How to make Fermi-Hubbard model in a tweezer array?

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This note elaborates how to derive (mainly single-band) Hubbard model from a general two-body interacting Hamiltonian [1, 2] and how the model parameters are calculated in basis of maximally localized Wannier functions (MLWFs) [3].

1 Model

Starting from a general many-body Hamiltonian with two-body interaction $V_2(\boldsymbol{r}-\boldsymbol{r'})$:

$$H = H_0 + H_{\text{int}} = \int d^d\boldsymbol{r}\psi^\dagger(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{r})\right]\psi(\boldsymbol{r}) + \frac{1}{2}\int d^d\boldsymbol{r}d^d\boldsymbol{r'}\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r'})V_2(\boldsymbol{r}-\boldsymbol{r'})\psi(\boldsymbol{r'})\psi(\boldsymbol{r}). \quad (1)$$

What we now want to do is to do a basis transformation, from position space $\psi(\boldsymbol{r})$ to a new basis $w_{i\mu}$:

$$\psi(\boldsymbol{r}) = \sum_{i\mu} w_{i\mu}(\boldsymbol{r})a_{i\mu} \quad (2)$$

where i is the lattice site label and μ is the band index[1]. $w_{i\mu}$ is the Wannier basis of which the exact form we don't know so far, but is assumed following properties (or more precisely, approximations):

1. $w_{i\mu}$ is local enough such that only nearest neighbor overlap is non-negligible
2. $w_{i\mu}$ in each band is constructed by linearly combining a non-overlapping set of eigenstates of single particle Hamiltonian[2] $w_{i\mu} = \sum_a c^a_{i\mu}\phi_a$, with $H_0\phi_a = \epsilon_a\phi_a$ and $\forall\mu\neq\nu$, $a(\mu)\neq a(\nu)$

The property 2 is safe only when groups of eigenstates used to form energy bands are far apart enough from each other, or in other words, the formed bandwidth is much smaller than the bandgap.

Rewrite Hamiltonian in the new basis:

$$H = \sum_{ij\mu\nu} t_{ij\mu\nu}a^\dagger_{i\mu}a_{j\nu} + \frac{1}{2}\sum_{ijkl\mu\mu'\nu\nu'} U_{ijkl\mu\mu'\nu\nu'}a^\dagger_{i\mu}a^\dagger_{j\mu'}a_{k\nu}a_{l\nu'}. \quad (3)$$

And each matrix element is

$$t_{ij\mu\nu} = \int d^d\boldsymbol{r}w^*_{i\mu}(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{r})\right]w_{j\nu}(\boldsymbol{r}) \quad (4)$$

$$U_{ijkl\mu\mu'\nu\nu'} = \int d^d\boldsymbol{r}d^d\boldsymbol{r'}w^*_{i\mu}(\boldsymbol{r})w^*_{j\mu'}(\boldsymbol{r'})V_2(\boldsymbol{r}-\boldsymbol{r'})w_{k\nu}(\boldsymbol{r'})w_{l\nu'}(\boldsymbol{r}). \quad (5)$$

[1] i and μ are countably many indices, they must be combined together to match number of basis elements in continuous basis $|\boldsymbol{r}\rangle$. Alternatively, we can think about folded free particle bands in Brillouin zone.

[2] Note that here we don't restrict on symmetries of the single particle states. We mix them, and only sort by eigenenergy.

Now for t, use property 2 of Wannier basis, thus term is reduced to two parts:

$$\begin{aligned} t_{ij\mu} &= \int d^d\boldsymbol{r} w^*_{i\mu}(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{r})\right] w_{j\mu}(\boldsymbol{r}) \\ &= \sum_{ab} \epsilon_b (c^a_{i\mu})^* c^b_{j\mu} \int d^d\boldsymbol{r} \phi^*_a(\boldsymbol{r})\phi_b(\boldsymbol{r}) \\ &= \sum_a \epsilon_a (c^a_{i\mu})^* c^a_{j\mu} \qquad\qquad i \neq j \end{aligned} \tag{6}$$

$$E_{i\mu} = \int d^d\boldsymbol{r} w^*_{i\mu}(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\boldsymbol{r})\right] w_{i\mu}(\boldsymbol{r}) = \sum_a \epsilon_a |c^a_{i\mu}|^2, \tag{7}$$

where we have assumed the orthogonality of single particle eigenstates ϕ_a.

Furthermore, if we also use the property 1 of Wanneir basis, we can further reduce matrix t_{ij} to be nonzero only when i, j are nearest neighbors. However, this is not very important in our practical calculations.

We should check the validity of using the property 2 here. For single particle parameters t and E, we need $t \ll \Delta E$, where ΔE is the band gap. In cold atom experiments, the band gap is typically trap frequency of one single atom trap ($\sim$ kHz), which is indeed much larger than the tunneling between different traps ($\sim 100\,\mathrm{Hz}$).

Let's come to the interacting part. This part is more complicated, as it requires us to make more assumptions on the interaction. We are considering atom-atom interaction at ultracold temperature, which is, to the leading order, the van der Waals interaction $\sim \frac{C_6}{r^6}$. This interaction is fast decaying, and more importantly, is only at the range of several to tens of Bohr radii, except for Rydberg atoms, while the atom spacing is at the order of laser wavelength. So we can safely assume it to be $V_2(\boldsymbol{r}-\boldsymbol{r'}) \propto \delta(\boldsymbol{r}-\boldsymbol{r'})$. With correct dimensions we say

$$V_2(\boldsymbol{r}-\boldsymbol{r'}) = \frac{4\pi\hbar^2 a_s}{m}\delta(\boldsymbol{r}-\boldsymbol{r'}), \tag{8}$$

where a_s is the s-wave scattering length. So in general for the s-wave scattering, the interaction is local but related to any combination of four bands:

$$U_{i\mu\nu\delta\sigma} = \frac{4\pi\hbar^2 a_s}{m} \int d^d\boldsymbol{r} w^*_{i\mu}(\boldsymbol{r}) w^*_{i\nu}(\boldsymbol{r}) w_{i\delta}(\boldsymbol{r}) w_{i\sigma}(\boldsymbol{r}) \tag{9}$$

More specifically in the system we are considering, the experiments are done at extremely low temperature such that only ground motion states in the trap are used. This clears for a single band approximation, with only atoms in degenerate bands with different spins are allowed to occupy and interact in one trap. Thus,

$$U_{i\mu} = \frac{4\pi\hbar^2 a_s}{m} \int d^d\boldsymbol{r} |w_{i\mu}(\boldsymbol{r})|^4 \tag{10}$$

This approximation is safe only when interaction $U \ll \Delta E$. In experiments, with $U/t \sim O(1)$ this is also well satisfied.

The model now is simplified as, with single band and nearest neighbor approximation

$$H = \sum_{\langle ij\rangle} t_{ij} a^\dagger_i a_j + \sum_i E_i n_i + \sum_i U_i a^\dagger_{i\uparrow} a^\dagger_{i\downarrow} a_{i\downarrow} a_{i\uparrow}, \tag{11}$$

which is exactly Hubbard model with site dependent parameters.

1.1 Side note: why SU(N) Fermi-Hubbard optical lattice has no spin-exchange term

The above assumptions reveal a simple fact that the SU(N) Fermi-Hubbard model has only the density-density interaction term. In general, SU(N)-symmetric models with the Columb (or contact interactions, even though the continuum limit model is density-density interacting, the general Waniierized model is not

(see above for the approximations we used to simplify the model). However, we argue that the same type of approximation can be made to simplify the model to be with only density-density interaction terms.

We go back to Eq. 9 with the short-range approximation intact, and we now have the density-density interaction terms and spin-exchange terms. The point here is that we can still apply the "single-band" approximation on each spin, reducing the interaction term to be

$$\sum_i U_{i\mu\nu} a^\dagger_{i\mu} a^\dagger_{i\nu} a_{i\nu} a_{i\mu}, \tag{12}$$

because the Zeeman splitting on each spin flavor is at the order of $\sim$ GHz, much higher than the $U \sim$ kHz itself. The huge energy penalty on the flavor flip effectively eliminates the flavor-hopping terms.

The last step we want to argue is why the U coupling is flavor-symmetric, i.e., $U_{\mu\nu} \to U$. This is not always true, as we can see from Ref. [4]. But in general, unless particularly chosen, the hyperfine levels with the same F inherently have the identical U independent of flavor, because the trapping laser (frequency $\sim$ 100THz) in general is not sensitive to the hyperfine level (in Zeeman split level $\sim$ GHz). Again, this is a natural outcome of order hierarchy. The effective SU(N) symmetry in this model is highly accurate, given the composite two huge order differences.

For this same reason, it's not easy for the SU(N) simulator to realize a spin-selective tunneling, unless you put the atoms on different orbitals, or you may "de-detune" a certain spin level on purpose so that it resonates with the trappin laser.

2 Maximally localized Wannier functions

The above discussion on the Wannier basis doesn't show how to build the basis. For periodic boundary systems, it is relatively easy, as it can be done by a discrete Fourier series expansion of Bloch wavefunction at each lattice site. But for the isolated open boundary systems we are now interested in, we need a special technique called maximally localized Wannier function (MLWF) to build the localized basis with the two desirable properties in the last section.

The key idea here is to find out the MLWF basis $\{w_{i\mu}\}$ of band μ by optimizing the spatial variance cost function

$$\Omega_\mu = \sum_i \left[\langle w_{i\mu}| r^2 |w_{i\mu}\rangle - \sum_a \langle w_{i\mu}| r_a |w_{i\mu}\rangle^2 \right]. \tag{13}$$

From now on we concentrate on one single band, and omit the band index μ.

According to [3], it is useful to decompose the cost function into two parts: a trace of some operator Ω_I and its remainder $\tilde{\Omega}$, as the trace is invariant under unitary transformation we don't need to optimize it in the later process

$$\begin{aligned}
\Omega &= \sum_i \left[\langle w_i| r^2 |w_i\rangle - \sum_a \langle w_i| r_a |w_i\rangle^2 \right] \\
&= \sum_i \left[\langle w_i| r^2 |w_i\rangle - \sum_a \left(\sum_j |\langle w_i| r_a |w_j\rangle|^2 - \sum_{j\neq i} |\langle w_i| r_a |w_j\rangle|^2 \right) \right] \\
&= \sum_a \mathrm{tr}\left[P r_a (1-P) r_a \right] + \sum_{i\neq j} \sum_a |\langle w_i| r_a |w_j\rangle|^2 \\
&= \Omega_I + \tilde{\Omega},
\end{aligned} \tag{14}$$

where $P = \sum_i |w_i\rangle \langle w_i|$ is the projector onto the μ-th band.

Then the problem is reduced to calculate all off-diagonal matrix elements $\langle w_i| r_a |w_j\rangle$ in eigenstate basis

$\{\phi_a\}$ and optimize over unitary matrix c_i^m:

$$\begin{aligned}\tilde{\Omega} &= \sum_{i\neq j}\sum_a |\langle w_i| r_a |w_j\rangle|^2 \\ &= \sum_{i\neq j}\sum_a |\sum_{mn}(c_i^m)^* c_j^n r_{a,mn}|^2,\end{aligned} \tag{15}$$

where $r_{a,mn}$ is a shorthand for $\langle\phi_m| r_a |\phi_n\rangle$.

This expression is non-negative, and the zero value can be taken if we can simultaneously diagonalize $r_a = x, y, z$. If we calculate a 1D lattice, only $r_a = x$ matrix would be non-zero (the reason will be seen below: reflection symmetry of bands), the solution states are just eigen states of x_{mn}, and is real given that eigenstates of real hermitian matrix are real (disregarding the overall phase).

What about higher dimensions? This is no longer true, as DVR basis is not complete, the matrices r_a are basis dependent and in general don't commute. The optimization needs to be done numerically. But we can play a trick so that the matrix c_i^m is simplified to be real entries only.

This is done as the following. We find 3 real (orthogonal) matrices O_{kl}^a to diagonalize $r_{a,mn}$ respectively:

$$r_{a,l}\delta_{kl} = \sum_{mn} r_{a,mn} O_{ln}^a O_{km}^a. \tag{16}$$

Then we decompose $c_i^m = \sum_l O_{ml}^a z_{li}^a$. We absorb all complex phases into unitary matrix z_{li}^a. For any a:

$$\begin{aligned}\sum_{i\neq j}|\sum_{mn}(c_i^m)^* c_j^n r_{a,mn}|^2 &= \sum_{i\neq j}|\sum_l (z_{li}^a)^* z_{lj}^a r_{a,l}|^2 \\ &= \sum_{i\neq j}\sum_l (z_{li}^a)^* z_{lj}^a r_{a,l}\sum_n (z_{nj}^a)^* z_{ni}^a r_{a,n} \\ &= \sum_{ln} r_{a,n} r_{a,l}\sum_{i\neq j}(z_{li}^a z_{nj}^a)^* z_{ni}^a z_{lj}^a \\ &= \sum_{ln} r_{a,n} r_{a,l}\left(\sum_{ij} - \sum_{j=i}\right)(z_{li}^a z_{nj}^a)^* z_{ni}^a z_{lj}^a \\ &= \sum_{ln} r_{a,n} r_{a,l}\left[\sum_i (z_{li}^a)^* z_{ni}^a \sum_j (z_{nj}^a)^* z_{lj}^a - \sum_i (z_{li}^a z_{ni}^a)^* z_{li}^a z_{ni}^a\right] \\ &= \sum_{ln} r_{a,n} r_{a,l}\left(\delta_{ln} - \sum_i |z_{li}^a|^2 |z_{ni}^a|^2\right).\end{aligned} \tag{17}$$

We can see that the cost function value is independent on phase of any matrix entry z_{li}^a. So it is safe to set all entries of c_i^m to be real.

This is done by, say, in symmetry-adapted sinc DVR basis:

$$\begin{aligned}\langle w_i| r_a |w_j\rangle &= \sum_{mn}(c_i^m)^* c_j^n \int d^d\boldsymbol{r}\,\phi_m^*(\boldsymbol{r}) r_a \phi_n(\boldsymbol{r}) \\ &= \sum_{mn}\sum_{kl}(c_i^m)^* c_j^n (\phi_{mk}^p)^* \phi_{nl}^q \int d^d\boldsymbol{r}(\Delta_k^p(\boldsymbol{r}))^* r_a \Delta_l^q(\boldsymbol{r}),\end{aligned} \tag{18}$$

where p, q are sector labels of the corresponding eigenstates k, l. Once k, l are determined, p, q are automatically determined so they are not independent indices. Values of k, l are related to symmetry sectors they are in:

$$k = \begin{cases} 0, 1, \ldots, N & p = 1 \\ 1, 2, \ldots, N & p = -1. \end{cases} \tag{19}$$

Immediate observation tells that for any dimension $b \neq a$, the orthogonality ensures symmetry sector $p_b = q_b$ must be satisfied; while for dimension a, $p_a = -q_a$ is the only way to make the integral nonvanishing. Combining with the quadrature rule of DVR basis integral, in eg. 3D the integral is calcualted as

$$\begin{aligned}
&\int d^d\boldsymbol{r}(\Delta_k^p(\boldsymbol{r}))^* r_a \Delta_l^q(\boldsymbol{r}) \\
&= \frac{\Delta x_a}{2}\delta_{p_a,-q_a}\prod_{b\neq a}\delta_{p_b,q_b}\sum_{\substack{i=-N\\ i\neq 0}}^{N} i(\delta_{ki}+p_a\delta_{k,-i})(\delta_{li}+q_a\delta_{l,-i}) \\
&= \frac{\Delta x_a}{2}\delta_{p_a,-q_a}\prod_{b\neq a}\delta_{p_b,q_b}\sum_{\substack{i=-N\\ i\neq 0}}^{N} [i\delta_{ki}\delta_{li}-(-i)\delta_{k,-i}\delta_{l,-i}] \\
&= \Delta x_a\delta_{p_a,-q_a}\prod_{b\neq a}\delta_{p_b,q_b}\sum_{i=1}^{N} i\delta_{ki}\delta_{li}.
\end{aligned} \tag{20}$$

So the matrix element is

$$\langle w_i|\, r_a\, |w_j\rangle = \sum_{mn}(c_i^m)^* c_j^n \Delta x_a \sum_{l=1}^{N} l(\phi_{ml}^p)^*\phi_{nl}^q\delta_{p_a,-q_a}\prod_{b\neq a}\delta_{p_b,q_b} = \sum_{mn}(c_i^m)^* c_j^n R_{mn}^a \tag{21}$$

By calculating the matrix element of tensor R_{mn}^a, we can derive the cost function needed by optimization.

For optimization of a unitary matrix, there are established algorithms for such kind of Riemannian manifold optimization, eg. the ones implemented in `pymanopt` package [5]. By using them the target unitary transformation is readily obtained.

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