QFT by Lancaster and Blundell Sections 4.4 and 4.5

Wayne Dam

Physics Cafe

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Outline

4.4 Two Particles

- We now consider the case of two particles interacting with each other.
- The second-quantized two particle operator $\hat{A}$ is given by

$$\hat{A} = \sum_{\alpha\beta\gamma\delta} A_{\alpha\beta\gamma\delta}\, \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\delta \tag{1}$$

  and the matrix elements are given by

$$A_{\alpha\beta\gamma\delta} = \langle \alpha\beta | \hat{A} | \gamma\delta \rangle \tag{2}$$

- Note the operators are written with the annihilation operators to the right and the creation operators on the left.
  This is known as *Normal Ordering* and is convenient for calculations.
- For example it ensures the operator has zero vacuum expectation value:
  $\langle 0 | A | 0 \rangle = 0$.

- Recall the decomposition of an observable operator, A, in terms of its eigenvalues and eigenvectors,

$$A = \sum_{\alpha} |\alpha\rangle\langle\alpha|, \tag{3}$$

where we are indexing the eigenvectors by the eigenvalues themselves.
The eigenvalues are the outcomes of measurements associated with the Hermitian operator A and the eigenvectors the resulting states after a measurement.

- Then we can write a function of the operator as,

$$f(A) = \sum_{\alpha} f(\alpha)|\alpha\rangle\langle\alpha|. \tag{4}$$

We covered this last fall.

- Writing this in our new language of creation and destruction operators of the eigenstates, we then have,

$$f(A) = \sum_{\alpha} f(\alpha)\hat{a}_{\alpha}^{\dagger}\hat{a}_{\alpha}. \tag{5}$$

- So for a scalar potential, $V(x)$, as a function of position its corresponding operator is,

$$\hat{V} = \int_x V(x) \cdot \hat{\psi}^\dagger(x)\hat{\psi}(x). \tag{6}$$

- We often will be dealing with particles that interact by a scalar potential that is a function of positions, for example, two charged particles interacting by a Coulomb field.
  The two particle potential in that case is given by,

$$V(x,y) = \frac{Q}{4\pi\epsilon_0}\frac{1}{|x-y|} = V(x-y). \tag{7}$$

  Notice it is a function of the *difference* of the two position variables.

- Recall the single particle operator of a scalar potential that is a function of position.
  Why? $\Longrightarrow$ Recall eigen-decomposition of operators.

- In the case of two position variables we need to integrate over both variables now. So,

$$\hat{V} = \frac{1}{2} \int_{xy} V(x,y) \cdot \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \hat{\psi}(y) \hat{\psi}(x). \tag{8}$$

- Notice in addition to the normal ordering of the creation/annihilation operators the variables are in the (x, y, y, x).
  This is again for convenience and avoids a self energy term that would appear in the case of fermions.

- We now follow the usual routine of translating it into a momentum representation. This turns out to give a very interesting interpretation of two particles interacting via a scalar potential.

- Recall the Fourier mode expansions of the creation and annihilation operators for particles at a position x,

$$\hat{\psi}^\dagger(x) = \sum_p e^{-ipx} \hat{a}_p^\dagger \tag{9}$$

$$\hat{\psi}(x) = \sum_p e^{ipx} \hat{a}_p \tag{10}$$

- Substitute this into our potential operator expression,

$$\hat{V} = \frac{1}{2} \int_{xy} V(x-y) \cdot \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \hat{\psi}(y) \hat{\psi}(x) \tag{11}$$

$$= \frac{1}{2} \int_{xy} \sum_{p_1 p_2 p_3 p_4} e^{-ip_1 x} e^{-ip_2 y} e^{ip_3 y} e^{ip_4 x} V(x-y) \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_3} \hat{a}_{p_4} \tag{12}$$

$$\tag{13}$$

- We now rewrite to introduce an $x-y$ in the exponentials to deal with the $V(x-y)$.

$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 p_3 p_4} \int_{xy} V(x-y) e^{i(p_4-p_1)(x-y)} \cdot e^{i(-p_1-p_2+p_3+p_4)y} \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_3} \hat{a}_{p_4}. \tag{14}$$

- Defining the new variable $z = x - y$ we can rewrite the integrals as,

$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 p_3 p_4} \hat{a}^\dagger_{p_1} \hat{a}^\dagger_{p_2} \hat{a}_{p_3} \hat{a}_{p_4} \int_z V(z) e^{i(p_4 - p_1)z} \cdot \int_y e^{i(-p_1 - p_2 + p_3 + p_4)y}. \tag{15}$$

- Recall the last integral is just a delta function in terms of momenta in the exponential,

$$\int_y e^{i(-p_1 - p_2 + p_3 + p_4)y} = \delta_{-p_1 - p_2 + p_3 + p_4}. \tag{16}$$

  That is it equals zero every except when $-p_1 - p_2 + p_3 + p_4 = 0$ and it evaluates to 1.

- This allows us to eliminate one of the momenta, setting $p_4 = p_1 + p_2 - p_3$. This gives us

$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 p_3} \hat{a}^\dagger_{p_1} \hat{a}^\dagger_{p_2} \hat{a}_{p_3} \hat{a}_{p_1 + p_2 - p_3} \int_z V(z) e^{-i(p_3 - p_2)z} \tag{17}$$

- And the last integral is just the Fourier transform of the potential function,

$$\int_z V(z) e^{-i(p_3 - p_2)z} = \tilde{V}(p_3 - p_2). \tag{18}$$

- Substituting this into our operator equation we have,

$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 p_3} \tilde{V}(p_3 - p_2) \hat{a}^\dagger_{p_1} \hat{a}^\dagger_{p_2} \hat{a}_{p_3} \hat{a}_{p_1+p_2-p_3} \tag{19}$$

- As a next to last step in interpreting this interaction operator we set $q = p_3 - p_2$ and eliminate p_3,

$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 q} \tilde{V}(q) \hat{a}^\dagger_{p_1} \hat{a}^\dagger_{p_2} \hat{a}_{p_2+q} \hat{a}_{p_1-q} \tag{20}$$

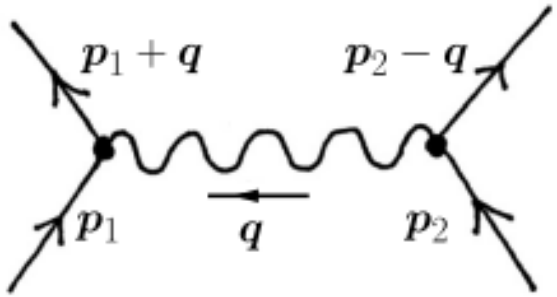
- Finally, we reindex the sum, subtracting q from p_2 and adding it to p_1.

- This gives the final two-particle interaction expression,

$$\boxed{\hat{V} = \frac{1}{2} \sum_{p_1 p_2 q} \tilde{V}(q) \hat{a}^\dagger_{p_1+q} \hat{a}^\dagger_{p_2-q} \hat{a}_{p_2} \hat{a}_{p_1}} \tag{21}$$

- We can interpret this expression diagrammatically as a scattering problem in momentum space – A Feynman diagram.

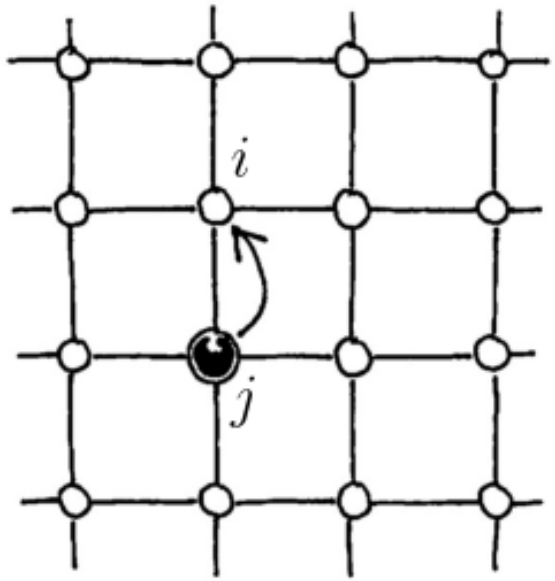
$$\hat{V} = \frac{1}{2} \sum_{p_1 p_2 q} \tilde{V}(q) \hat{a}^{\dagger}_{p_1+q} \hat{a}^{\dagger}_{p_2-q} \hat{a}_{p_2} \hat{a}_{p_1} \tag{22}$$



- A particle comes in with momentum p_2.
- It sends out a force-carrying particle with momentum q, reducing its final momentum to $p_2 - q$.
- The force-carrying particle is absorbed by a second particle which ends up with a final momentum of $p_1 + q$.
- Notice momentum is conserved.

4.5 The Hubbard Model, introduction

- Recall from last week the tight binding model of particles in a discrete lattice which are allowed to hop from one site to a another.



- Going from site j to site i is represented by the operator $\hat{c}_i^\dagger \hat{c}_j$ and lowers the system's energy by $-t_{ij}$.

- Assuming only nearest neighbour hopping with a constant energy saving per hop, the Hamiltonian of the system is given by the sum over all possible sites i and nearest neighbours per site, $i + \tau$,

$$\hat{H}_{tb} = -t \sum_{i\tau} \hat{c}_{i+\tau}^\dagger \hat{c}_i. \tag{23}$$

- In the *Hubbard model* we extend the Tight Binding model which only has kinetic energy terms to include a repulsive force.
  This models the two body repulsive force that electrons would experience from each other on a lattice.

- As a gross simplification we assume the lattice sites are far enough apart that we need to only include electrons on the same site.

- Thus the two particle potential operator

$$\hat{V} = \frac{1}{2} \sum_{ijkl} V_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l \tag{24}$$

  becomes

$$\hat{V} = \frac{1}{2} \sum_{i} V_{iiii} \hat{c}_i^\dagger \hat{c}_i^\dagger \hat{c}_i \hat{c}_i \tag{25}$$

$$\equiv \frac{U}{2} \sum_{i} \hat{c}_i^\dagger \hat{c}_i^\dagger \hat{c}_i \hat{c}_i \tag{26}$$

- Note that $U > 0$ so two particles on the same site raises the potential energy.

- The Hamiltonian of the Hubbard Model is then,

$$\boxed{\hat{H}_h = -t \sum_{i\tau} \hat{c}^\dagger_{i+\tau} \hat{c}_i + \frac{U}{2} \sum_i \hat{c}^\dagger_i \hat{c}^\dagger_i \hat{c}_i \hat{c}_i} \tag{27}$$

- The trade-off in the kinetic energy terms (which encourage hopping with the negative $-t$ factor) and the Coulomb potential (which encourages repulsion by the positive U factor) gives rise to interesting behaviour.

- $\Longrightarrow$ To Be Continued ...

- We have not included electron spin in this model yet. This changes the Hamiltonian to,

$$\hat{H}_h = -t \sum_{i\tau\sigma} \hat{c}^\dagger_{i+\tau,\sigma} \hat{c}_{i\sigma} + \frac{U}{2} \sum_{i\sigma\sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}^\dagger_{i\sigma'} \hat{c}_{i\sigma'} \hat{c}_{i\sigma} \tag{28}$$

- The ordering of the σ and σ' in the second term follows from the interaction diagram.

- We can simplify the second term using the commutation properties of Fermions to put the unprimed and primed σ operators together.

- First note that if $\sigma = \sigma'$ in the double sum then the two destruction operators on the right hand side will evaluate to zero since a site can contain at most one electron of a given spin by the Pauli exclusion principle.

- Dropping the i for now we can rewrite the sum as,

$$\sum_{\sigma \neq \sigma'} \hat{c}^\dagger_\sigma \hat{c}^\dagger_{\sigma'} \hat{c}_{\sigma'} \hat{c}_\sigma \tag{29}$$

- Recall the commutation relations of Fermions,

$$c_\alpha c_\beta + c_\beta c_\alpha = 0 \tag{30}$$

$$c^\dagger_\beta c_\alpha + c_\alpha c^\dagger_\beta = \delta_{\alpha\beta} \tag{31}$$

- The first relation lets us swap the last two annihilation operators with introducing a minus sign, propogating the σ' operator to the left by one.

$$\hat{c}_\sigma^\dagger \hat{c}_{\sigma'}^\dagger, \hat{c}_{\sigma'} \hat{c}_\sigma = -\hat{c}_\sigma^\dagger \hat{c}_{\sigma'}^\dagger, \hat{c}_\sigma \hat{c}_{\sigma'} \tag{32}$$

- We now swap the middle two operator using the second commutation relation,

$$c_\beta^\dagger c_\alpha = \delta_{\alpha\beta} - c_\alpha c_\beta^\dagger. \tag{33}$$

- So,

$$-\hat{c}_\sigma^\dagger \hat{c}_{\sigma'}^\dagger, \hat{c}_\sigma \hat{c}_{\sigma'} = -\hat{c}_\sigma^\dagger \left(\delta_{\sigma\sigma'} - \hat{c}_\sigma \hat{c}_{\sigma'}^\dagger, \right) \hat{c}_{\sigma'} \tag{34}$$

$$= -\delta_{\sigma\sigma'} \hat{c}_\sigma^\dagger \hat{c}_{\sigma'} + \underbrace{\hat{c}_\sigma^\dagger \hat{c}_\sigma \hat{c}_{\sigma'}^\dagger, \hat{c}_{\sigma'}}_{\hat{n}_\sigma \hat{n}_{\sigma'}} \tag{35}$$

- Placing this back into the sum over $\sigma \neq \sigma'$ the term with the delta function is zero and we have (note number operators commute),

$$\frac{U}{2} \sum_{\sigma \neq \sigma'} \hat{n}_\sigma \hat{n}_{\sigma'} = \frac{U}{2} \left(\hat{n}_\uparrow \hat{n}_\downarrow + \hat{n}_\downarrow \hat{n}_\uparrow \right) \tag{36}$$

$$= U \cdot \hat{n}_\uparrow \hat{n}_\downarrow \tag{37}$$

- This lets us write the Hubbard model as,

$$\boxed{\hat{H}_h = -t \sum_{i\tau\sigma} \hat{c}^{\dagger}_{i+\tau,\sigma} \hat{c}_{i\sigma} + U \cdot \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}} \tag{38}$$

- Note the nice physical interpretation of this equation.
- The number operators will add U to the Hamiltonian only if there is a spin up and a spin down together on the same site. This increases the total energy.
- A single electron with either spin or no electron at all at a site will evaluate to zero and not contribute to the Hamiltonian.

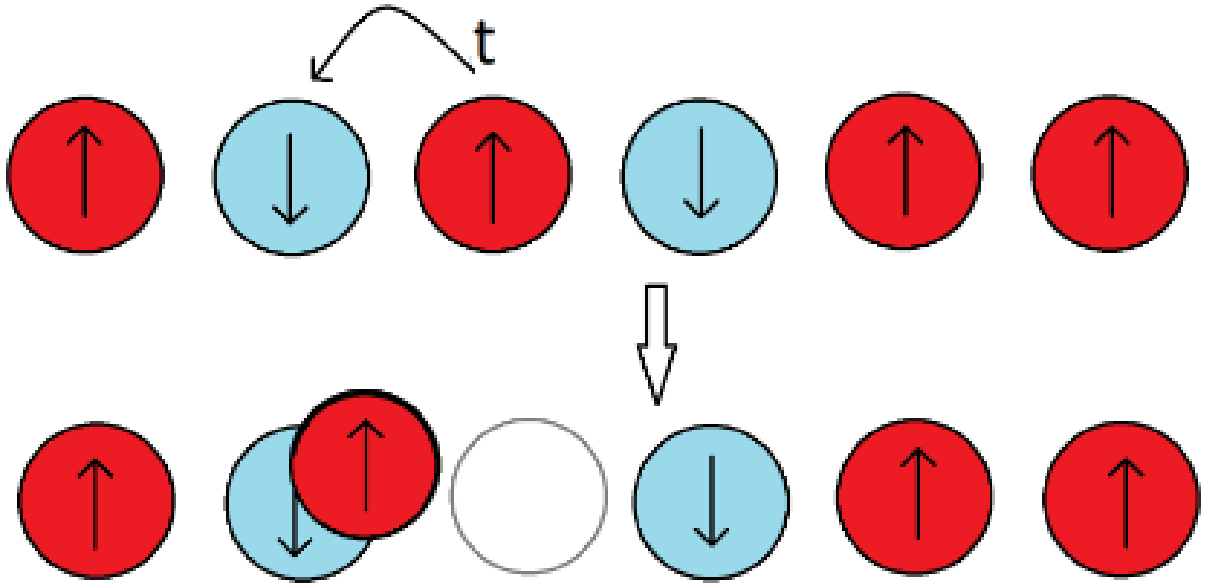


FIG. 2: Pictoric representation of the kinetic term t in the Hubbard Hamiltonian.

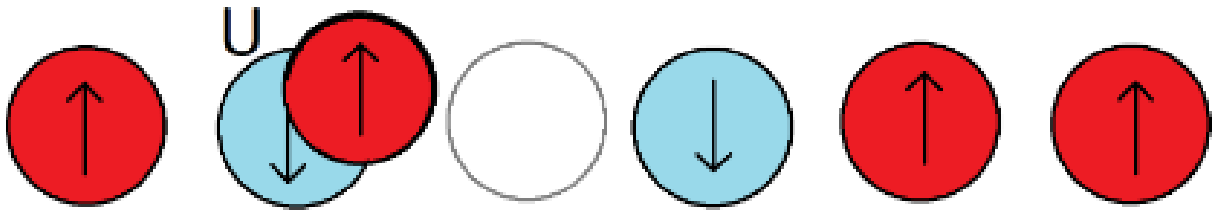


FIG. 3: Pictoric representation of the one site repulsion term U in the Hubbard Hamiltonian.

Example (4.11 Two Site Hubbard Model, Two Electrons with Same Spins Hydrogen H_2 Molecule, 1s shells)

- Consider the two site case with two electrons. There are two possibilities to here. One were the two electrons have the same spin and one where they are opposite.
- When the two electrons have the same spin they are forced by the Pauli exclusion principle to occupy one site each. They both can't be on the same site.
- This makes our Hilbert space one dimensional with the basis vector $|\Psi\rangle = |\uparrow,\uparrow\rangle$ for two spin up electrons, for example.
- Let's expand out our Hamiltonian here,

$$H = -t\left(\hat{c}^{\dagger}_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^{\dagger}_{2\uparrow}\hat{c}_{1\uparrow} + \hat{c}^{\dagger}_{1\downarrow}\hat{c}_{2\downarrow} + \hat{c}^{\dagger}_{2\downarrow}\hat{c}_{1\downarrow}\right) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right) \tag{39}$$

- From inspection you can see that H operating on the state $|\uparrow,\uparrow\rangle$ yields zero. That is,

$$H|\uparrow,\uparrow\rangle = 0|\uparrow,\uparrow\rangle. \tag{40}$$

- Thus the energy (i.e., eigenvalue) associated with the single state is zero, $E = 0$. The same happens for the two spin down state.

Example (4.11 Two Site Hubbard Model, Two Electrons with Opposite Spins)

- Our Hilbert space is now 4-dimensional with a basis $|\uparrow\downarrow, 0\rangle$, $|\uparrow, \downarrow\rangle$, $|\downarrow, \uparrow\rangle$, $|0, \uparrow\downarrow\rangle$.
- We now form the Hamiltonian matrix in this basis by taking its matrix elements with respect to the inner products of the basis with H.
  That is, $H_{11} = \langle\uparrow\downarrow, 0|\hat{H}|\uparrow\downarrow, 0\rangle$, $H_{21} = \langle\uparrow, \downarrow|\hat{H}|\uparrow\downarrow, 0\rangle$, etc.

$$[H] = \begin{array}{c|cccc} & |\uparrow\downarrow, 0\rangle & |\uparrow, \downarrow\rangle & |\downarrow, \uparrow\rangle & |0, \uparrow\downarrow\rangle \\ \hline \langle\uparrow\downarrow, 0| & \langle\uparrow\downarrow,0|\hat{H}|\uparrow\downarrow,0\rangle & \cdots & & \\ \langle\uparrow, \downarrow| & \langle\uparrow,\downarrow|\hat{H}|\uparrow\downarrow,0\rangle & \cdots & & \\ \langle\downarrow, \uparrow| & \vdots & & & \\ \langle 0, \uparrow\downarrow| & & & & \end{array} \tag{41}$$

- For the (1,1) element first evaluate $H|\uparrow\downarrow, 0\rangle$:

$$-t\left(\hat{c}^\dagger_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}_{1\uparrow} + \hat{c}^\dagger_{1\downarrow}\hat{c}_{2\downarrow} + \hat{c}^\dagger_{2\downarrow}\hat{c}_{1\downarrow}\right) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right)\cdot|\uparrow\downarrow, 0\rangle \tag{42}$$

$$= -t\left(0 + |\downarrow, \uparrow\rangle + 0 + |\uparrow, \downarrow\rangle\right) + U(1\cdot 1 + 0)|\uparrow\downarrow, 0\rangle \tag{43}$$

$$= -t|\downarrow, \uparrow\rangle + 0 - t|\uparrow, \downarrow\rangle + U|\uparrow\downarrow, 0\rangle \tag{44}$$

- We can then read the first column as $U, -t, -t, 0$, which agrees with the text.

Example (4.11 Two Site Hubbard Model, Two Electrons with Opposite Spins, cont'd)

- Working out the full H gives us the matrix,

$$H = \begin{pmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{pmatrix} \tag{45}$$

- We now solve for the eigenvalues and eigenvectors algebraically by hand or using a computer algebra system.
  $\Longrightarrow$ Note that for particular values of U and t the calculation can also be done numerically with Matlab or Octave.

- There are four eigenvalues and eigenvectors in general. We take both U (repulsive force) and t to be positive.

- The eigenvalues, i.e., system energies, in order from lowest to highest are:

$$\begin{pmatrix} \frac{1}{2}\left(U - \sqrt{U^2 + 16t^2}\right) \\ 0 \\ U \\ \frac{1}{2}\left(U + \sqrt{U^2 + 16t^2}\right) \end{pmatrix} \tag{46}$$

Example (4.11 Two Site Hubbard Model, Two Electrons with Opposite Spins, cont'd)

- Fixing $U = 1$ and plotting the eigenvalues as a function of t we have,

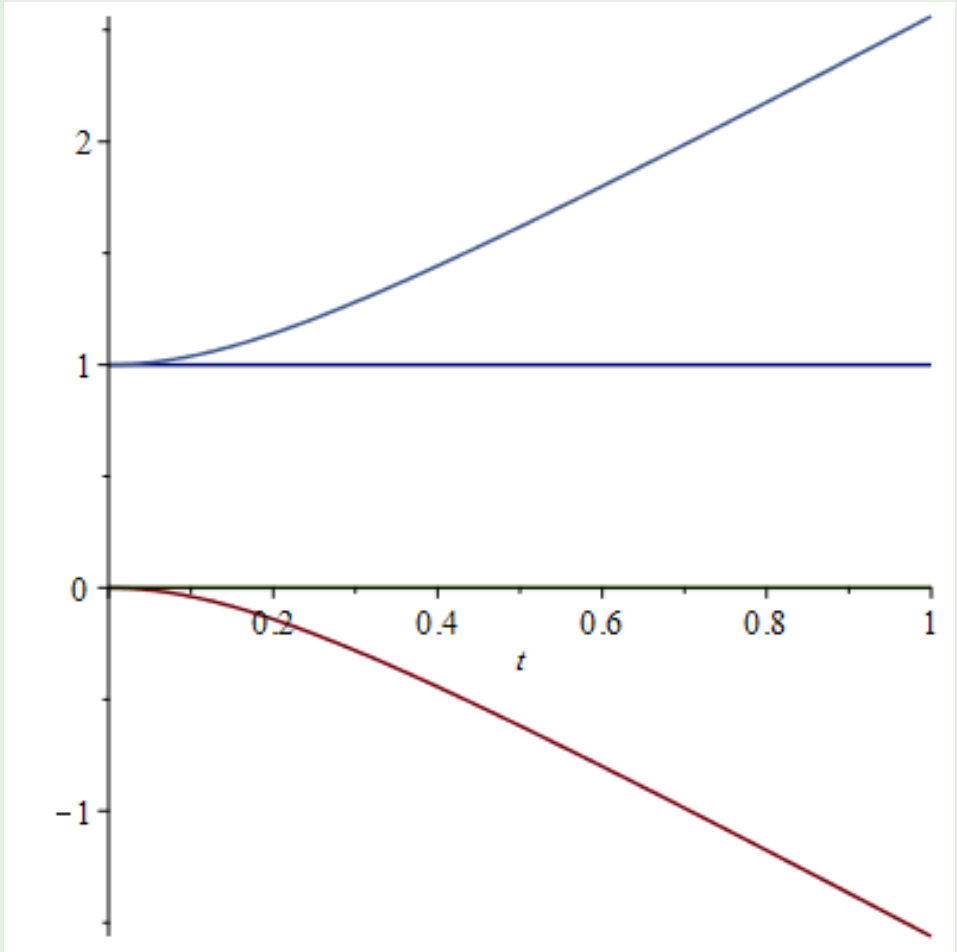


Figure: Energy levels of two site Hubbard model as a function of t for $U = 1$.

Example (4.11 Two Site Hubbard Model, Two Electrons with Opposite Spins, cont'd)

- The ground state energy and corresponding state eigenvector are,

$$E_{GS} = \frac{1}{2}\left(U - \sqrt{U^2 + 16t^2}\right) \tag{47}$$

$$|\Psi_{GS}\rangle = \begin{pmatrix} 1 \\ \frac{4t}{-U+\sqrt{U^2+16t^2}} \\ \frac{4t}{-U+\sqrt{U^2+16t^2}} \\ 1 \end{pmatrix}. \tag{48}$$

- At low enough temperatures we expect the system to be in the ground state. There are two interesting cases.
- One where $t << U$ and the repulsive force term dominates. Here the ground state approaches the limit, $|\Psi_{GS}\rangle = (0, 1, 1, 0) = |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle$.
- The other case is $t >> U$ and the kinetic hopping term dominates. The ground state then approaches, $|\Psi_{GS}\rangle = (1, 1, 1, 1) = |\uparrow\downarrow, 0\rangle + |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle + |0, \uparrow\downarrow\rangle$
- The first state is analogous to an insulator where the electrons are each frozen into a single site while the second is like a metal where electrons are free to move between all sites.

Example (Four Site Hubbard Model, Two Electrons Spin Up, Two Spin Down)

- With some calculation you find in this case the Hilbert space dimension is 30 and it is spanned by the 30 basis vectors, $|\uparrow,\uparrow,\downarrow,\downarrow\rangle$, $|\uparrow\downarrow,\uparrow,\downarrow,0\rangle$, etc.
  Evaluating the Hamiltonian just as before we get the matrix,