peak roughly centered around the value of \( U \) in the periodic limit \( (0.36 E_R) \) with a 1% relative width. We fit this distribution to Laplace function

\[
P(u) = \frac{1}{2\Delta} \exp \left(- \frac{|u - u_0|}{\Delta} \right)
\]

with \( u_0 \approx 0.36 E_R \) and \( \Delta = 2 \times 10^{-3} E_R \). For \( S_L = 14 \) and for \( 10^{-2} \leq S_D \leq 1 \), \( \delta u / \langle u \rangle \) ranges from \( 10^{-4} \) to \( 10^{-2} \). Hence one can assume that the on-site interaction is roughly constant even in the presence of disorder. Fig. 13 shows the probability distribution of nearest neighbor overlap \( u \). We observe that the magnitude of off-site interactions is almost 4 orders of magnitude smaller than the on-site interaction; evidently negligible in the many-body interacting Hamiltonian.

On-site energies are usually assumed to be almost uncorrelated between different sites. We calculated the nearest neighbor covariance function. For \( S_L = 14 \) and \( S_D = 1 \), with \( \langle ij \rangle \) nearest neighbor pairs:

\[
\frac{\langle \varepsilon_i \varepsilon_j \rangle - \langle \varepsilon_i \rangle \langle \varepsilon_j \rangle}{\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2} \approx 0.49
\]

The \( \varepsilon_i \)'s are correlated between nearest neighboring sites for this disordered potential.

Fig. 15 shows the correlation pattern between the on-site energy difference of nearest neighboring sites and the hopping coefficient. Fit to this joint distribution gives \( \langle t(ij) \rangle - t_0 \sim \langle |\varepsilon_i - \varepsilon_j| \rangle^{\delta} \) with \( \delta = 1.05 \). In White et. al., the orientation of laser speckles does not coincide with the lattice axes; the laser speckle has a cylindrical shape whose longitudinal direction points along \( \frac{1}{2} \mathbf{n}_1 + \frac{1}{2} \mathbf{n}_2 + \frac{1}{\sqrt{2}} \mathbf{n}_3 \). The insert of Fig. 15 displays the correlation pattern for bonds in \( \mathbf{n}_3 \)-direction if the longitudinal direction of the speckles is aligned with the \( \mathbf{n}_3 \)-axis of the lattice. This illustrates the directional effect of laser speckles.

The characteristics of the speckle field is reflected in other aspects of the parameters. According to the orientation of laser speckles with respect to the lattice axes, we should expect that the average hopping coefficient along \( \mathbf{n}_1 \) and \( \mathbf{n}_2 \) to be equal and the hopping along \( \mathbf{n}_3 \) to be different. As shown in Table 1, \( \langle t_3 \rangle \) differs from those of \( \langle t_2 \rangle \) because of the cylindrical symmetry of the speckle. However, the difference is small because the correlation length of the speckle is only slightly larger than the lattice spacing, such that the nearest neighbor hopping is not sensitive to the anisotropy induced by the speckle.

In Fig. 16 the variation of the distribution widths of all 4 Hubbard parameters versus speckle intensity is shown.
for $S_L = 14$. Fig. 16(a) shows the dependence of the width $\sigma_\epsilon = \sqrt{\langle (\epsilon_i - \langle \epsilon_i \rangle)^2 \rangle}$ for the onsite energy on the disorder strength $S_D$ for $S_L = 14$. It can be seen from the graph that $\sigma$ increases linearly with the disorder strength, approximately equal to the speckle potential shift. Hence, the width is an appropriate measure of the disorder strength. The linear fit of this functional dependence gives $\sigma_\epsilon = 0.95 \times S_D$. The distribution width of nearest neighbor hopping coefficients and Hubbard $U$ are shown in Fig. 16(b) and Fig. 16(c) respectively. In Fig. 16(d), we show the disorder dependence of the mean value of Hubbard $U$. It can be seen from the graph that $\langle u \rangle$ is not sensitive to the disorder strength.

FIG. 15: Correlation between the on-site energy difference and hopping coefficient between nearest neighbor sites for $S_L = 14$ and $S_D = 1$. The insert displays the correlation pattern for bonds in $\mathbf{n}_3$-direction if the longitudinal direction of the speckles is aligned with the $\mathbf{n}_3$-axis of the lattice. The line in the insert is a fit to a power function.

FIG. 16: (Color online) The width of the probability distribution for $\epsilon$, $t_{ij}$, $u_i$ and $\langle u \rangle$ for $S_L = 14$.

### V. CONCLUSION

In this paper, we developed a method to construct low energy basis states and applied the method to calculate the Hubbard parameters in a disordered lattice created by an optical speckle field. The imaginary time projection method introduced in this paper generates a type of Wannier-like localized basis that satisfies several conditions imposed by a reasonable coarse-grained, effective lattice Hamiltonian.

Detailed many-body calculations using the determined parameters with comparison to experiments are in progress. The method can be extended to include interactions.

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**TABLE I: Directional effect of speckles for $S_L = 14$**

| $S_D(E_R)$ | $\langle \epsilon \rangle(10^{-3} E_R)$ | $\langle t \rangle(10^{-3} E_R)$ | $\langle t \rangle(10^{-3} E_R)$ |
|------------|--------------------------------|-------------------------------|-------------------------------|
| 0.050      | $8.00 \pm 2 \times 10^{-4}$ | $8.10 \pm 1 \times 10^{-4}$ | $8.10 \pm 1 \times 10^{-4}$ |
| 0.100      | $8.02 \pm 4 \times 10^{-4}$ | $8.02 \pm 4 \times 10^{-4}$ | $8.01 \pm 3 \times 10^{-4}$ |
| 0.250      | $8.10 \pm 1 \times 10^{-4}$ | $8.10 \pm 1 \times 10^{-4}$ | $8.07 \pm 1 \times 10^{-4}$ |
| 0.375      | $8.20 \pm 2 \times 10^{-4}$ | $8.20 \pm 2 \times 10^{-4}$ | $8.16 \pm 1 \times 10^{-4}$ |
| 0.500      | $8.32 \pm 3 \times 10^{-4}$ | $8.33 \pm 3 \times 10^{-4}$ | $8.26 \pm 2 \times 10^{-4}$ |
| 0.750      | $8.59 \pm 4 \times 10^{-4}$ | $8.60 \pm 4 \times 10^{-4}$ | $8.48 \pm 3 \times 10^{-4}$ |
| 1.000      | $8.72 \pm 3 \times 10^{-4}$ | $8.73 \pm 3 \times 10^{-4}$ | $8.57 \pm 2 \times 10^{-4}$ |
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[16] S is Hermitian and positive definite, so $h$ exists uniquely.
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