

**COMPARATIVE STUDY ON THE HUBBARD MODEL ON ANTIFERROMAGNETIC INSULATORS USING QUANTUM ELECTRON SIMULATION TOOLBOX (QUEST)****Tantasso Sabo<sup>1</sup>, Micheal Oboh<sup>2</sup>**

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**ABSTRACT**

Magnetic property of a 2D Hubbard model is inferred from the result of Monte Carlo simulation. Lattice size of 4x4, and temperature down to  $T = 0.25$  where studied. The plots of  $\rho$  versus  $\mu$  exhibit some of the fundamental physics of the Hubbard model, namely the “Mott insulating gap”. At  $T = 0$  the chemical potential has the property that  $\mu = \partial E / \partial \rho$ . In words,  $\mu$  tells us how much the energy changes when we change the density of the system. Thus a jump in  $\mu$  reflects the existence of a gap (and hence that our system is insulating). It turns out that even when interactions are turned on, and we cannot describe the system in terms of a bunch of energy levels, a jump in  $\mu$  still indicates the existence of a gapped, insulating phase. This is the most simple indication of a ‘Mott’ insulating phase in the half-filled Hubbard model. The half-filled system is found to exhibit antiferromagnetic order for coulomb repulsion  $U = 4$ . Generally, antiferromagnetic order may exist at sufficiently low temperatures, vanishing at and above a certain temperature, the Néel temperature (named after Louis Néel (1948), who had first identified this type of magnetic ordering). The low temperature magnetic properties are found to be well described by the existence of a gapped insulating phase. Numerical evidence presented confirm the existence of a ‘Mott’ insulating phase for the half-filled Hubbard model, when interaction between electrons are switch off, for  $U = 4$ , and temperature as low as  $T = 0.25$ .

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## INTRODUCTION

The Hubbard model offers one of the simplest ways to get insight into how the interactions between electrons can give rise to insulating, magnetic, and even novel superconducting effects in a solid. It was written down in the early 1960's and initially applied to understanding the behavior of the transition metal monoxides (FeO, NiO, CoO), compounds which are anti-ferromagnetic insulators, yet had been predicted to be metallic by methods which treat strong interactions less carefully.

Over the intervening years, the Hubbard model has been applied to the understanding of many systems, from 'heavy fermion' systems in the 1980's, to high temperature super-conductors in the 1990's. Indeed, it is an amazing feature of the model that, despite its simplicity, it exhibits behavior relevant to many of the most subtle and beautiful properties of solid state systems.

The Hubbard model has been studied by the full range of analytic techniques developed by condensed matter theorists, from simple mean field approaches to field theoretic methods employing Feynman diagrams, expansions in the degeneracy of the number of flavors' (spin, orbital angular momentum), etc. It has also been extensively attacked with numerical methods like diagonalization and quantum monte carlo.

The Hubbard model is written in terms of 'fermions' creation and destruction operators. These operators differ in several respects from the operators  $\hat{a}^+$ ;  $\hat{a}$  for a single harmonic oscillator. Perhaps most confusing is a conceptual difference: the fermions operators in the Hubbard model are not introduced in terms of familiar position and momentum operators. Rather they stand on their own.

Also, instead of just one creation and one destruction operator, in the Hubbard model there is a set of such operators, which are distinguished by attaching indices  $j$  and  $\sigma$ . Thus we write  $C_{j\sigma}^+$  and  $C_{j\sigma}$  the index  $j$  labels the spatial lattice site and the index  $\sigma$  labels the electron spin (up or down).

As a consequence, the occupation number states are no longer characterized by a single number  $n_{j\sigma}$ , as for a single harmonic oscillator, but instead by a collection of occupation numbers  $n_{j\sigma}$ . One writes such states as  $n_{1\sigma}, n_{2\sigma}, n_{3\sigma} \dots$ . Because these operators are meant to describe fermions, they are defined to have certain anti-commutation relations. (The anti-commutator of two operators  $\{ \hat{A}; \hat{B} \}$  is defined to be  $(AB + BA)$ )

$$[c_{j\sigma} c_{j\sigma}^+] = \delta_{j1} \delta_{\sigma, \sigma^1} \quad (1.1)$$

$$[c_{j\sigma}^+ c_{1\sigma^1}^+] = 0 \quad (1.2)$$

$$[c_{j\sigma} c_{1\sigma^1}] = 0 \quad (1.3)$$

An immediate consequence of these anti-commutation relations is the Pauli principle: the maximum occupation of a particular site with a given spin is 1.

### THE HUBBARD HAMILTONIAN

Having introduced creation and annihilation operators, we can now write down the Hubbard Hamiltonian. Before doing so, let's think about how we might simply describe the motion and interactions of electrons in a solid. First, we need to account for the fact that there is a regular array of nuclear positions in a solid, which for simplicity we consider to be fixed. (In other words, we will not worry about lattice vibrations.) This suggests that we begin with a lattice of atoms (sites) on which the electrons move. A single atom is already a very complex structure, with many different energy levels. The most simple 'atom' we can imagine would have a single energy level. Then, the Pauli principle would tell us that at most two electrons (one with spin up and one with spin down) can sit on this 'atom'. In a solid where electrons can move around, the electrons interact via a screened Coulomb interaction. The biggest interaction will be for two electrons on the same atom. For simplicity, Hubbard stops just there, so that interactions are modeled by a term which is zero if the atom is empty of electrons or has only a single electron on it, but has the value  $U$  if the atom has two electrons. There is no interaction between electrons on different sites.

Our kinetic energy will consist of an expression which allows electrons to move from one site to its neighbors. The energy scale  $t$  which governs this 'hopping' will be determined by the overlap of two wave functions on the pair of atoms. Since wave functions die off exponentially, we can begin by allowing hopping only between the closest atoms in our lattice. Now let's formalize this construction. We define  $c_{j\sigma}^+$  to be the operator which creates an electron of spin

$\sigma$  on lattice site  $j$ . Similarly  $c_{j\sigma}$  is the destruction operator, and  $n_{j\sigma} = c_{j\sigma}^+ c_{j\sigma}$  is the number operator.

The Hubbard Hamiltonian is then,

$$H = -t \sum_{(ji)\sigma} c_{j\sigma}^+ c_{i\sigma} + u \sum_j n_{j\uparrow} n_{j\downarrow} - \mu \sum_j (n_{j\uparrow} + n_{j\downarrow}) \quad (1.4)$$

The first term is the kinetic energy: It describes the destruction of an electron of spin  $\sigma$  on site  $i$  and its creation on site  $j$  (or vice-versa). The symbol  $(ji)$  emphasizes that hopping is allowed only between two sites which are adjacent. The second term is the interaction energy. It goes through all the sites and adds an energy  $U$  if it finds that the site is doubly occupied. The final term is a chemical potential which controls the filling.

We refer to the situation where the filling is one electron per site as 'half filling' since the lattice contains half as many electrons as the maximum number (two per site). Studies of the Hubbard model often focus on the half filled case because it exhibits a lot of interesting phenomena (Mott insulating behavior, anti-ferromagnetic order, etc.)

## THE MONTE CARLO METHOD

The Monte Carlo method is often referred to as a 'computer experiment'. One might think of this as a way of conveying the fact that the output of simulations is not an equation, as in conventional theory. Instead, numbers appear on the computer screen in somewhat the same way that numbers appear on a measuring device in the laboratory. Thus there is the implication that somehow simulations are a bit of a 'black box' and that the use of the computer is hiding the underlying physics. It is not a happy accident that the computer is generating configurations with the desired probability distribution! Indeed, the fundamental equations underlying simulations are the same as analytic theories and one can view simulations as a way of solving the mathematics (differential equations) when it becomes too complicated for analytic techniques.

With all that said, it is still useful to pursue the ‘Monte Carlo as experiment’ point of view. Consider the process of making a measurement in the laboratory. Nature prepares a ‘configuration’ of the system, and the experimentalist takes that configuration and records a value for some quantity of interest. To get better statistics (or perhaps inevitably because of finite measuring time) nature actually produces many configurations, and the experimentalist averages over the values obtained. It is useful to emphasize that no matter how long the experimentalist measures, the configurations he sees are an incredibly small subset of those that the system is capable of exploring. Nature uses some very complex rules for time evolving the system from configuration to configuration, for example the many particle Newton or Schrödinger equations. These rules govern the states that the experimentalist sees, and hence the data he takes. Here’s one useful way to think about computer simulations: The goal of a computer simulation is to devise a method where the computer plays a similar role to that of nature for the experimentalist. That is, the computer generates configurations upon which we make measurements. This leaves us with the problem of devising instructions for the computer that replicate nature’s way of generating configurations.

One approach to constructing a simulation would be actually coding up the microscopic equations governing the system’s time evolution. Simulations of classical systems going under the name ‘molecular dynamics’ are actually done precisely this way. One computes the force  $F_n$  on each particle  $n$ , uses the force to compute the acceleration  $a_n = F_n/m$ , and then moves the velocity and position forward a small time interval  $dt$  with,

$$v_n \rightarrow v_n + a_n dt; x_n \rightarrow x_n + v_n dt.$$

But in the spirit of statistical mechanics, we really don’t care about the microscopic time evolution and the paths  $x_n(t)$  and  $v_n(t)$  the particles take in phase space. All we really need is to replicate the probability  $P(\{x_n, v_n\})$  that nature uses to generate her configurations. If we can do that, we’ll get the same answers as the experimentalist!

If we were doing classical statistical mechanics, the probability distribution that we would be attempting to emulate would be the Boltzmann distribution  $P(\{x_n, v_n\}) = Z^{-1} e^{-\beta E(\{x_n, v_n\})}$ . However, let’s discuss Monte Carlo within the context of a general probability distribution. This will emphasize that Monte Carlo is by no means limited to Boltzmann statistics. To make the notation less unwieldy, we will also label our probabilities by a single index  $i$  which will be

understood to represent particular values of all the degrees of freedom of the system we are studying (for example  $i$  could mean a collection of positions and velocities  $\{x_n, v_n\}$ ). In the remainder of this note we will denote the inverse temperature

by  $\beta = 1/T$ , and set Boltzmann's constant to unity. As we shall see, to do Monte Carlo, we actually don't need to know  $p_i$ , but only ratios of  $p_j/p_i$  for two configurations. This is certainly an important point for statistical mechanics since  $p_j/p_i = e^{-\beta(E_j-E_i)}$  is known, but the individual  $p_i$  involve the unknown partition function  $Z$ .

For the purpose of this project quantum electron simulation toolbox (QUEST) has been used as a DQMC simulation technique. The values of the chemical potential( $\mu$ ) were varied for  $a; 4\text{electrons on }4\text{sites}$

### QUANTUM ELECTRON SIMULATION TOOLBOX (QUEST)

Quantum Electron Simulation Toolbox (QUEST) is a FORTRAN 90/95 package for performing determinant quantum Monte Carlo (DQMC) simulations for strongly correlated electron systems. Its development was motivated by a FORTRAN 77 DQMC code<sup>1</sup> written and maintained by Richard Scalettar at the University of California, Davis (UCD). Currently the development of QUEST is led by Zhaojun Bai and Richard Scalettar at UCD. Several research groups have also participated the effort: Mark Jarell (Louisiana State University), Eduardo D'Azevedo and Thomas Maier (ORNL), Sergey Savrasov (UCD), and Karen Tomko (Ohio Supercomputer Center).

In QUEST 1.0, structure of the legacy code has been modernized. In particular, BLAS and LAPACK numerical linear algebra libraries and new techniques such as delayed-updating are integrated into QUEST's computational kernel. These developments have improved the efficiency of DQMC simulation and generated fruitful research applications. Recognizing the increasing appeal of using hybrid multicore processors and graphics processing unit (GPU) systems, QUEST 2.0 is released with a new optimized computational kernel designed for such heterogeneous multicore CPU + GPU architecture. This project presents a basic implementation of QUEST and describes a minimum number of input parameters required for configuring a DQMC simulation. The example is the 2D one-band Hubbard model on a square lattice. A sample input file `sample.in` for a  $4 \times 4$ ,  $6 \times 6$ ,  $8 \times 8$  square lattices with  $U = 4t, 6t, 8t$  at half-filling and temperature  $\beta = 8t$  is provided. To run the simulation, simply execute the command:

```
$ ./test sample.in sample.out
```

This will launch the simulation and redirect all standard outputs to the file sample.out.

### Input file

A QUEST input file is a text file containing a collection of keywords and their values. Broadly speaking, QUEST keywords fall into two categories: keywords that set up the Hubbard Hamiltonian and those that control the dynamics of Monte Carlo simulation. Keyword value is specified by a single line statement:

```
keyword = value
```

sample input file has the following keywords

- nx (integer): linear dimension of the lattice in the x-direction.
- ny (integer): linear dimension of the lattice in the y-direction.
- U (real): strength of the onsite interaction U.
- t up (real): hopping integral for spin- $\uparrow$  electrons.
- t dn (real): hopping integral for spin- $\downarrow$  electrons.
- mu up (real): chemical potential  $\mu\uparrow$  for spin- $\uparrow$  electrons.
- mu dn (real): chemical potential  $\mu\downarrow$  for spin- $\downarrow$  electrons.
- L (integer): number of imaginary time slices L. In the DQMC simulation, the inverse temperature  $\beta$  is discretized into L “imaginary time” intervals  $\beta = L\Delta T$
- dtau (real): size of the imaginary time (Trotter) step  $\Delta T$
- nwarm (integer): number of sweeps in the warmup (thermalization) phase.
- npass (integer): number of sweeps in the measurement phase.
- nbin (integer): determines the number of bins for measurement data. In the current example, physical observables are measured at each Monte Carlo sweep during the measurement phase. In order to reduce autocorrelation, QUEST groups measurement data into several bins before analyzing statistics.
- seed (integer): random number seed. If seed is set to zero, QUEST will generate a seed automatically. The above keywords constitute a minimal set of parameters to perform DQMC simulation of the 2D Hubbard model.

**RESULTS**

The following results were obtained, for values of  $U = 4$ ,  $T = 2$ ,  $T = 1$ ,  $T = 0.25$  after varying the values of chemical potential ( $\mu$ ) from the range(-4,-3.8,-3.6,-3.4,...4.0): For a  $4 \times 4 = 16$  sites, the results were tabulated as shown below

**Table 1.0:  $U = 4$ ,  $T = 2$ ,  $t = 0$** 

s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$
01	-4.0	0.4456	16	-1.0	0.8740	31	2.0	1.2771
02	-3.8	0.4726	17	-0.8	0.8928	32	2.2	1.3051
03	-3.6	0.4996	18	-0.6	0.9197	33	2.4	1.3329
04	-3.4	0.5274	19	-0.4	0.9465	34	2.6	1.3610
05	-3.2	0.5342	20	-0.2	0.9733	45	2.8	1.3902
06	-3.0	0.5844	21	0.0	1.0000	46	3.0	1.4198
07	-2.8	0.6129	22	0.2	1.0270	47	3.2	1.4496
08	-2.6	0.6415	23	0.4	1.0542	38	3.4	1.4771
09	-2.4	0.6697	24	0.6	1.0805	39	3.6	1.5050
10	-2.2	0.6983	25	0.8	1.1089	40	3.8	1.5333
11	-2.0	0.7261	26	1.0	1.1360	41	4.0	1.5602
12	-1.8	0.7531	27	1.2	1.1641			
13	-1.6	0.7821	28	1.4	1.1920			
14	-1.4	0.8104	29	1.6	1.2208			
15	-1.2	0.8382	30	1.8	1.2499			

**Table 1.1  $U = 4$ ,  $T = 1$ ,  $t = 0$** 

s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$
01	-4.0	0.2223	16	-1.0	0.8700	31	2.0	1.3232
02	-3.8	0.2505	17	-0.8	0.9076	32	2.2	1.3728
03	-3.6	0.2914	18	-0.6	0.9324	33	2.4	1.4252
04	-3.4	0.3405	19	-0.4	0.9566	34	2.6	1.4741
05	-3.2	0.3813	20	-0.2	0.9784	45	2.8	1.5345
06	-3.0	0.4337	21	0.0	1.0000	46	3.0	1.5703
07	-2.8	0.4820	22	0.2	1.0238	47	3.2	1.6219
08	-2.6	0.5287	23	0.4	1.0483	38	3.4	1.6661
09	-2.4	0.5810	24	0.6	1.0744	39	3.6	1.7128
10	-2.2	0.6347	25	0.8	1.1026	40	3.8	1.7552
11	-2.0	0.6797	26	1.0	1.1329	41	4.0	1.7852
12	-1.8	0.7271	27	1.2	1.1665			
13	-1.6	0.7670	28	1.4	1.1999			
14	-1.4	0.8035	29	1.6	1.2380			
15	-1.2	0.8359	30	1.8	1.2789			

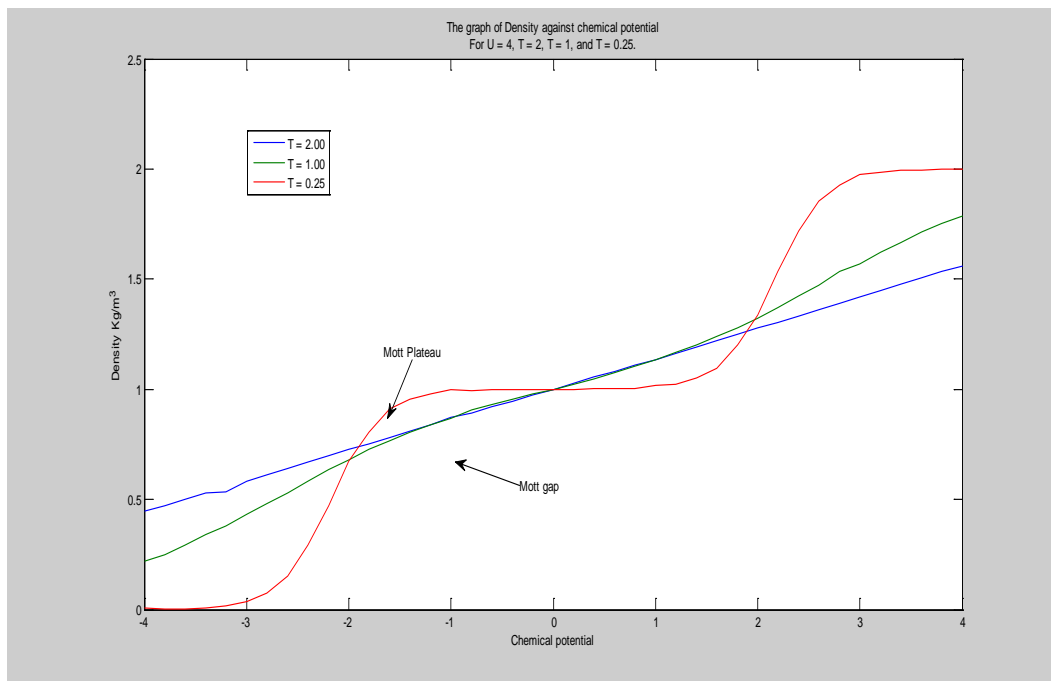


**Table 1.2:  $U = 4, T = 0.25, t = 0$**

s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$	s/no	$\mu$	$\rho$
01	-4.0	0.0060	16	-1.0	0.9966	31	2.0	1.3394
02	-3.8	0.0014	17	-0.8	0.9958	32	2.2	1.5365
03	-3.6	0.0048	18	-0.6	0.9982	33	2.4	1.7172
04	-3.4	0.0076	19	-0.4	0.9992	34	2.6	1.8537
05	-3.2	0.0179	20	-0.2	0.9996	35	2.8	1.9291
06	-3.0	0.0384	21	0.0	1.0000	36	3.0	1.9772
07	-2.8	0.0743	22	0.2	1.0005	37	3.2	1.9848
08	-2.6	0.1541	23	0.4	1.0011	38	3.4	1.9936
09	-2.4	0.2931	24	0.6	1.0023	39	3.6	1.9970
10	-2.2	0.4708	25	0.8	1.0043	40	3.8	1.9990
11	-2.0	0.6763	26	1.0	1.0160	41	4.0	2.0012
12	-1.8	0.8053	27	1.2	1.0224			
13	-1.6	0.9094	28	1.4	1.0503			
14	-1.4	0.9532	29	1.6	1.0949			
15	-1.2	0.9803	30	1.8	1.2023			

**Graphical interpretation**

The plots of  $\rho$  versus  $\mu$  exhibit some of the fundamental physics of the Hubbard model, namely the “Mott insulating gap”.



**Figure 1 Density as a function of chemical potential for the single site( $t=0$ )Hubbard Model at  $U = 4$  for three different temperatures. At low temperature a ‘mott plateau’ is developed.**

At  $T = 0$  the chemical potential has the property that  $\mu = \partial E / \partial \rho$ . In words,  $\mu$  tells us how much the energy changes when we change the density of the system. If we have a noninteracting system described by a set of energy levels, and we have filled the levels up to some 'Fermi energy'  $E_F$  the cost to add a particle is the next energy level just above the last level we filled, that is,  $\mu = E_F$ . If we reach a gap, a region of energy where there are no further levels to be filled, then  $\mu$  has to take a jump from the energy at the top of the band which has just been filled to the energy at the bottom of the next band. Thus a jump in  $\mu$  reflects the existence of a gap (and hence that our system is insulating). It turns out that even when interactions are turned on, and we cannot describe the system in terms of a bunch of energy levels, a jump in  $\mu$  still indicates the existence of a gapped, insulating phase. This is the most simple indication of a 'Mott' insulating phase in the half-filled Hubbard model.

Notice that at half-filling  $\rho = 1$  when  $\mu = U/2$ . Because half-filling is so often studied, it is convenient to write the Hubbard Hamiltonian as,

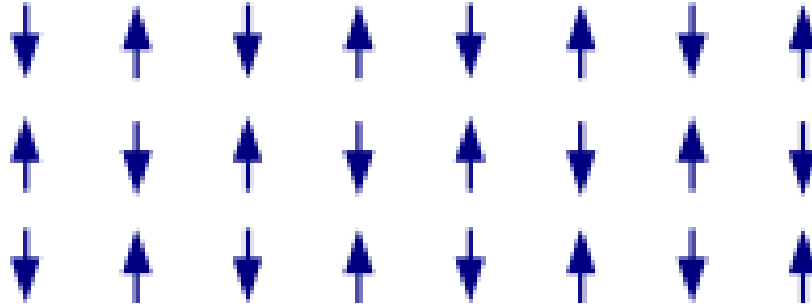
$$H = -t \sum_{(ji)\sigma} C_{j\sigma}^+ C_{i\sigma} + U \sum_j (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) - \mu \sum_j (n_{j\uparrow} + n_{j\downarrow}) \quad (3.1)$$

This just corresponds to a shift in the chemical potential  $\mu$  by  $U/2$ . When this is done, half-filling conveniently occurs always at  $\mu = 0$  for any value of  $t$ ;  $T$ ;  $U$ . To emphasize, the properties of this 'new' model are identical to the old one, if one compares them at the same density. It's just that the chemical potentials used to get those densities are offset.

## RESULT ANALYSIS

Spins of electrons, align in a regular pattern with neighboring spins (on different sublattices) pointing in opposite directions. This is, like ferromagnetism and ferrimagnetism, a manifestation of ordered magnetism. Generally, antiferromagnetic order may exist at sufficiently low temperatures, vanishing at and above a certain temperature, the Néel temperature (named

after Louis Néel (1948), who had first identified this type of magnetic ordering). Above the Néel temperature, the material is typically paramagnetic. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, are usually related to the.



### Antiferromagnetic ordering

When no external field is applied, the antiferromagnetic structure corresponds to a vanishing total magnetization. In an external magnetic field, a kind of ferrimagnetic behavior may be displayed in the antiferromagnetic phase, with the absolute value of one of the sublattice magnetizations differing from that of the other sublattice, resulting in a nonzero net magnetization. Although the net magnetization should be zero at a temperature of absolute zero, the effect of spin canting often causes a small net magnetization to develop, as seen for example in hematite.

The magnetic susceptibility of an antiferromagnetic material typically shows a maximum at the Néel temperature. In contrast, at the transition between the ferromagnetic to the paramagnetic phases the susceptibility will diverge. In the antiferromagnetic case, a divergence is observed in the *staggered susceptibility*.

Various microscopic (exchange) interactions between the magnetic moments or spins may lead to antiferromagnetic structures. In the simplest case, one may consider an Ising model on an bipartite lattice, e.g. the simple cubic lattice, with couplings between spins at nearest neighbor sites. Depending on the sign of that interaction, ferromagnetic or antiferromagnetic order will

result. Geometrical frustration or competing ferro- and antiferromagnetic interactions may lead to different and, perhaps, more complicated magnetic structures.

### **Antiferromagnetic materials**

Antiferromagnetic materials occur commonly among transition metal compounds, especially oxides. An example is the heavy-fermion superconductor URu<sub>2</sub>Si<sub>2</sub>. Better known examples include hematite, metals such as chromium, alloys such as iron manganese (FeMn), and oxides such as nickel oxide (NiO). There are also numerous examples among high nuclearity metal clusters. Organic molecules can also exhibit antiferromagnetic coupling under rare circumstances, as seen in radicals such as 5-dehydro-m-xylylene.

Synthetic antiferromagnets (often abbreviated by SAF) are artificial antiferromagnets consisting of two or more thin ferromagnetic layers separated by a nonmagnetic layer. Due to dipole coupling of the ferromagnetic layers which results in antiparallel alignment of the magnetization of the ferromagnets. Antiferromagnetism plays a crucial role in giant magnetoresistance, as had been discovered in 1988 by the Nobel prize winners Albert Fert and Peter Grünberg (awarded in 2007) using synthetic antiferromagnets. There are also examples of disordered materials (such as iron phosphate glasses) that become antiferromagnetic below their Néel temperature. These disordered networks 'frustrate' the antiparallelism of adjacent spins; i.e. it is not possible to construct a network where each spin is surrounded by opposite neighbour spins. It can only be determined that the average correlation of neighbour spins is antiferromagnetic. This type of magnetism is sometimes called *speromagnetism*.

In numerous strongly correlated electron systems different degrees of freedom, such as the spin, orbitals and lattice deformations are inextricably coupled, usually by Coulomb interactions and the specifics of the crystal structure, but also due to alloying. Such systems are often characterized by competing ground states susceptible to external perturbations such as magnetic field, pressure or chemical doping. Tuning the external parameters may lead to a quantum critical point and stabilize novel ground states with exotic properties. This point is well illustrated in the cuprate superconductors.

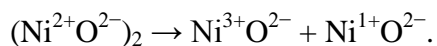
## Mott Insulators

Mott insulators are a class of materials that should conduct electricity under conventional band theories, but are insulators when measured (particularly at low temperatures). This effect is due to electron-electron interactions which are not considered in conventional band theory.

The bandgap in a Mott insulator exists between bands of like character, such as 3d character, while the bandgap in charge transfer insulators exists between anion and cation states, such as between O 2p and Ni 3d bands in NiO.

Although the band theory of solids had been very successful in describing various electrical properties of materials, in 1937 Jan Hendrik de Boer and Evert Johannes Willem Verwey pointed out that a variety of transition metal oxides predicted to be conductors by band theory (because they have an odd number of electrons per unit cell) are insulators. Nevill Mott and Rudolf Peierls then (also in 1937) predicted that this anomaly can be explained by including interactions between electrons.

In 1949, in particular, Mott proposed a model for NiO as an insulator, where conduction is based on the formula



In this situation, the formation of an energy gap preventing conduction can be understood as the competition between the Coulomb potential  $U$  between 3d electrons and the transfer integral  $t$  of 3d electrons between neighboring atoms (the transfer integral is a part of the tight-binding approximation). The total energy gap is then

$$E_{\text{gap}} = U - 2zt,$$

where  $z$  is the number of nearest-neighbor atoms

In general, Mott insulators occur when the repulsive Coulomb potential  $U$  is large enough to create an energy gap. One of the simplest theories of Mott insulators is the 1963 Hubbard

model. The crossover from a metal to a Mott insulator as  $U$  is increased can be predicted within the so-called Dynamical Mean Field Theory.

### Mottness

*Mottness* denotes the additional ingredient, aside from antiferromagnetic ordering, which is necessary to fully describe a Mott Insulator. In other words, we might write

$$\text{antiferromagnetic order} + \text{mottness} = \text{Mott insulator}$$

Thus, mottness accounts for all of the properties of Mott insulators that cannot be attributed simply to antiferromagnetism.

There are a number of properties of Mott insulators, derived from both experimental and theoretical observations, which cannot be attributed to antiferromagnetic ordering and thus constitute mottness. These properties include

- Spectral weight transfer on the Mott scale
- Vanishing of the single particle Green function along a connected surface in momentum space in the first brillouin zone
- *Two* sign changes of the Hall coefficient as electron doping goes from  $n = 0$  to  $n = 2$  (band insulators have only one sign change at  $n = 1$ )
- The presence of a charge  $2e$  (with  $e < 0$  the charge of an electron) boson at low energies
- A pseudogap away from half-filling ( $n = 1$ )

### Comparison between QUEST Results and theoretical values

R.T Scalettar(2007) in his work on ‘Numerical studies of disordered Tight-Binding Hamiltonian’ considered Strong Coupling Limit ( $t=0$ ) for the non interacting Hubbard model. Each of the states  $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$  is an eigenstate of  $H$  with eigenvalues  $0, -\mu, -\mu, U-2\mu$  respectively. The partition function is

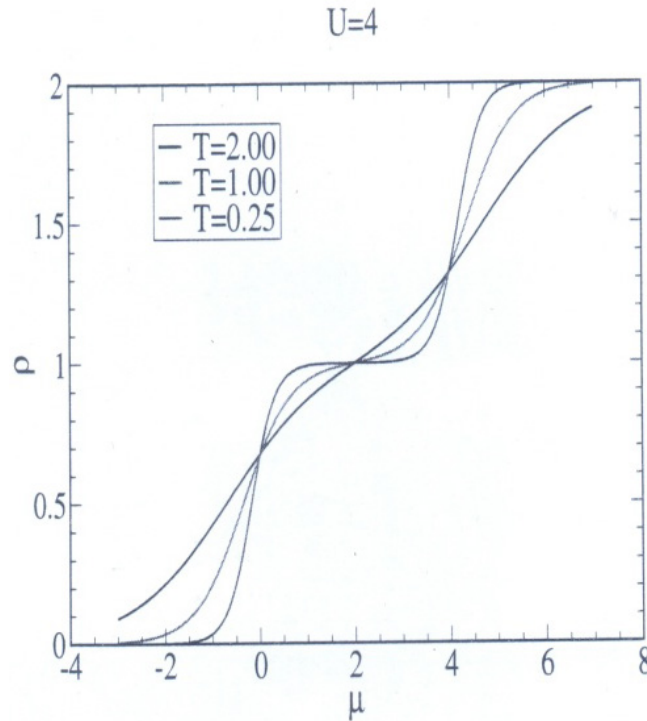
$$Z = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle = 1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U} \quad (4.1)$$

and the energy is,

$$E = \langle H + \mu n \rangle = Z^{-1} \sum_{\alpha} \langle \alpha | H e^{-\beta H} | \alpha \rangle = U e^{2\beta\mu - \beta u} (1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta u})^{-1} \quad (4.2)$$

The occupation is given by,

$$\rho = \langle n \rangle = 2(e^{\beta\mu} + e^{2\beta\mu - \beta u})(1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta u})^{-1} \quad (4.3)$$



**Fig. 2** is a plot of  $\rho$  vs.  $\mu$  for  $U = 4$  and  $T = 2$   $T=1$  and  $T = 0.25$  and exhibits one of the fundamental features of the Hubbard model, namely the .Mott insulating gap. As shown in his work below.

Now comparing his numerical work with the simulation results we obtain from QUEST, in both cases there exhibits one of the fundamental futures of the Hubbard model , namely the `Mott insulating gap' . This means that In a non interacting system described by a set of energy levels, with levels filled up to some `Fermi energy'  $E_F$  , the cost to add a particle in the next energy level just above the last occupied level, that is,  $\mu = E_F$  . The jump in  $\mu$  at  $\rho = 1$  arises from the

interactions: Consider a nearly empty lattice and ask the energy cost to add an electron. This cost need not involve  $U$  because empty sites are abundant. When one gets to half-filling, however, suddenly the cost to add an electron jumps by  $U$  since inevitably an added electron must sit on top of an electron which is already there. This sudden jump in the cost to add a particle is referred to as the "Mott gap". Besides the plateau in  $\rho(\mu)$ , Mott and band gaps are characterized by a density of states (spectral function) which vanishes at the Fermi surface.

Similar jumps in  $\mu$  also occur in the context of band theory, where a gap between two bands likewise causes  $\mu$  to change discontinuously. In both cases, the jump in  $\mu$  indicates the existence of a gapped, insulating phase. However, band and Mott insulators are very different in other ways. 'Anderson insulators', arising from disorder, differ from both by having a finite  $N(E_F)$ .

## SUMMARY

The physical picture for the way in which the Hubbard Hamiltonian can describe metal-insulator transitions is simple. Imagine a half-filled lattice in which each site has one electron. In order for an electron to move, it will have to go onto a site which is already occupied. This costs an energy  $U$ . It is plausible to imagine that if  $U$  is very large, the electrons will not want to move at all, and one will have an Mott insulator.

The Mott insulator can be described in a slightly more subtle way which however connects a bit better with one's picture of energy gaps as giving rise to insulators. Imagine a nearly empty lattice and asking what the energy cost is to add an electron. This cost will not involve  $U$  because it is easy to find a site which is empty. When one gets to half-filling, however, suddenly the cost to add an electron jumps by  $U$  since inevitably an added electron must sit on top of an electron which is already there. This sudden jump in the cost to add a particle is referred to as the mott gap and is similar in a way to the fact that the cost to add an electron jumps by some amount if there is a gap in the energy bands. It is worth noting, though, that this



analogy goes only so far, and the Mott gap differs in a number of very fundamental ways from band gaps.

In the half-filled sector, one electron per site, the states with antiferromagnetic order (neighboring sites have electrons with opposite spins) are lower in energy than ferromagnetic ones (neighboring sites have parallel spins). Although this has come out of consideration of only two sites, it is a general feature: The Hubbard model has antiferromagnetic order at half-filling. Indeed, the antiferromagnetic 'exchange' energy scale  $J = t^2/U$  that we found is precisely the energy scale for this order even in the thermodynamic limit. In addition to antiferromagnetism, one can see the Mott gap in this little two site model by looking at the eigenvalues of the sector with one up and one down electron. More precisely, the eigenvalues are shifted by values involving the hopping  $t$  away from  $\pm U/2$ . The separation  $U$  between  $\pm U/2$  is the Mott gap, and, as one increases  $t$  the separation becomes less and less clear. This puts a very simple quantitative face on the statement that when  $U$  is large one has an insulator (a Mott gap) but when  $U$  is small, the electrons can still move around.

This analysis of the two site model can be extended quite easily to somewhat larger lattices by writing a program which generates the matrix elements of  $H$  and diagonalizes the resulting matrices. In fact, this is one important way that information has been gained concerning the Hubbard model. Although it is limited to 10-20 sites (depending on how much computational effort one is willing to put up with) the results obtained are exact and any possible quantity, including time dependent ones, can be computed.

## FINDINGS

- The plots of  $\rho$  versus  $\mu$  exhibit some of the fundamental physics of the Hubbard model, namely the "Mott insulating gap".
- At  $T = 0$  the chemical potential has the property that  $\mu = \mu(\rho)$ . In words,  $\mu(\rho)$  tells us how much the energy changes when we change the density of the system.

- Magnetic moments of atoms or molecules, are usually related to the spins of electrons, align in a regular pattern with neighboring spins (on different sublattices) pointing in opposite directions.
- Generally, anti-ferromagnetic order may exist at sufficiently low temperatures, vanishing at and above a certain temperature, the Néel temperature (named after Louis Néel (1948).
- Anti-ferromagnetic materials occur commonly among transition metal compounds, especially oxides. Better known examples include hematite, metals such as chromium, alloys such as iron manganese (FeMn), and oxides such as nickel oxide (NiO).
- Mott insulators occur when the repulsive Coulomb potential  $U$  is large enough to create an energy gap.
- *Anti-ferromagnetic order + mottness = Mott insulator.*

## CONCLUSION

- The Hubbard model has anti-ferromagnetic order at half-filling.
- The Mott insulator can be described in a slightly more subtle way which however connects a bit better with one's picture of energy gaps as giving rise to insulators.
- The Quantum Monte Carlo method using QUEST is faster in getting the property of mott insulators, than the numerical method.

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