Theory of the Luttinger surface in doped Mott insulators

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Abstract

In this paper, we give a general introduction to Luttinger's theorem and Mott insulators followed by a discussion on the characterization of Mottness using divergence of self energy and subsequently arriving at the Luttinger surface. Different scenarios in presence and absence of particle-hole symmetry are explored along with validity of Luttinger's theorem in the former and its breakdown in the latter. A modification of Luttinger's theorem is presented.

1 Luttinger's theorem

Luttinger's theorem relates the particle density of a Fermi liquid with the volume enclosed by its Fermi surface. Taking n_e in d dimensions

$$n_e = 2 \int_{G(\omega=0,p)>0} \frac{d^d x}{(2\pi)^d} \tag{1}$$

The factor of 2 comes from spin degenaracy.

2 Mott insulators and Luttinger's surface

We are familiar with explanation of conduction of electricity in materials using band theory. Mott insulators are materials that are expected to be electrical conductors under conventional band theories. However they show insulating behaviour, especially at low temperatures. To understand their behaviour we need a theory which takes into account strong electron-electron correlation.

2.1 Band Insulator

A typical band insulator has a Hamiltonian of the form:

$$H_{BI} = -t \sum_{j\sigma}(c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma}) + V \sum_{j\sigma}(-1)^j c_{j,\sigma}^\dagger c_{j,\sigma} = H_t + H_V \tag{2}$$

We can go to momentum space by doing a Fourier transform of the particle operator, i.e. $c_{n\sigma} = \dfrac{1}{\sqrt{N}} \sum_{k\sigma}$ and we get

$$H_{BI} = H_t + H_V = -t \sum_{k\sigma} \psi^\dagger_{k\sigma'} \begin{pmatrix} \epsilon(k) & V \\ V & -\epsilon(k) \end{pmatrix} \psi_{k\sigma'} \qquad (3)$$

Where $\psi_{k\sigma'} = \begin{pmatrix} c_{k\sigma} \\ c_{(k-\pi/a)\sigma} \end{pmatrix}$ and eigenvalues of the matrix sandwiched in between are $\varepsilon(k) = \pm \sqrt{\epsilon^2 + V^2}$ These eigenvalues correspond to different bands, i.e. the filled valence band (lower energy) and the empty conduction band (higher energy). As long as the valence band is full there is a band gap, i.e. a cost associated with placing an additional electron into the system.

In the absence of interactions for band insulator bands are strict eigenstates of single particle operators, and the occupying of valence band does not affect the conduction band; indeed the bands are static in the filling. For Mott insulator however, the bands are rigid as the spectral weight of each band depends upon the electron filling.

2.2   Mott Gap

NiO is supposed to be a conducting material according to conducting band theory as Ni ($3d^8 4s^2$ gives 2 electrons to O and therefore Ni$^+$ has 2 unpaired electrons. However the material is an insulator due to the electron repulsions which add an energy cost U for doubly occupying an orbital. At zero temperature, if U exceeds a certain value, there are no conduction electrons resulting in a charge gap which we call the Mott gap.

So now the Hamiltonian becomes

$$H = -t \sum_{ij\sigma} g_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{j\sigma} \qquad (4)$$

μ being the chemical potential.

2.3   Green function

To obtain the bands and their spectral weights' dependance on the filling we use the single particle Green function.

$$G_{i\sigma} = -i\theta(t) \langle \{c^\dagger_{i\sigma}, c_{j\sigma}\} \rangle \qquad (5)$$

Differentiating and Using the Heisenberg equations of motion we obtain

$$\partial_t G_{i\sigma} = -i\delta(t) - i\theta(t) \langle \{ \dot{c}_{i\sigma}, c^\dagger_{i\sigma} \} \rangle \qquad (6)$$

where $\dot{c}_{i\sigma} = U c_{i\sigma} n_{i\bar{\sigma}}$ - $\mu c_{i\sigma}$. To solve this we define

$$\tilde{G}_{i\sigma} = \theta(t) \langle \{c_{i\sigma}(t) n_{i\sigma}(t), c^\dagger_{i\sigma}(0) \rangle \qquad (7)$$

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and inserting it into the differential of the Green function, we get

$$\partial_t G_{i\sigma} = -i\delta(t) - U\tilde{G}_{i\sigma}(t,0) + i\mu\tilde{G}_{i\sigma}(t,0) \tag{8}$$

Differentiating $\tilde{G}_{i\sigma}$ and using Fourier transform we obtain a solution for it as

$$\tilde{G}_{i\sigma}(\omega) = \frac{n_{i\bar{\sigma}}}{\omega - U + \mu} \tag{9}$$

Then we can obtain the single particle Green function as

$$G_{i\sigma}(\omega) = \frac{1}{\omega = \mu} + \frac{U\langle n_{i\bar{\sigma}}\rangle}{(\omega + \mu)(\omega + \mu - U)}) \tag{10}$$

Summing over the spin degrees of freedom and shifting μ to $\mu + U/2$ we get

$$G_i(\omega) = \frac{2-n}{\omega + \mu} + \frac{n}{\omega + \mu - U} = \frac{1+x}{\omega + \mu} + \frac{1-x}{\omega + \mu - U} \tag{11}$$

where x is the hole number (fraction of number of holes out of total number of electrons and holes) equal to 1-n, n being the number of electrons (again a fraction). Clearly there is a dynamic dependence on the filling. Further analyzing the spectral function $A(\omega) = \dfrac{-1}{\pi}G_i(\omega + i\Gamma)$ we get

$$A(\omega) = (1+x)\delta(\omega - \mu + U/2) + (1-x)\delta(\omega - \mu - U/2) \tag{12}$$

The Real part of the Green function would be

$$R(\omega) = ReG_i(\omega) = \int_{-\infty}^{\infty} d\omega \frac{A(\omega)}{\omega - \omega'} \tag{13}$$

Since the spectral function vanishes in the Mott gap, we can write the real part as

$$R(\omega) = -\int_{-\infty}^{-\Delta_-} d\omega \frac{A(\omega)}{\omega} - \int_{\Delta_+}^{\infty} d\omega \frac{A(\omega)}{\omega'} \tag{14}$$

Where $\Delta_\pm$ are the upper and lower edges of the Mott gap. The integral can vanish under some particular conditions as $A(\omega)$ is always positive definite, In fact in the atomic limit, x=0. Using (12), $R(\omega) = 0$ for all momenta at $\mu = 0$. Away from the limit, $R(\omega) = 0$ for specific values of momentum. Indeed there exists a surface in momentum space for which the real part of the single particle Green function vanishes. This is called the Luttinger surface.

3 Particle-hole symmetry

To find out the exact location of the zeroes in a material where particle hole symmetry is present, we shall first do a particle-hole transformation

$$c_{i\sigma} \to e^{iQr}c_{i\sigma}^\dagger \tag{15}$$

For invariance of the Hamiltonian undere the transformation with $\mu = U/2$, $Q = (\pi, \pi)$, i.e. it is π along the x and y axes. This leads to the identity

$$A_{\sigma(\omega, k)} = A_{\sigma(-\omega, -k-Q+2n\pi)} \tag{16}$$

For $k = Q/2 + 2n\pi$, the spectral function is an even function of frequency.

In 1D and nearest neighbour hopping, the Fermi points (there can be no surface in 1D) at half filling are $\pm\pi$. in 2D, we can also use this to get 2 points but to get the surface we utilize the symmetry of interchanging x and y axes leaving the Hamiltonian unchanged as long as hopping t is isotropic ($t_x = t_y$). For $Q = (q,q)$, the components of momentum along the X and Y axes can be interchanged to give us

$$k_y = -k_x - q + 2n\pi \tag{17}$$

and by reflection symmetry we get

$$-k_y = -k_x - q + 2n\pi \tag{18}$$

Then we get the condition from (17) and (18)

$$k_x \pm k_y = -\pi + 2n\pi = (2n-1)\pi \tag{19}$$

giving us $\cos k_x + \cos k_y = 2\cos(\dfrac{k_x + k_y}{2}) \cos(\dfrac{k_x - k_y}{2}) = 2\cos^2(\dfrac{(2n-1)\pi}{2}) = 0$

This gives us the surface of zeroes.

Even in the non-isotropic case, we can use a different prescription to find the zeroes of the Green function.

$$t(k) = t_x \cos k_x + t_y \cos k_y \tag{20}$$

where $t_x \neq t_y$.

Let's us define the moment

$$M_n^\sigma(k) = \int d\omega \omega^n A_\sigma(\omega, x) = \int d\omega \omega^n \int dt e^{i\omega} (\langle c_i(t), c_j^\dagger(0)\rangle + \langle c_j^\dagger(0), c_i(t)\rangle) \tag{21}$$

Using $\omega^n e^{i\omega t} = (\text{-i})^n \partial^n e^{i\omega t}$ we get $\int \dfrac{d\omega}{2\pi} \omega^n A_\sigma ij(\omega) = M_n^\sigma(\text{i,j})$ where

$$M_n^\sigma(i,j) = \frac{1}{2}(\langle\{[H,[H,...[H,c_{i\sigma}]]...]_{ntimes}, c_{j\sigma}^\dagger\}\rangle + \langle\{c_{i\sigma}, [H,[H,...[H,c_{j\sigma}^\dagger]]...]_{ntimes}c_{i\sigma}\}\rangle) \tag{22}$$

is a string of commutators of the Hubbard Hamiltonian H. Decomposing the Hubbard Hamiltonian into its H_U and H_t parts we can get the commutator (for n commutations) as

$$K_{i\sigma}^n = [...[c_{i\sigma}, H],...H]_{ntimes} = \sum_j t_{ij}\Lambda_{j\sigma}^n + Q_{i\sigma}^n \tag{23}$$

Where $Q_{i\sigma}^n = [...[c_{i\sigma}, H_U],...H_U$ and $\Lambda_{j\sigma}^n$ contains the H_t term. So in the moments, for only the H_U part, we get

$$\langle\{Q_{i\sigma}^n, c_{j\sigma}^\dagger\rangle = \delta_{ij}\gamma_n \tag{24}$$

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and so the moment is

$$M_n^\sigma(i,j) = \delta_{ij}\gamma_n + \frac{1}{2}\sum_l t_{il}(\langle\{\Lambda_{j\sigma}^n, c_{j\sigma}^\dagger\}\rangle + h.c.) \tag{25}$$

Applying the constraint that (15) must be symmetric under parity, at half filling and $\mu = U/2$ we get

$$\gamma_n = (\frac{U}{2})^n\frac{1 + (-1)^n}{2} \tag{26}$$

which shows that it vanishes for odd n. As the Green function itself is the zeroth moment, all we have to do to make sure it's an even function is make the second term vanish. This term which is proportional to t(k) can vanish for certain values of momentum, which happen to be the Fermi momentum k_F (and the anisotropy plays no role here as both components are zero at the Fermi surface). Therefore G(0, k=k_F = 0 for a Mott insulator. This is an exact result. In this case, the volume enclosed by the surface of zeroes is equal to the particle density which shows that in the presence of particle hole symmetry, Luttinger's theorem holds in a Mott insulator.

A remarkable result we arrive at further is that the self energy Σ of the electron (arises when the electron interacts with itself) defined by :

$$G_{i\sigma}(\omega) = \frac{1}{\omega + \mu + U/2 - \Sigma} \tag{27}$$

diverges at the Luttinger surface as all the other terms in the denominator are finite. This differentiates the Mott insulator from the Fermi liquid where the self energy vanishes at the chemical potential.

4 Absence of particle-hole symmetry

Let's now discuss what happens to Luttinger's theorem in the absence of particle hole symmetry. Since we are now working away from the non-interacting limit we must consider certain modifications to our previously known formulations. The particle density in terms of Green function can be expressed as can be expressed as

$$n = -2i\sum_k \lim_{t\to\infty}\int\frac{d\omega}{2\pi}G(k,i\omega)e^{i\omega t} \tag{28}$$

Where the factor of 2 comes due to spin degeneracy. We further use the identity

$$G(k,i\omega) = \frac{\partial}{\partial i\omega}lnG^{-1}(k,i\omega) + G(k,i\omega)\frac{\partial}{\partial i\omega}\Sigma(k,i\omega) \tag{29}$$

Then we can rewrite the particle density as the difference between two integrals I_1 and I_2

$$n = -2i\sum_k\int_\infty^\infty\frac{d\omega}{2\pi}\frac{\partial}{\partial i\omega}lnG^{-1}(k,i\omega) - 2i\sum_k\int_\infty^\infty G(k,i\omega)\frac{d\omega}{2\pi}\Sigma(k,i\omega) = I_1 - I_2 \tag{30}$$

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Now to establish whether on not Luttinger's theorem breaks down with particle hole asymmetry, we must evaluate the second integral I_2. To do so we must first define the Luttinger-Ward functional $\Phi[G]$ which is a scalar functional of the electron-electron interaction and the self-energy depends on it as follows:

$$\Sigma = \frac{\delta\Phi[G]}{\delta G} \tag{31}$$

The Luttinger-Ward functional has a perturbative expansion generally, so at first we will expect similar behavior in Mott insulators as well. From (27) we know where Σ fits into the Green function. In the atomic limit the form we obtain for it is

$$\Sigma = \frac{U}{2} + \frac{U}{2}\frac{1}{\omega + \mu} = \frac{U}{2} + \frac{-1 \pm \sqrt{1 + U^2 G^2}}{2G} \tag{32}$$

but to in a perturbative expansion of the LW functional, $\Sigma = U$ up to all orders. This is a contradiction. Clearly we cannot arrive at the Mott gap perturbative expansion as the latter form of the self energy has no ω or rather G dependence and so we must therefore adopt some different prescription.

To get the exact form of the LW function, we follow what Altshuler et al did by integrating Σ with respect to G, i.e.

$$\delta\Phi[G] = \sum_k \int \frac{d\omega}{\omega} \sum(k, i\omega)\delta G(k, i\omega) \tag{33}$$

keeping in mind that the approximate LW functional obtained must contain a singular part and that I_2 obtained thus must agree with direct calculation as in (30). The result was then

$$\Phi(i\omega) = \frac{1}{2}[-lnG(i\omega) \pm \sqrt{1 + U^2 G^2(\omega)} \pm \frac{1}{2}ln(\frac{\sqrt{1 + U^2 G^2(\omega)} - 1}{\sqrt{1 + U^2 G^2(\omega)} + 1})] \tag{34}$$

From this we obtain I_2 as

$$I_2 = -2I \int \frac{d\omega}{2\pi}\frac{\delta\phi(i\omega)}{\delta i\omega} = 2\Theta(\mu) - \Theta(-\mu + U/2) - \Theta(-mu - U/2) \tag{35}$$

It is to be observed that in the presence of particle hole shymmetry, i.e. $\mu = 0$, I_2 completely. Which gives us the modified Luttinger theorem as

$$n = \int_{G(0,k)} \frac{d^2 k}{(2\pi)^2} + \Theta(\mu) \tag{36}$$

5 Consequences and Results

5.1 Self Energy Divergence

As mentioned previously, the self energy diverges at the Luttinger surface as the Green function vanishes at the Luttinger surface. In presence of particle

hole symmetry, this happens linearly.i.e. the Green function is proportional to the difference between k (particle momentum) and k_L (momentum at Luttinger surface). This could give us the dependence of the real part of the self energy of the form :

$$Re\Sigma(k, \omega 0) \propto \frac{1}{k - k_L} \tag{37}$$

thus showing the divergence at the surface. Indeed such a divergence keeps the energy band (after taking self energy into consideration) $\epsilon(k) + Re\Sigma(k,\omega)$ from crossing the Fermi energy, thus making the material an insulator.

Additionally we state that the Green function's zeroes are defining characteristic of a Mott insulator and independent of the spin ordering of the ground state. That last point is to emphasize that the associated divergence of the self energy is not specifically a consequence of antiferromagnetism as has been claimed by other others, rather is the cause of the insulating properties of the material without doping.

5.2 Projected models

In projected models of t-J model of doped Mott insulators where we truncate upto a certain number of terms, we don't see the single particle Green's function's zeroes. This is because projecting out the double occupancy cause only the spectral weight below the chemical potential at half filling to remain which leaves us with only the first integral in (14) which is non zero and has no other term to cancel it.

This in turn points us to the location of chemical potential in a doped Mott insulator at half filling. Say if it were higher than the lower Hubbard band (- $\sqrt{V^2 + \epsilon^2}$) and U=∞. Then according to (12) the spectral function would have an infinite energy denominator above the Mott gap and so the second term in (14) disappears so the real part of the Green function doesn't vanish (no surface of zeroes then).

How then can we define a Mott insulator in the absence of the Luttinger surface then? In such conditions where the chemical potential may have any arbitrary value (at zero temperature), we rely on the fact that the spectral weight is always evenly distributed above and below the gap at half filling which in turn makes sure that the Green function must change sign over some surface of momentum within the gap. Therefore, even if a given model (which may not be realistic) does not give a surface if zeroes, a sign change in the Re G(k) is sufficient establish "Mottness'

5.3 Weak and Strong Violations of Luttinger surface

Let's consider doping of the material. The location of the zeroes is not so trivial as it was in the particle hole symmetric case. We know at least that a that the Green function's real part must be zero along some surface in momentum space
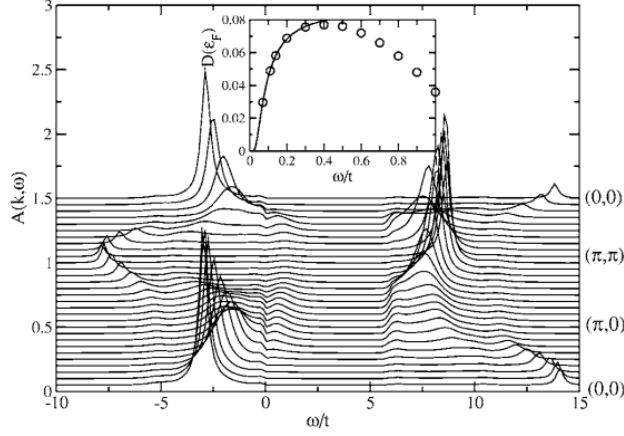
Figure 1:

because the spectral weight at half filling changes across the chemical potential. Most of it at $(k_x, k_y) = (\pi, \pi)$ lies above μ while the spectral wight at $(0,0)$ lies below.

To satisfy (14), we need the spectral wight to lie above μ. We could redistribute the spectral weight to get the zero of Re G(K) however its symmetric distribution around the chemical potential or lack thereof will determine the severity of the violation of the Luttinger.

Here in we introduce two types of violations of the Luttinger volume:

- Weak Violation

- Strong Violation

5.3.1   Weak Violation

Following (19), we seek to keep the Luttinger surface close to $k_x + k_y = \pi$ line. Using results obtained from Fig. 1, to stick to such a surface the spectral weight above μ must be small compared to spectral weight below μ and therefore the chemical potential asymmetric within the Mott gap for Re G to vanish.

5.3.2   Strong Violation

On the other hand the Luttinger volume could be strongly violated at the cost of keeping the distribution of the spectral weight more symmetrical about the chemical potential. The surface of zeroes is close to $(k_x, k_y) = (\pi, \pi)$. Both of these are demonstrated in panels (b) (for weak violation) and (c) (for strong violation) in Fig. 2.
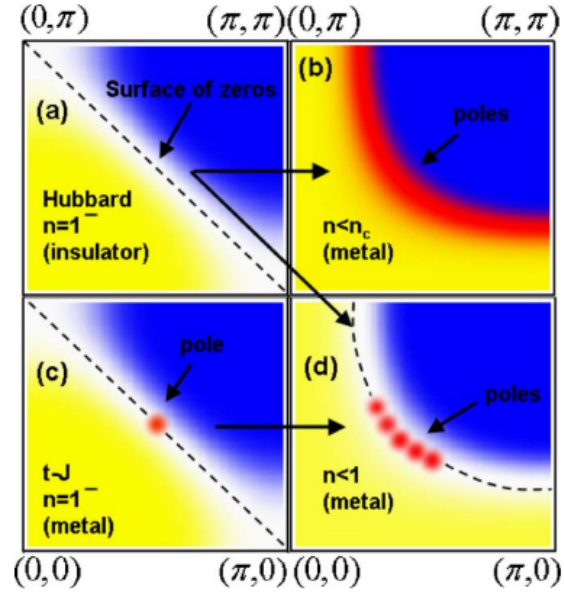
Figure 2:

6 Conclusion

7 References