

Metal Insulator Transition

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Abstract

Metal Insulator transition(MIT) is characterized by the conductivity which will be zero in the insulator phase. In this term paper, we focus on Mott insulator, and a simple theoretical way to describe this MIT is the Hubbard Model .Finally, we will look at the experiments of Mott insulator transition .

1 Introduction

Mott Insulator is a typical example of strongly correlated system. It was first proposed by Mott[1] in 1949. Since then, it continuously receive attention from physics society. Specially after the discovery of High Tc superconductor, it serves as the start point to High-Tc superconductor in most research. The most successful model for metal insulator transition is the Hubbard model, which is non-solvable in high dimensions; still can generate many predication of metal insulator transition.

2 Band theory of Metal and Insulator

The first quantum version of electron behavior in solid is the Sommerfeld Theory, which treat electron as free and do not include the underlying ion field and the electron-electron interaction. The band theory is the next step after Sommerfeld theory, which take the ion field into account. One of the important triumphs of Band theory is its explanation of the Metal and Insulator. Insulator is corresponding to the fully filled band and Metal just partially filled.

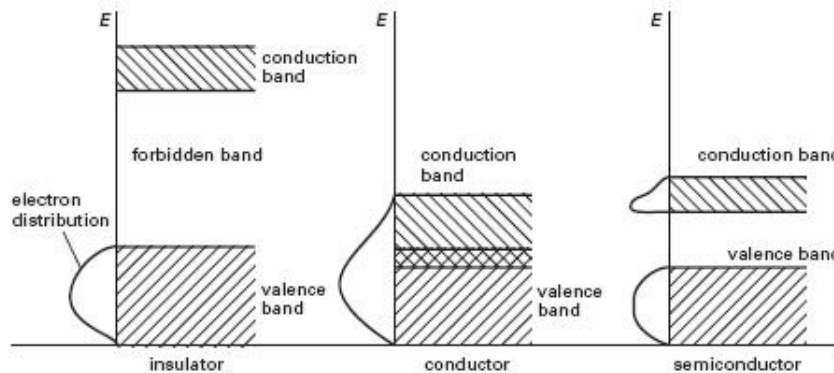


FIG.1[5]

However, despite its great explanation of metal and insulator, its ignorance of electron-electron interaction will certainly bring itself into trouble.

One example of this is NiO[2], which should be metallic according to the Band theory. Nevertheless, Band theory is just one-particle quantum mechanics, which we can not count on too much, specially in the front of complicated condensed matter system.

3 Mott Insulator

The Mott Insulator is an insulator due to the electron-electron interaction. If there is no electron-electron interaction in crystal solid, the only length scale is just the lattice spacing d , (besides the length scale of ion field) however, if we introduce the interaction between electrons, we will also have another length scale associated with this electron-electron interaction, which is Bohr radius a_B for Coulomb interaction. Then the Mott's argument is the following:

$$d \gg a_B \quad \text{Insulator}$$

$$d \ll a_B \quad \text{Metal}$$

Thus there should be a critical value of $d = d_0$ at which metal insulator transition occur at zero temperature. $d < d_0$ is a metal, $d > d_0$ is an insulator.

To clarify this Mott introduce the pseudo "order parameter" ϵ [2]

$$\epsilon = I - E$$

I is the ionization energy and E the electron affinity of one atom inside the crystal.

If there is no electron-electron interaction, then $I = E$, $\epsilon = 0$, however, for electron-electron interaction case, $I > E$, $\epsilon > 0$. Clearly, I , E will change as the varying of lattice spacing d . Generally, as d becomes smaller, ϵ will decrease. There are two ways for the change of ϵ as proposed by Mott:

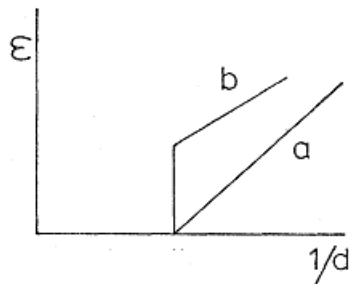


FIG.2[2]

If ϵ drops like curve b , then we will have a first order phase transition, if it drops like curve a then we will have a continuous phase transition.

Mott[1] argued that the drop must be discontinuous (curve b). Since the Coulomb attraction between electron and hole will lead them to form a pair

which will have discrete binding energy, and the activation energy in the insulating state cannot be less than this binding energy, thus ϵ will drop discontinuously.

It turns out ϵ can behavior in much complicated way than just discontinuous.

4 Hubbard Model of Metal Insulator Transition

If we try to include the effect of electron interaction, we will end up with a very complex many body problem, and in general can not be solved. Thus we have to simplify our problem. One way of these is to introduce a model which only have the essential physics but ignore the details. The Hubbard model for Mott insulator is:

$$\begin{aligned} H_H &= H_t + H_u - \mu N \\ H_t &= -t \sum (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \\ H_u &= U \sum (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \end{aligned}$$

and $N = \sum n_{i\sigma}$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$
 $c_{i\sigma}^\dagger$ is the electron creation operator.

H_t is just the nearest-neighbor hopping Hamiltonian which is diagonalized in the momentum space:

$$\begin{aligned} c_{k\sigma} &= \sum_j e^{-ikr_j} c_{j\sigma} \\ H_t &= \sum_{k\sigma} \epsilon_0(k) c_{k\sigma}^\dagger c_{k\sigma} \end{aligned}$$

H_u represents the onsite Coulomb interaction, which only include the short range part.

In this model the Mott insulator phase will emerge at half filling $\langle n_{i\sigma} \rangle = \frac{1}{2}$

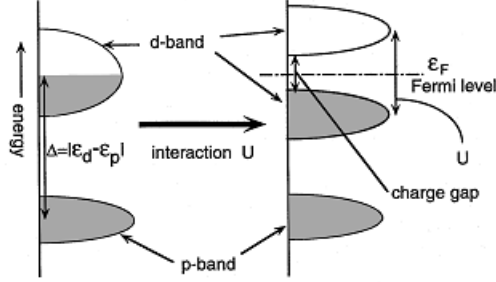


FIG.3[3]

In the above figure, p band remain unchanged after including the interaction U , however, the d band splits into two subband and open up a charge gap. The corresponding state becomes an insulator.

If the interaction is very strong $U \gg t$ then we can expand this theory in terms of t/U , which behavior like a small parameter.

Moreover, the second-order perturbation theory in terms of t/U leads to the $t - J$ model[3]:

$$H_{t-J} = - \sum P_d (t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c.) P_d + J \sum \vec{S}_i \cdot \vec{S}_j$$

here P_d is a projection operator to exclude the double occupancy of particles at the same site.

The metal insulator transition in Hubbard model has two types: the filling control transition(FC-MIT) and the bandwidth control transition(BC-MIT)

The FC-MIT is varying the electron concentration or the chemical potential μ/U . The BC-MIT is varying hopping energy of electron or the bandwidth t/U . The following is the phase diagram of metal insulator in the Hubbard model and the two kinds of phase transition:(we will see below that the scaling behavior of these two type phase transition is different)

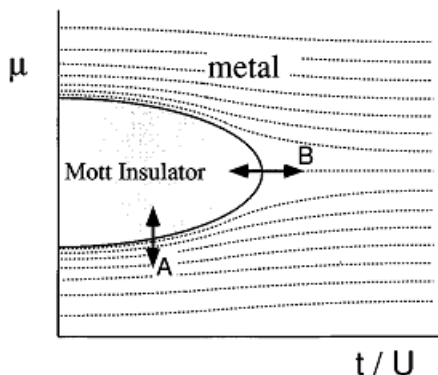


FIG.4[3]

Route A shows filling control transition (FC-MIT), while route B is the bandwidth control transition (BC-MIT). Dotted curves illustrate density contour lines.[3]

5 Scaling behavior of metal insulator transition

Hyperscaling assumes that near the critical point there will be a single characteristic length scale ξ and energy scale or frequency scale Ω to follow:

$$\begin{aligned}\xi &\sim |\Delta|^{-\nu} \\ \Omega &\sim \xi^{-z} \sim |\Delta|^{z\nu}\end{aligned}$$

Here Δ is the control parameter measure the distance from the critical point, which will be μ in the case of FC-MIT, t in the case of BC-MIT.

z is called the dynamical exponent. The reason here to have frequency Ω in addition to the correlation length is that we are treating with Quantum Phase Transition, thus the time dimension is special not behaves like space dimension. In the usual phase transition we only have spatial dimension, it is enough to just introduce the correlation length, since we are in thermal equilibrium there is no time scale anymore.

under the assumption of Hyperscaling the free energy density f_s will have the following form:

$$f_s(\Delta) \sim \Delta^{\nu(d+z)}$$

In the case of finite size L and the inverse temperature β , there will be a finite-size scaling function:

$$f_s(\Delta) \sim \Delta^{\nu(d+z)} F(\xi/L, \Omega/\beta^{-1})$$

There are two most relevant quantities for discussing metal insulator transition in Hubbard model, Drude weight and the charge compressibility.

5.1 Drude weight

The most obvious quantity to characterize metal insulator transition is just the conductivity, since metal conducts electricity while insulator not. The Drude weight is just the singular part of the frequency-dependent conductivity $\sigma(w)$

$$\sigma(w) = D\delta(w) + \sigma_{reg}(w)$$

Numerical calculation of Drude weight from Hubbard model shows that it vanishes at half filling which signals the transition to the Mott insulator.

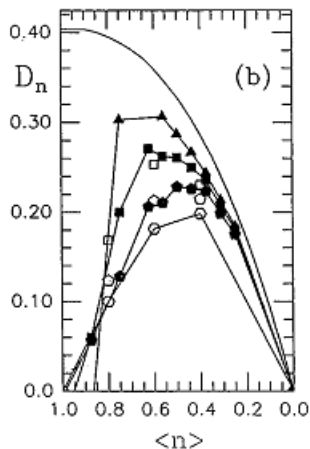


FIG.5 Drude weight D as a function of electron filling $\langle n \rangle$ [4]

5.2 Charge susceptibility

In contrast to the vanish of Drude weight, a charge excitation gap opens at the half filling as demonstrated in FIG.3. The definition of the charge susceptibility χ_c is :

$$\chi_c = n^2 \kappa = \frac{\partial n}{\partial \mu}$$

where κ is the charge compressibility.

as we approach the critical point the scaling behavior of Drude weight and charge compressibility will be:

$$\begin{aligned} D &\sim \Delta^\varsigma \\ \kappa &\sim \Delta^{-\alpha} \end{aligned}$$

$$\varsigma = \nu(d + z - 2), \alpha = \nu(z - d)$$

However, the scaling law is not always the same for FC-MIT (filling control transition) and BC-MIT (bandwidth control transition) define the doping concentration δ as

$$\delta = -\frac{\partial f_s}{\partial \mu} = -\frac{\partial f_s}{\partial \Delta}$$

it scales as:

$$\delta \sim \Delta^{\nu(d+z)-1}$$

For FC-MIT we have the following scaling law[3]:

$$\begin{aligned} \xi &\sim \delta^{-1/d} \\ \Delta &\sim \delta^{z/d} \\ \kappa &\sim \delta^{1-z/d} \\ D &\sim \delta^{1+(z-2)/d} \end{aligned}$$

For BC-MIT (1D Hubbard model) we have different scaling law from FC-MIT[3]:

$$\begin{aligned} D &\sim \delta \\ \chi_c &\sim \delta^{-1} \end{aligned}$$

This means FC-MIT and BC-MIT belong to different universal classes at least for 1D Hubbard model.

6 Experimental evidence for Metal Insulator transition

Direct observation of Metal Insulator transition is a great challenge for experimentalist, for example in Mott's argument we should change lattice spacing d continuously, and then at some point $d = d_0$ we will observe the transition, however, this lattice changing cannot be done easily in the current experimental situation. But some experiments do confirm the predication of Hubbard model, for example the Mott-Hubbard gap(FIG.3 labeled by charge gap)

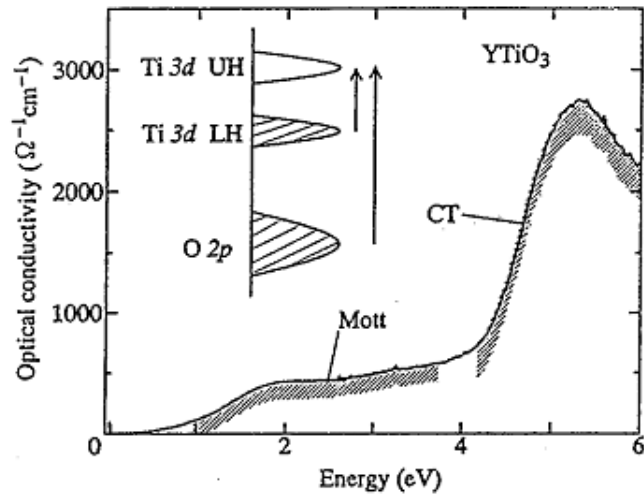


FIG.6 Optical conductivity in YTiO₃. [6]

The rise around 1 eV is identified as Mott-Hubbard gap(gap between UH and LH) and the rise around 4 eV is ascribed to the gap between O 2p and Ti 3d upper Hubbard band.

Another way to observe the Metal Insulator transition is by doping experiments, since doping effectively changes the chemical potential μ in Hubbard model, thus we will observe FC-MIT.

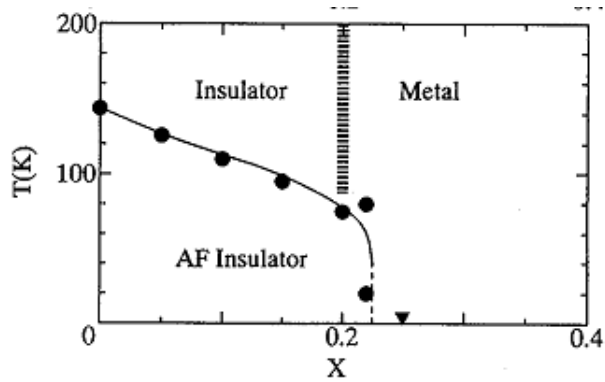


FIG.7 Phase diagram of $La_{1-x}Sr_xVO_3$ [7]
 The FC-MIT(filling control transition) occurs at $x_c \approx 0.2$

References

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