PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Plan for Lecture 30

Quantum Mechanics of the Hubbard Model

1. Motivation and history of model
2. Two-site example
3. N-site example in one-dimension

26	Wed: 04/06/2022	Chap. 10 (review)	Multiparticle systems and second quantization		
27	Fri: 04/08/2022		Multi electron atoms	#21	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	#22	04/18/2022
29	Wed: 04/13/2022		Multi electron atoms		
	Fri: 04/15/2022	*No class*	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons	#23	04/22/2022
31	Wed: 04/20/2022		Hubbard model with multiple electrons		
32	Fri: 04/22/2022		BCS model of superconductivity		
33	Mon: 04/25/2022		BCS model of superconductivity		

PHY 742 -- Assignment #23

April 18, 2022

The material for this homework follows Lecture 30

1. Consider the two site Hubbard model, described by Hamiltonian H, with two electrons and zero total spin in the two electron basis of states |A>, |B>, and |C> discussed in the lecture. Evaluate the matrix element <A| H |C>.

Electron Correlations in Narrow Energy Bands
Author(s): J. Hubbard
Source: *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. 276, No. 1365 (Nov. 26, 1963), pp. 238-257
Published by: The Royal Society
Stable URL: http://www.jstor.org/stable/2414761
Accessed: 15-04-2015 03:16 UTC

Electron correlations in narrow energy bands

By J. Hubbard

Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(*Communicated by B. H. Flowers, F.R.S.—Received* 23 *April* 1963)

It is pointed out that one of the main effects of correlation phenomena in *d*- and *f*-bands is to give rise to behaviour characteristic of the atomic or Heitler–London model. To investigate this situation a simple, approximate model for the interaction of electrons in narrow energy bands is introduced. The results of applying the Hartree–Fock approximation to this model are examined. Using a Green function technique an approximate solution of the correlation problem for this model is obtained. This solution has the property of reducing to the exact atomic solution in the appropriate limit and to the ordinary uncorrelated band picture in the opposite limit. The condition for ferromagnetism of this solution is discussed. To clarify the physical meaning of the solution a two-electron example is examined.

The Hubbard Hamiltonian:

Using Fermi particle second quantization operators

$c_{l\sigma}$ and $c^\dagger_{l\sigma}$

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -\mathrm{t}\left[\hat{c}^\dagger_{l\sigma}\hat{c}_{l'\sigma} + \hat{c}^\dagger_{l'\sigma}\hat{c}_{l\sigma}\right] + U\sum_l \hat{c}^\dagger_{l\uparrow}\hat{c}_{l\uparrow}\hat{c}^\dagger_{l\downarrow}\hat{c}_{l\downarrow},$$

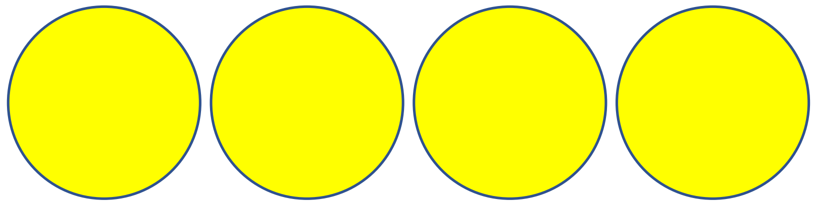
single particle contribution

two particle contribution

$$\{c_{l\sigma}, c_{l'\sigma'}\} = 0$$

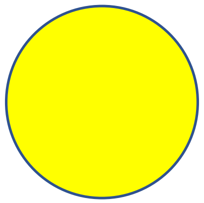
$$\{c^\dagger{}_{l\sigma}, c^\dagger{}_{l'\sigma'}\} = 0$$

$$\{c_{l\sigma}, c^\dagger{}_{l'\sigma'}\} = \delta_{ll'}\delta_{\sigma\sigma'}$$

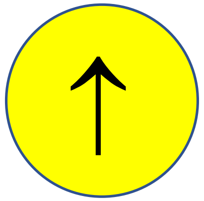


l = 1 2 3 4

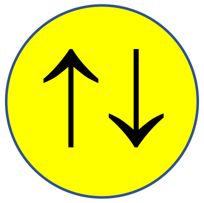
Possible configurations of a single site



$$|0\rangle$$



$$c_\uparrow^\dagger |0\rangle$$



$$c_\uparrow^\dagger c_\downarrow^\dagger |0\rangle$$

Hubbard model -- continued

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -\mathrm{t}\left[\hat{c}^{\dagger}_{l\sigma}\hat{c}_{l'\sigma} + \hat{c}^{\dagger}_{l'\sigma}\hat{c}_{l\sigma}\right] + U\sum_{l}\hat{c}^{\dagger}_{l\uparrow}\hat{c}_{l\uparrow}\hat{c}^{\dagger}_{l\downarrow}\hat{c}_{l\downarrow},$$

t represents electron "hopping" between sites, preserving spin

U represents electron repulsion on a single site

Two-site Hubbard model

$$H = -t\left(c^{\dagger}{}_{1\uparrow}c_{2\uparrow} + c^{\dagger}{}_{2\uparrow}c_{1\uparrow} + c^{\dagger}{}_{1\downarrow}c_{2\downarrow} + c^{\dagger}{}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

where

$$n_{l\sigma} \equiv c^{\dagger}{}_{l\sigma}c_{l\sigma}$$

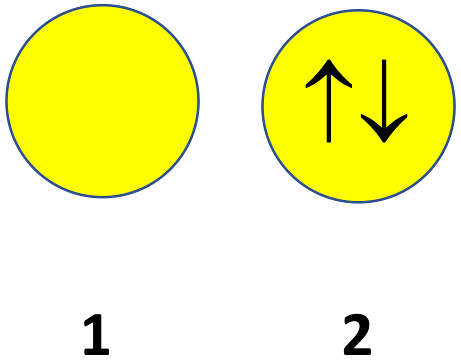
Consider all possible 2 particle states with zero spin:

$$\left|A\right\rangle \equiv c^{\dagger}{}_{1\uparrow}c^{\dagger}{}_{1\downarrow}\left|0\right\rangle$$

$$\left|B\right\rangle \equiv c^{\dagger}{}_{2\uparrow}c^{\dagger}{}_{2\downarrow}\left|0\right\rangle$$

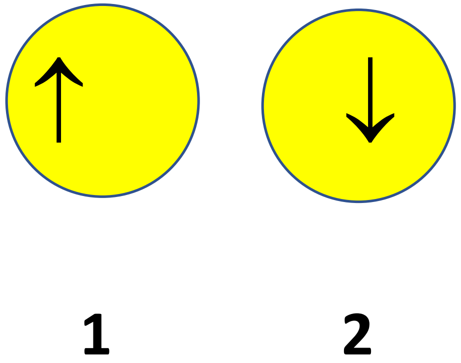
$$\left|C\right\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}{}_{1\uparrow}c^{\dagger}{}_{2\downarrow} + c^{\dagger}{}_{2\uparrow}c^{\dagger}{}_{1\downarrow}\right)\left|0\right\rangle$$

$$H = -t\left(c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{2\uparrow}c_{1\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow} + c^{\dagger}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$



$$c^{\dagger}_{1\uparrow}c_{2\uparrow}$$

➔



Two-site Hubbard model

$$H = -t\left(c^\dagger{}_{1\uparrow}c_{2\uparrow} + c^\dagger{}_{2\uparrow}c_{1\uparrow} + c^\dagger{}_{1\downarrow}c_{2\downarrow} + c^\dagger{}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Matrix elements of Hamiltonian for all 2 particle states with spin 0:

$$H = \begin{array}{c} \\ A \\ B \\ C \end{array}\begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{pmatrix} U & 0 & -\sqrt{2}t \\ 0 & U & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & 0 \end{pmatrix} \end{array}$$

$$|A\rangle \equiv c^\dagger{}_{1\uparrow}c^\dagger{}_{1\downarrow}|0\rangle$$

$$|B\rangle \equiv c^\dagger{}_{2\uparrow}c^\dagger{}_{2\downarrow}|0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^\dagger{}_{1\uparrow}c^\dagger{}_{2\downarrow} + c^\dagger{}_{2\uparrow}c^\dagger{}_{1\downarrow}\right)|0\rangle$$

Eigenvalues of Hamiltonian:

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)$$

$$E_2 = U$$

$$E_3 = +2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)$$

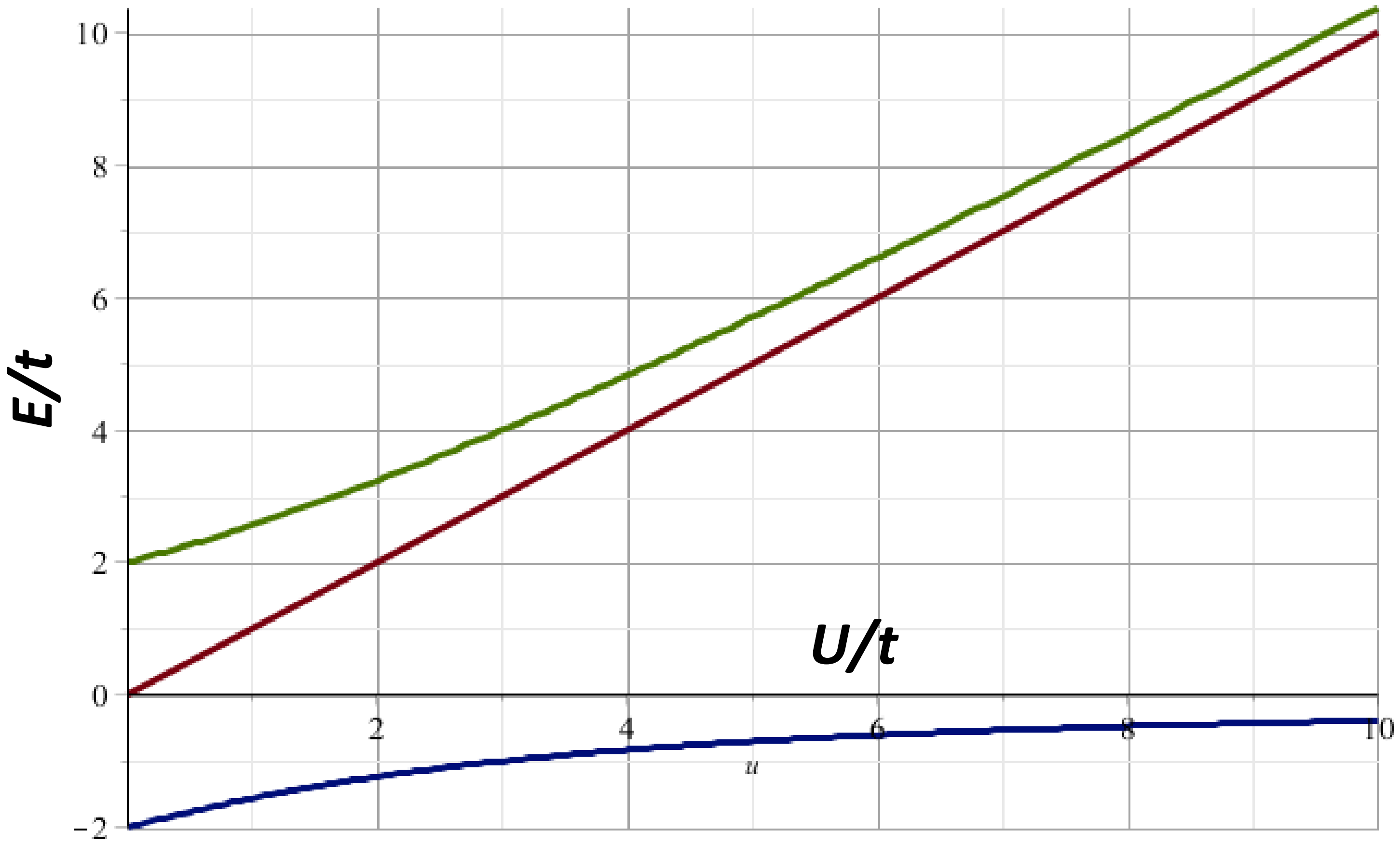
Eigenvectors of the Hamiltonian:

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}|C\rangle + \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)\left(|A\rangle + |B\rangle\right)$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{2}}\left(|A\rangle - |B\rangle\right)$$

$$|\Psi_3\rangle = \frac{1}{\sqrt{2}}|C\rangle - \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)\left(|A\rangle + |B\rangle\right)$$

Eigenvalues of the 2-site Hubbard model



Eigenvalues of Hamiltonian:

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)$$

$$E_2 = U$$

$$E_3 = +2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)$$

Two-site Hubbard model

$$H = -t\left(c^\dagger{}_{1\uparrow}c_{2\uparrow} + c^\dagger{}_{2\uparrow}c_{1\uparrow} + c^\dagger{}_{1\downarrow}c_{2\downarrow} + c^\dagger{}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Ground state of the two-site Hubbard model

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right) \qquad \left|\Psi_1\right\rangle = \frac{1}{\sqrt{2}}\left|C\right\rangle + \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)\left(\left|A\right\rangle + \left|B\right\rangle\right)$$

Single particle limit ($U \rightarrow 0$)

$$E_1 = -2t \qquad \left|\Psi_1\right\rangle = \frac{1}{\sqrt{2}}\left|C\right\rangle + \frac{1}{2}\left(\left|A\right\rangle + \left|B\right\rangle\right)$$

$$\left|A\right\rangle \equiv c^\dagger{}_{1\uparrow}c^\dagger{}_{1\downarrow}\left|0\right\rangle \qquad \left|B\right\rangle \equiv c^\dagger{}_{2\uparrow}c^\dagger{}_{2\downarrow}\left|0\right\rangle$$

$$\left|C\right\rangle \equiv \frac{1}{\sqrt{2}}\left(c^\dagger{}_{1\uparrow}c^\dagger{}_{2\downarrow} + c^\dagger{}_{2\uparrow}c^\dagger{}_{1\downarrow}\right)\left|0\right\rangle$$

Two-site Hubbard model Single particle limit $(U \rightarrow 0)$

Full spectrum for spin 0 eigenstates

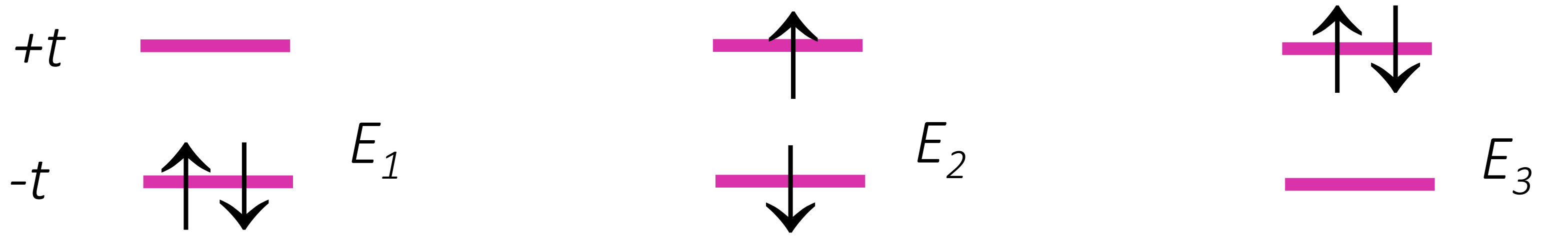
$$E_1 = -2t \qquad |\Psi_1\rangle = \frac{1}{2}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle$$

$$E_2 = 0 \qquad |\Psi_2\rangle = \frac{1}{4}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} - c^\dagger_{2\downarrow}\right)|0\rangle$$

$$+\frac{1}{4}\left(c^\dagger_{1\uparrow} - c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle$$

$$E_3 = +2t \qquad |\Psi_1\rangle = \frac{1}{2}\left(c^\dagger_{1\uparrow} - c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} - c^\dagger_{2\downarrow}\right)|0\rangle$$

Single particle picture:



N-site system in one dimension

$$H = -t\sum_{n=1}^{N-1}\sum_{\sigma=\uparrow}^{\downarrow}\left(c^{\dagger}_{n\sigma}c_{n+1\sigma} + c^{\dagger}_{n+1\sigma}c_{n\sigma}\right) + U\sum_{n=1}^{N} c^{\dagger}_{n\uparrow}c_{n\uparrow}c^{\dagger}_{n\downarrow}c_{n\downarrow}$$

Solved analytically in 1968 **Extension to 2 and 3 dimensions has remained elusive…..**

VOLUME 20, NUMBER 25 PHYSICAL REVIEW LETTERS 17 JUNE 1968

ABSENCE OF MOTT TRANSITION IN AN EXACT SOLUTION OF THE SHORT-RANGE, ONE-BAND MODEL IN ONE DIMENSION

Elliott H. Lieb* and F. Y. Wu
Department of Physics, Northeastern University, Boston, Massachusetts
(Received 22 April 1968)

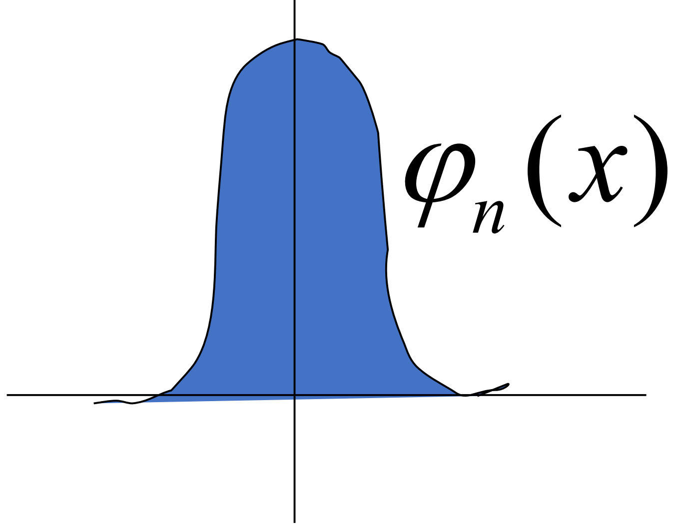
The short-range, one-band model for electron correlations in a narrow energy band is solved exactly in the one-dimensional case. The ground-state energy, wave function, and the chemical potentials are obtained, and it is found that the ground state exhibits no conductor-insulator transition as the correlation strength is increased.

https://doi.org/10.1103/PhysRevLett.20.1445 https://doi.org/10.1103/PhysRevLett.21.192.2
https://doi.org/10.1016/S0378-4371(02)01785-5 reminiscence and proofs

Consider the single particle term --

$$H_{SP} = -t \sum_{n=1}^{N-1} \sum_{\sigma=\uparrow}^{\downarrow} \left(c_{n\sigma}^{\dagger} c_{n+1\sigma} + c_{n+1\sigma}^{\dagger} c_{n\sigma} \right)$$

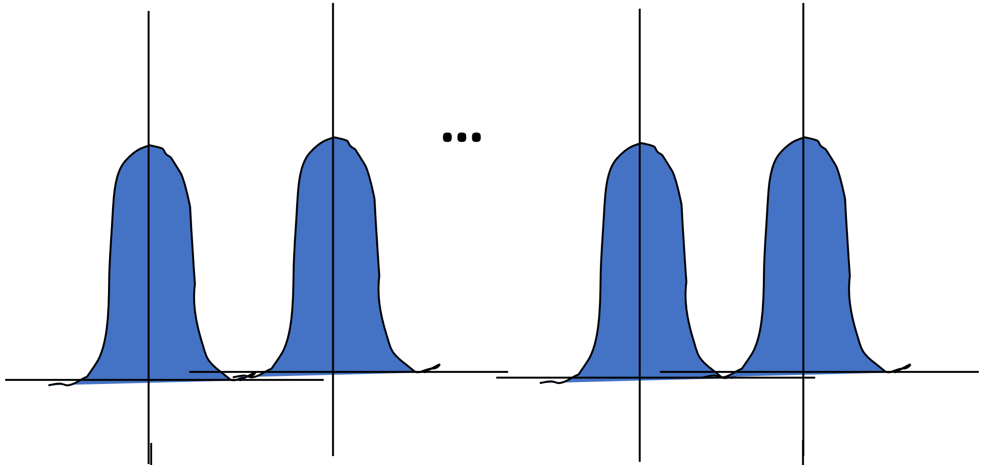
Here we imagine that the basis functions for a site *n* are localized on that site – Wannier functions --



Now we assume that we have *N* electrons (*N* → ∞) and that all of the states have equal probability of being on any of the sites.

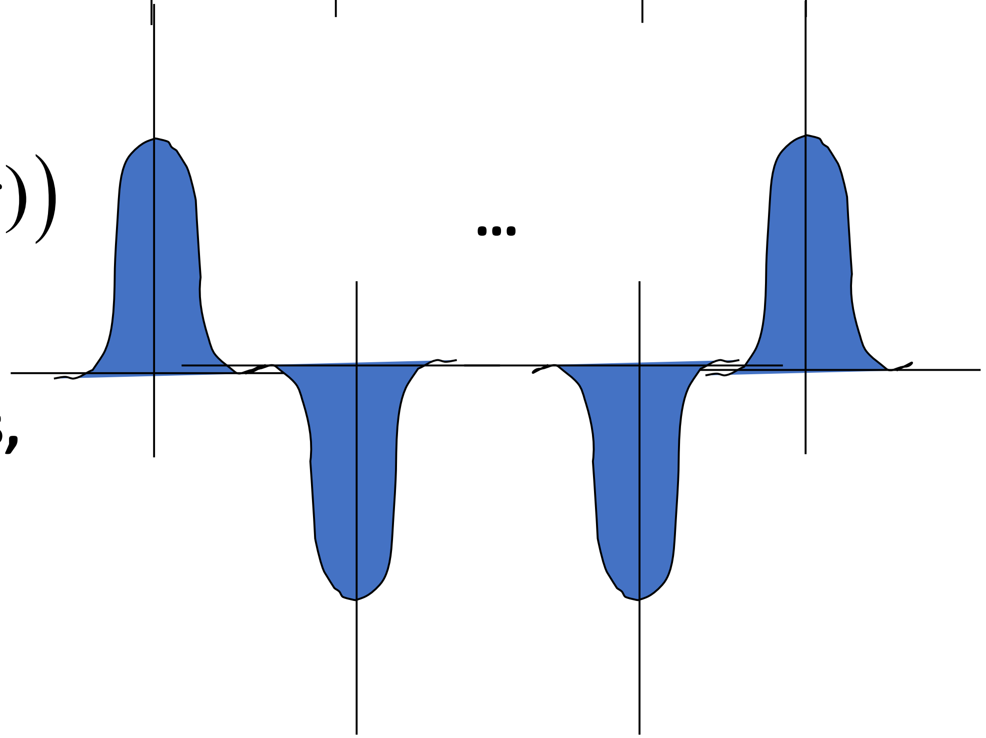
Example N-particle wavefunction:

$$\Psi_N^a = \frac{1}{\sqrt{N}}\left(\varphi_1(x) + \varphi_2(x) + \ldots \varphi_n(x) + \ldots \varphi_N(x)\right)$$



Another example N-particle wavefunction:

$$\Psi_N^z = \frac{1}{\sqrt{N}}\left(\varphi_1(x) - \varphi_2(x) + \ldots - \varphi_{N-1}(x) + \varphi_N(x)\right)$$



These are only two examples of possible wavefunctions, all of which have have different energies

Systematic approach using Bloch symmetry --

Systematic approach using Bloch symmetry

$$\Psi^{k}_{N\sigma} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikan} \varphi_{n\sigma}(x)$$

Here we assume that the Wannier functions $\varphi_{n\sigma}(x)$ are centered at the position na and have the extent

$-\frac{a}{2} \leq x \leq \frac{a}{2}$. There are N distinct values of k:

$-\frac{\pi}{a} \leq k < \frac{\pi}{a}$, which becomes a continuum as $N \rightarrow \infty$.

Analysis within second-quantized framework:

$$H_{SP} = -t\sum_{n=1}^{N-1}\sum_{\sigma=\uparrow}^{\downarrow}\left(c_{n\sigma}^{\dagger}c_{n+1\sigma} + c_{n+1\sigma}^{\dagger}c_{n\sigma}\right)$$

Define new operators in the Bloch basis:

$$A_{k\sigma} = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{ikan} c_{n\sigma}$$

$$\{A_{k\sigma}, A_{k'\sigma'}\} = 0$$

$$\{A^{\dagger}{}_{k\sigma}, A^{\dagger}{}_{k'\sigma'}\} = 0$$

$$\{A_{k\sigma}, A^{\dagger}{}_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}$$

$$H_{SP} = -2t\sum_{k}\sum_{\sigma=\uparrow}^{\downarrow}\left(\cos(ka)\, A_{k\sigma}^{\dagger}A_{k\sigma}\right)$$

Single particle eigenstates --

Note that we are considering the case were there are N sites and N electrons (called "half-filling" case)

$$H_{SP} = -2t \sum_k \sum_{\sigma=\uparrow}^{\downarrow} \left(\cos(ka) \; A^\dagger_{k\sigma} A_{k\sigma} \right)$$

$$\psi_{k\sigma} = A^\dagger_{k\sigma} \left| 0 \right\rangle$$

$$H_{SP}\psi_{k\sigma} = \varepsilon_k \psi_{k\sigma} \qquad \varepsilon_k = -2t\cos(ka)$$

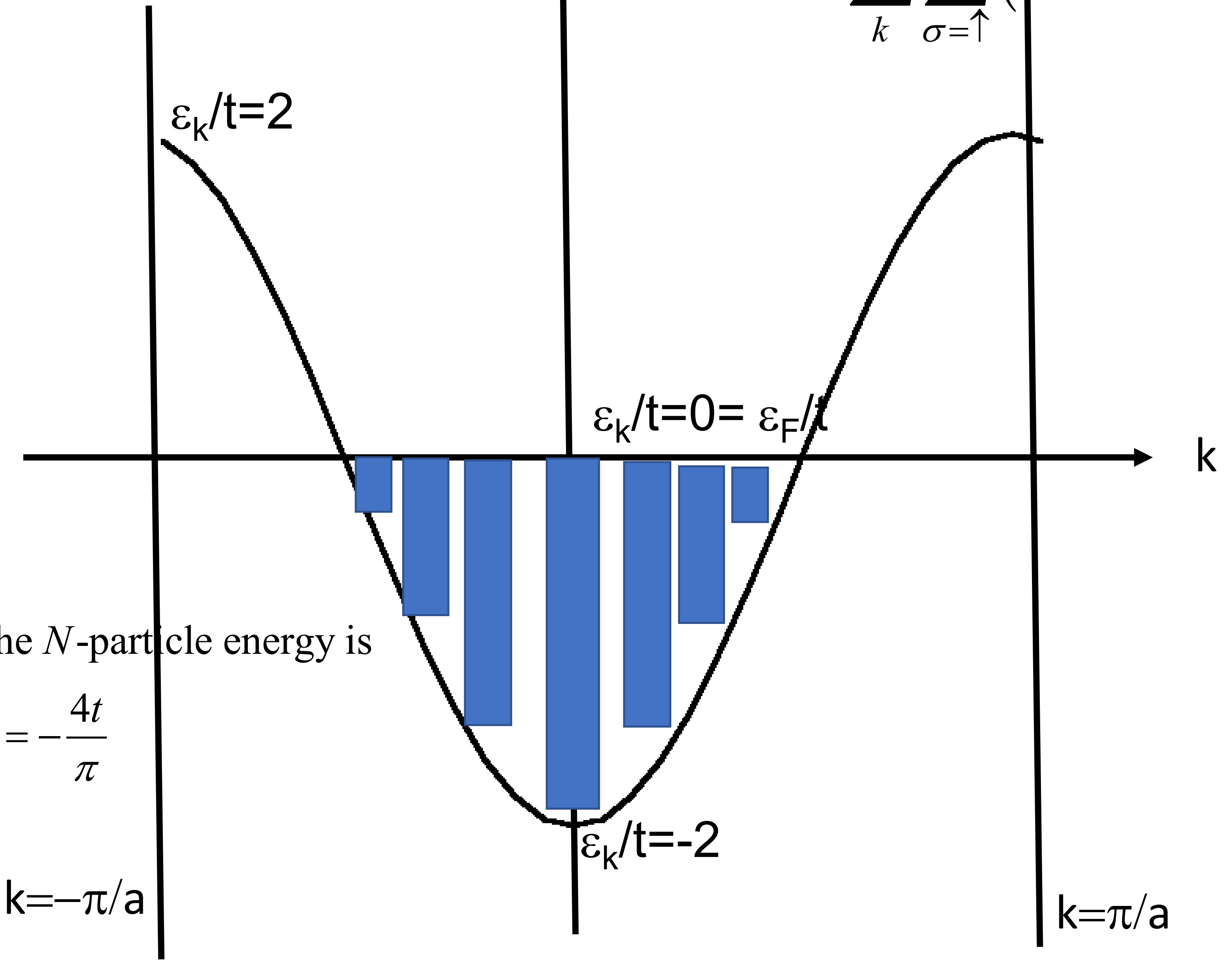
N particle state: $\Psi_N = \prod_{k\sigma} A^\dagger_{k\sigma} \left| 0 \right\rangle$

The range of k is $-k_F \leq k \leq k_F$ where $2\sum_k = N$

It can be shown that: $k_F = \dfrac{\pi}{2a}$

Single particle contributions --

$$H_{SP} = -2t\sum_{k}\sum_{\sigma=\uparrow}^{\downarrow}\left(\cos(ka)\, A^{\dagger}_{k\sigma}A_{k\sigma}\right)$$



It can be shown that the N-particle energy is

$$\frac{E_N}{N} = -4t\sum_{k=-k_F}^{k_F}\cos(ka) = -\frac{4t}{\pi}$$

Treatment of the full one-dimensional Hubbard model -- using the Bloch basis --

$$H = -2t\sum_{k\sigma}\cos\left(ka\right)A^{\dagger}_{k\sigma}A_{k\sigma} + \frac{U}{2N}\sum_{kq\sigma k'q'\sigma'}A^{\dagger}_{k\sigma}A^{\dagger}_{k'\sigma'}A_{q'\sigma'}A_{q\sigma}\delta(-k-k'+q+q')$$

where the delta function must be satisfied modulo a reciprocal lattice vector $\frac{2\pi}{a}$

VOLUME 20, NUMBER 25 PHYSICAL REVIEW LETTERS 17 JUNE 1968

Exact solution --

ABSENCE OF MOTT TRANSITION IN AN EXACT SOLUTION OF THE SHORT-RANGE, ONE-BAND MODEL IN ONE DIMENSION

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$$E \equiv E(\tfrac{1}{2}N_a, \tfrac{1}{2}N_a; U)$$

$$= -4N_a \int_0^\infty \frac{J_0(\omega)J_1(\omega)d\omega}{\omega[1+\exp(\frac{1}{2}\omega U)]}, \qquad (20)$$

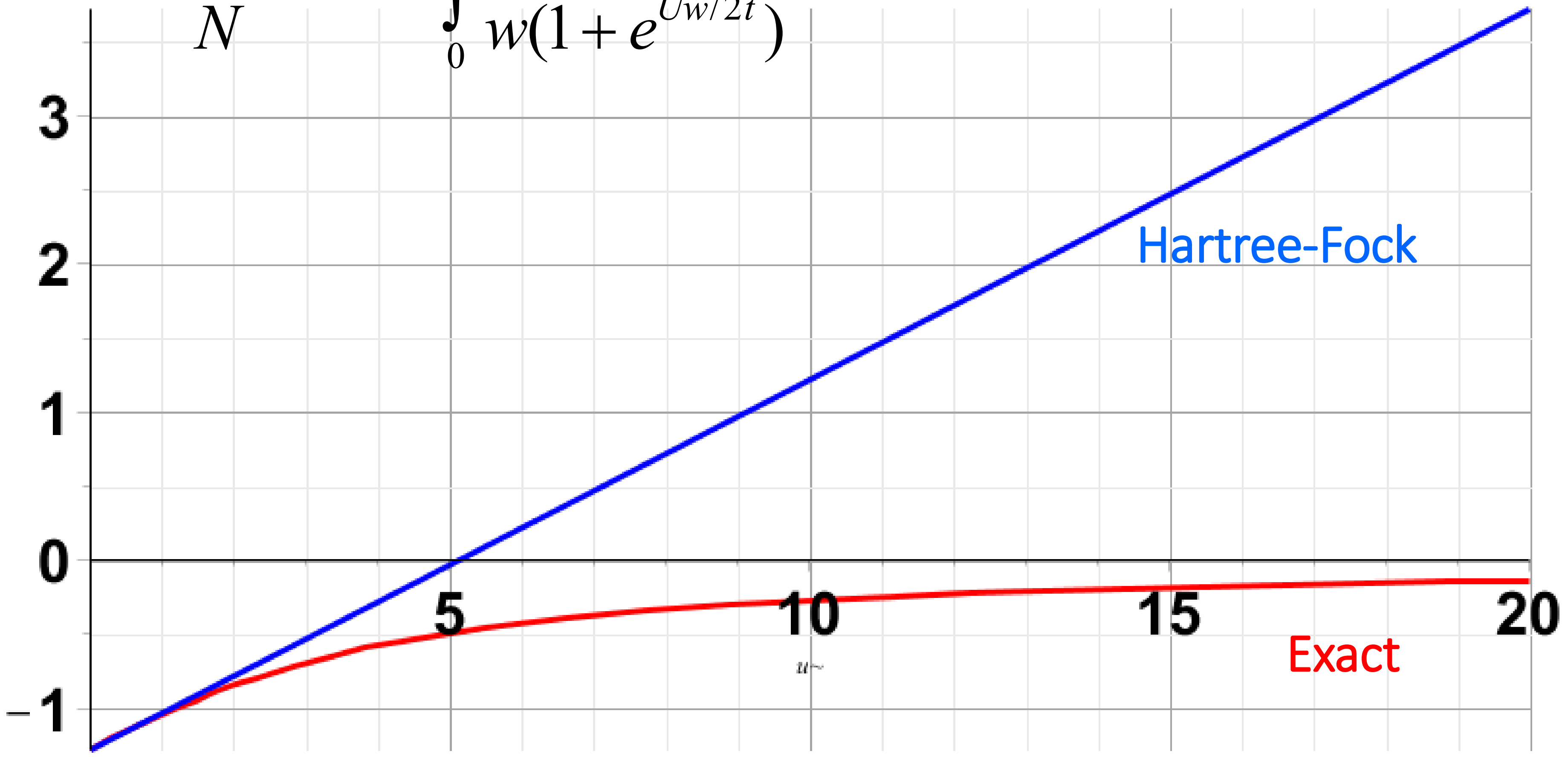
In our notation:

$$\frac{E_{exact}}{N} = -4t\int_0^\infty \frac{J_0(w)J_1(w)}{w(1+e^{Uw/2t})}dw$$

Evaluation of exact model in comparison with Hartree-Fock approximation

Lieb-Wu solution:

$$\frac{E_{exact}}{N} = -4t\int_0^\infty \frac{J_0(w)J_1(w)}{w(1+e^{Uw/2t})}dw$$



Some details of Hartree-Fock approximation, first using 2-site, 2 electron example --

$$H = -t\left(c^{\dagger}{}_{1\uparrow}c_{2\uparrow} + c^{\dagger}{}_{2\uparrow}c_{1\uparrow} + c^{\dagger}{}_{1\downarrow}c_{2\downarrow} + c^{\dagger}{}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Wave function assumed to be product of single particle states

Zero order approximation:

Define: $a_{\sigma}^{\dagger} \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}{}_{1\sigma} + c^{\dagger}{}_{2\sigma}\right)$

Let $\left|\Psi_1^{HF}\right\rangle = a_{\uparrow}^{\dagger}a_{\downarrow}^{\dagger}\left|0\right\rangle$

$$E_1^{HF} = \left\langle \Psi_1^{HF}\right|H\left|\Psi_1^{HF}\right\rangle = -2t + \frac{1}{2}U$$

Two-site Hubbard model -- Hartree-Fock approximation

$$H = -t\left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

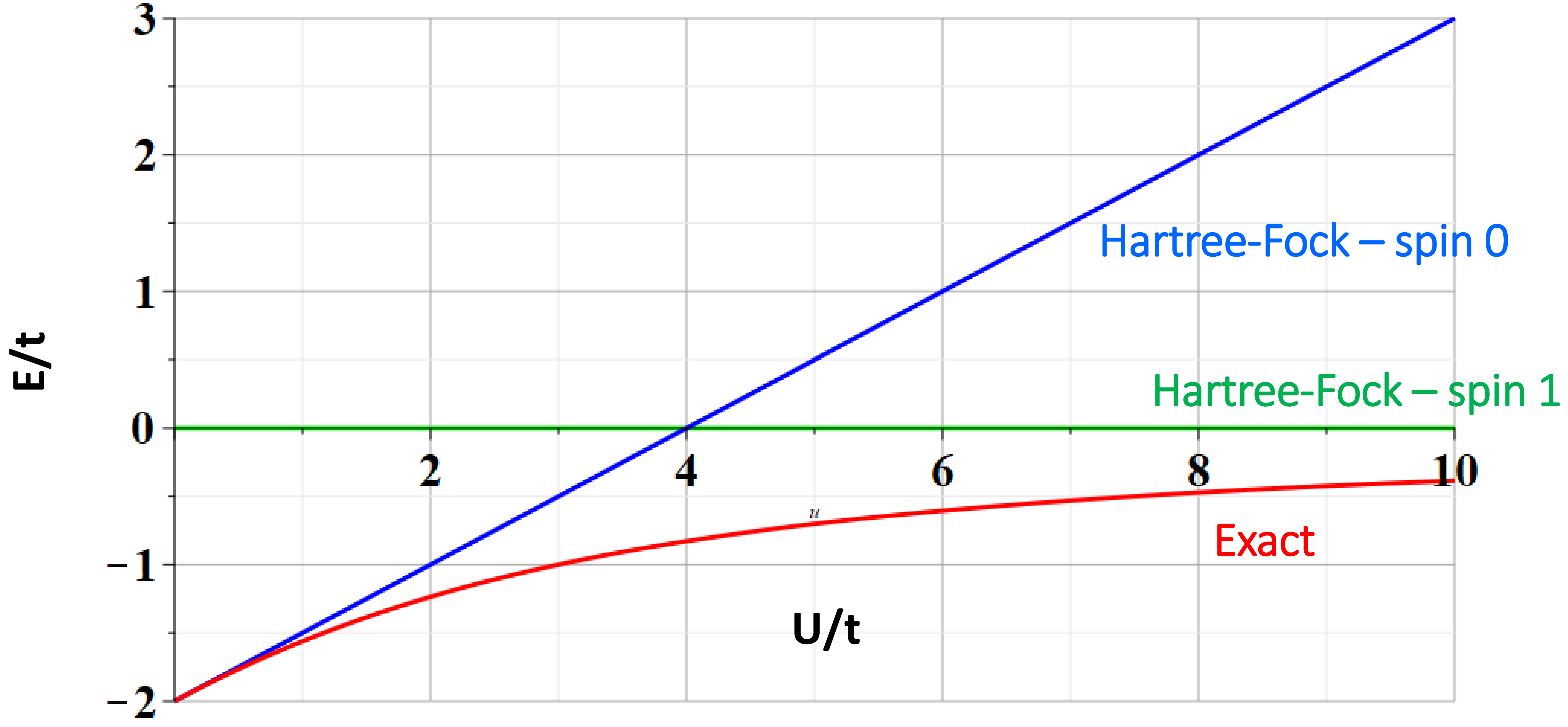
Variational search for lower energy solutions

High spin solution

Let $\left|\Psi_1^{Spin}\right\rangle = c^\dagger_{1\uparrow}c^\dagger_{2\uparrow}\left|0\right\rangle$

$$E_1^{Spin} = \left\langle\Psi_1^{Spin}\middle|H\middle|\Psi_1^{Spin}\right\rangle = 0$$

Comparison of 2-site Hubbard model – solutions for ground state --



Some details of the Hartree-Fock treatment of the full one-dimensional Hubbard model --

In the *k*-basis, the Hubbard model takes the form:

$$H = -2t\sum_{k\sigma}\cos\left(ka\right)A^{\dagger}_{k\sigma}A_{k\sigma} + \frac{U}{2N}\sum_{kq\sigma k'q'\sigma'}A^{\dagger}_{k\sigma}A^{\dagger}_{k'\sigma'}A_{q'\sigma'}A_{q\sigma}\delta(-k-k'+q+q')$$

where the delta function must be satisfied modulo a reciprocal lattice vector $\frac{2\pi}{a}$

Simple Hartree-Fock approximation

$$\left|\Psi_{HF}\right\rangle = \prod_{-k_F \le k \le k_F} A^{\dagger}_{k\uparrow}A^{\dagger}_{k\downarrow}\left|0\right\rangle$$

$$E_{HF} = \left\langle\Psi_{HF}\left|H\right|\Psi_{HF}\right\rangle$$

Evaluating the ground state energy in this simple Hartree Fock approximation, we find that

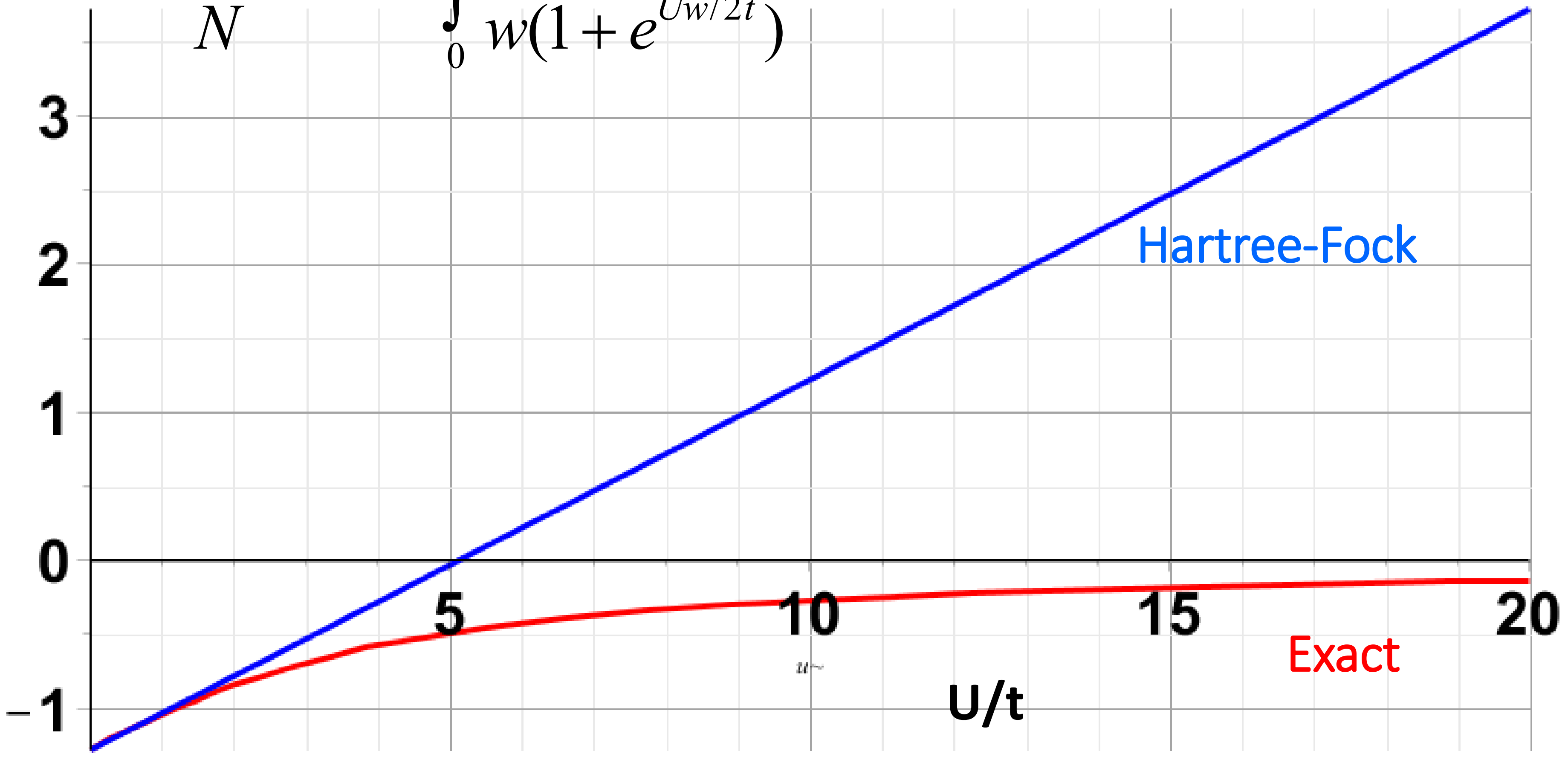
$$\frac{E_{\rm HF}}{\mathcal{N}} = -4 \sum_{-k_F \leq k \leq k_F} \cos(ka) + u \left(\frac{1}{2}\right)^2 = -\frac{4}{\pi} + \frac{u}{4}. \qquad (15)$$

note that $k_F=\pi/(2a)$

Evaluation of exact model in comparison with Hartree-Fock approximation

Lieb-Wu solution:

$$\frac{E_{exact}}{N} = -4t\int_0^\infty \frac{J_0(w)J_1(w)}{w(1+e^{Uw/2t})}dw$$



To be continued…