ICTS School on Strongly Correlated Systems

Many body physics review

Kinematics

We are interested in electronic systems. Electrons are fermions. Our collection of electrons may be modeled to live in the continuum or on a lattice depending on the problem of interest.

In the continuum, $c^{\dagger}_{\sigma}(\vec{r})$ creates an electron at position $\vec{r}$, and similarly on a lattice we may create an electron at site i with ~~index~~ $c^{\dagger}_{i\sigma}$. ~~where~~ where σ stands for the spin label which may be $\uparrow$ or $\downarrow$. The fermion operators satisfy

$$\{c_{\sigma}(\vec{r}),\ c^{\dagger}_{\sigma'}(r')\} = \delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}')$$

$$\{c_{\sigma}(\vec{r}),\ c_{\sigma'}(r')\} = 0$$

or

$$\{c_{i\sigma},\ c^{\dagger}_{j\sigma'}\} = \delta_{ij}\,\delta_{\sigma\sigma'}$$

$$\{c_{i\sigma},\ c_{j\sigma'}\} = 0.$$

where $\{\ \}$ is the anticommutator.

We will move freely between real and k space via

$$c^\dagger_\sigma(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}}' e^{-i\vec{k}\cdot\vec{r}} c^\dagger_\sigma(\vec{k})$$

and

$$c^\dagger_{i\sigma}(\vec{r}) = \frac{1}{\sqrt{N}} \underbrace{\sum_{\vec{k}}'}_{\vec{k} \in BZ} e^{-i\vec{k}\cdot\vec{r}} c^\dagger_\sigma(\vec{k})$$

where V and N are volume and number of sites respectively.

<u>Dynamics</u>: The dynamics of the system is determined by its Hamiltonian. The Hamiltonian is written down typically by

1. Identifying the symmetries of the system
2. Identifying the energy scales

For example, the problem of electrons in a ~~solid~~ ~~clean~~ solid has a well known Hamiltonian

$$\mathcal{H} = \int d^d\vec{r}\, \psi^\dagger_\sigma(\vec{r}) \left(-\frac{\nabla^2}{2}\right) \psi_\sigma(\vec{r}) + \underbrace{\int d^d r\, v(\vec{r})}_{\text{Ionic potential}} \psi^\dagger_\sigma(\vec{r}) \psi_\sigma(\vec{r})$$

$$\underbrace{- \mu \int d^d r\, \psi^\dagger_\sigma(\vec{r}) \psi_\sigma(\vec{r})}_{\text{(chemical potential)}}$$

$$+ \frac{e^2}{\cancel{2}} \int d^d r\, d^d r'\, \psi^\dagger_\sigma(\vec{r}) \psi^\dagger_{\sigma'}(\vec{r}') \frac{1}{|\vec{r}-\vec{r}'|} \psi_{\sigma'}(\vec{r}') \psi_\sigma(\vec{r})$$

Or, the Hubbard model on the a lattice.

$$\mathcal{H} = -t \sum_{\langle ij \rangle}' (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c) - \mu \sum_{i}' c^{\dagger}_{i\sigma} c_{i\sigma}$$
$$+ U \sum_{i}' c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow}$$

Discuss: what is strong correlation?

Note that both these Hamiltonians are endowed with all the usual symmetries such as ① Translation ② Rotation/lattice ~~[illegible]~~ symmetries ③ Time reversal ④ Phase symmetry etc:

~~Hypothetically,~~ Let us suppose that we can diagonalize this Hamiltonian and write

$$\mathcal{H} |\Psi_n\rangle = E_n |\Psi_n\rangle$$

where $|\Psi_n\rangle$ are the energy eigenvectors and E_n are the energy eigenvalues. Lets say the $|G\rangle$ is the ground state. If $\mathcal{U}$ is a symmetry of the system ($\mathcal{U}^{\dagger}\mathcal{H}\mathcal{U} = \mathcal{H}$), then if $\mathcal{U}|G\rangle \neq |G\rangle$, then $|G\rangle$ breaks a symmetry. A symmetry is broken if the ~~[illegible]~~ state of the system does not have all the symmetries of the Hamiltonian. While this is quite clear at $T=0$ (temperature), what can we say about finite temperature?

At a finite ($T = \frac{1}{\beta}$) temperature, the state is described by a density matrix

$$\rho = \frac{1}{Z} e^{-\beta \mathcal{H}} \qquad \text{where } Z = \mathrm{tr}\, e^{-\beta \mathcal{H}}$$

$$Z = \sum_n e^{-\beta E_n} \qquad \text{and } \rho = \frac{1}{Z} \sum_n e^{-\beta E_n} |\psi_n\rangle\langle\psi_n|$$

$$(|\psi_n\rangle \equiv |n\rangle) \qquad = \sum_n \overset{\boxed{e^{-\beta E_n}/Z}}{p_n} |n\rangle\langle n|$$

Again if $\mathcal{U}^{\dagger}\rho\,\mathcal{U} \neq \rho$ then we will have broken a symmetry (if $\mathcal{U}$ is ~~the~~ a symmetry of $\mathcal{H}$).

~~While the intentions of the discussion so far~~

~~Discussion~~: Suppose we knew the state of the system ρ, then we can obtain the expectation value of any observable A as

$$\langle A \rangle = \mathrm{tr}(\rho A).$$

This discussion, in principle (only in principle) solves all problems!

Responses: As introduced, we are also interested in obtaining/predicting the responses of the systems. Responses in General can be nonlinear. We will focus only on linear response. Suppose, I go on to apply a "stimulus" to the system, changing the Hamiltonian to

$$\mathcal{H}_f \to \mathcal{H} - \underbrace{f(t)}_{\text{"force"/ stimulus}} \underbrace{B}_{\text{some operator}}$$

Where $f(t)$ is the force and B is the operator of the system. We now look for the response of the system via the expectation value of an operator A

$$\Delta A(t) = \langle A \rangle_f^{(t)} - \langle A \rangle \equiv \int dt' \, \chi_{AB}(t-t') f(t')$$

$\chi_{AB}(t-t')$ is the response function. (Generically this will be $\chi_{AB}(t,t')$, but we focus on nice systems). This looks much nicer in frequency domain as

$$\Delta A(\omega) = \chi_{AB}(\omega)\, f(\omega).$$

The fourier tranforms are defined as

$$f(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} f(t) \quad \& \quad f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} f(\omega)$$

The impatant thing to remember is that $\chi_{AB}(t-t')$ is a causal function. i.e,

$$\chi_{AB}(t-t') = 0 \quad \text{if } t-t' < 0.$$

This is the statement that furture cannot affect the present, only the past can.

What is our predicted $\chi_{AB}(t-t')$? Kubo and others provided the answer to this question. The Kubo formula

$$\chi_{AB}(t-t') = -i\, \Theta(t-t') \langle [A(t), B(t')] \rangle$$

where $A(t) = e^{i\mathcal{H}t} A e^{-i\mathcal{H}t}$ (and a similar formula for $B(t')$) is the Heisenberg operator. This is a formally exact relation but is not generally easy to calculate. We can also get more revealing expressions for $\chi_{AB}(\omega)$

For this we need some mathematical results.

① The fourier transform of the θ function

$$\theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t \le 0 \end{cases}$$

$$\Theta(\omega) = \int_{-\infty}^{\infty} dt\, e^{+i\omega t}\, \theta(t)$$

is not well defined. So we do $\omega = \omega + i\eta = \omega^+$

$\eta > 0$ is a small +ve quantity. Then

$$\Theta(\omega^+) = + \frac{i}{\omega^+}$$

② $$\frac{1}{\omega^+} = P\left(\frac{1}{\omega}\right) - i\pi\delta(\omega)$$

For example for a ~~real~~ nice function $f(\omega)$

$$\int_{-\infty}^{\infty} d\omega\, f(\omega) \frac{1}{\omega^+} = P\int_{-\infty}^{\infty} d\omega \frac{f(\omega)}{\omega} - i\pi f(0)$$

We are ready to obtain $\chi_{AB}(\omega)$.

Define $p_n = \dfrac{e^{-\beta E_n}}{Z}$. $\rho = \sum_n{}' p_n |n\rangle\langle n|$

(we have changed notation $|\psi_n\rangle \equiv |n\rangle$)

$$-i\,\theta(t-t') \sum_n{}' p_n \langle n| [A(t), B(t')] |n\rangle .$$

$$-i\,\theta(t-t') \sum_{n,m}{}' p_n \left[\langle n| A(t) |m\rangle\langle m| B(t') |n\rangle \ldots\right.$$

$$-i\theta(t-t')\sum_{m,n}{}' p_n\Big[\langle n|A|m\rangle\langle m|B|n\rangle e^{-i\omega_{mn}(t-t')}$$

$$\langle n|B|m\rangle\langle m|A|n\rangle e^{i\omega_{mn}(t-t')}$$

$$\omega_{mn} = E_m - E_n$$

change $m \Leftrightarrow n$ in second term

$$\chi_{AB}(t-t') =$$

$$-i\,\theta(t-t') \times \sum_{m,n}{}' (p_n - p_m)\langle n|A|m\rangle\langle m|B|n\rangle e^{-i\omega_{mn}(t-t')}.$$

$\Rightarrow$

$$\chi_{AB}(\omega^+) = \sum_{m,n}{}' \frac{(p_n - p_m)\langle n|A|m\rangle\langle m|B|n\rangle}{\omega^+ - \omega_{mn}}.$$

This is the famous Lehmann representation.

$$\chi_{AB}(\omega^+) = \chi^r_{AB}(\omega) + i\chi^i_{AB}(\omega)$$

$$\chi^i_{AB}(\omega) = -\pi\sum_{m,n}{}' (p_n - p_m)\langle n|A|m\rangle\langle m|B|n\rangle\,\delta(\omega-\omega_{mn})$$

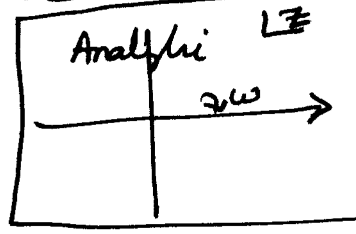
Note that $\chi^r_{AB}(\omega)$ is completely determined by $\chi^i_{AB}(\omega)$. This is called the

the Kramer's Kröning relation. By the same token if $\chi^{r}_{AB}(\omega)$ is known, then one can obtain $\chi^{i}_{AB}(\omega)$.

One can define $\chi_{AB}(z)$ for any complex frequency

$$\chi_{AB}(z) = \sum_{m,n}' (P_n - P_m) \frac{\langle n|A|m\rangle\langle m|B|n\rangle}{z - \omega_{mn}}$$

by analytic continuation. The key thing for causality and stability, is that this function of z is analytic in the upper half ~~plane~~ of z-plane.



~~Note~~ In the discussion so far, A and B are observable operators and are usually quadratic in the fermion operator. for examples, to obtain the magnetic susceptibility $B = \vec{S}_{tot}$ (total spin operator)

~~B(t)~~ and $A = \frac{\vec{S}_{tot}}{N}$ (also!). $\vec{S}_{tot} = \sum_i' c^{+}_{i\sigma} \vec{\tau}_{\sigma\sigma'} c_{i\sigma'}$

In practice we are also interested in other ~~[illegible]~~ correlation functions

A case in point is the retarded Green's function

$$G_{ab}(t-t') = -i\,\theta(t-t')\langle\{c_a(t), c_b^\dagger(t')\}\rangle$$

where a and b label some one particle
state of the system. We will see
later that this is a very important
correlation function from the point
of view of experiments. Lets analyse
this in some detail. We will begin
with a Lehmann representation of the
retarded Green's function:

$$G_{ab}(t-t') = -i\,\theta(t-t') \times$$

$$\sum_{m,n}' p_n \Big[\langle n|c_a|m\rangle\langle m|c_b^\dagger|n\rangle e^{-i\omega_{mn}(t-t')} + \langle n|c_b^\dagger|m\rangle\langle m|c_a|n\rangle e^{i\omega_{mn}(t-t')} \Big\}$$

$$G_{ab}(\omega^+) = \sum_{m,n}' (p_n + p_m)\frac{\langle n|c_a|m\rangle\langle m|c_b^\dagger|n\rangle}{\omega^+ - \omega_{mn}}.$$

Now imaginary part of this

$$-\frac{1}{\pi} G_{ab}(\omega^+) = \sum_{m,n}' (p_n + p_m)\langle n|c_a|m\rangle\langle m|c_b^\dagger|n\rangle\,\delta(\omega-\omega_{mn})$$

$$A_{ab}(\omega) = \sum_{m,n}{}' (P_n + P_m) \langle n | c_a | m \rangle \langle m | c_b^\dagger | n \rangle \, \delta(\omega - \omega_{mn}).$$

Now consider

$$\int_{-\infty}^{\infty} \cancel{A_{ab}} \, d\omega \, A_{ab}(\omega)$$

$$= \sum_{m,n}{}' (P_n + P_m) \langle n | c_a | m \rangle \langle m | c_b^\dagger | n \rangle$$

$$= \sum_{n}{}' P_n \left(\langle n | c_a c_b^\dagger + c_b^\dagger c_a | n \rangle \right)$$

$$= \langle \{ c_a, c_b^\dagger \} \rangle = \delta_{ab}$$

if a and b are orthonormal 1-particle states. In particular, in this case,

$$\int_{-\infty}^{\infty} d\omega \, A_{aa}(\omega) = 1.$$

Note that

$$A_{aa}(\omega) = \underbrace{\sum_{m,n}{}' (P_n + P_m) | \langle m | c_a^\dagger | n \rangle |^2 \, \delta(\omega - \omega_{mn})}_{>0}.$$

We now see that $A_{aa}(\omega)$ has the interpretation of a probability. In fact, $A_{aa}(\omega)$ is the probability that an added particle in the state a has an energy ω. Let us get a better understanding. At $T=0$,

$$A_a(\omega) = \sum_m |\langle m | c_a^\dagger | G\rangle|^2 \, \delta(\omega - \omega_{mG})$$

since only the ground state is occupied. If the ground state has M particles then the state $|m\rangle$ must have M+1 particles. The state $c_a^\dagger|G\rangle$ may have matrix element with many such M+1 particle states, ~~and~~ which have different energy eigenvalues. Thus the added particle "can have any energy" depending on the matrix elements. Let us see some of these things in action. The best place to start the discussion is the free fermi gas.

For the free fermi gas

$$\mathcal{H} = \sum_{\vec{k}}' \left(\frac{k^2}{2} - \mu\right) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} = \sum_{k}' \xi(\vec{k})\, c^\dagger_{k\sigma} c_{k\sigma}$$

where μ is determined at any temperature to ~~fixed~~ fix the number of particles

~~[illegible]~~ We have chosen the one particle states as the momentum states

~~[illegible]~~

$$G_{\vec{k}\sigma,\vec{k}'\sigma'}(t-t') = -i\,\theta(t-t')\left\langle\left\{ c_{\vec{k}\sigma}(t), c^\dagger_{\vec{k}'\sigma'}(t')\right\}\right\rangle$$

$\Rightarrow$ Now what are $c^\dagger_{k'\sigma'}(t')$ and $c_{\vec{k}\sigma}(t)$

~~[illegible]~~ for the free gas?

Note that the $|n\rangle$ states are the slater determinants with filled momentum states

$$c^\dagger_{k\sigma}(t)\; e^{iHt}\, c^\dagger_{k\sigma}\, e^{-iHt}\, |m\rangle = e^{i\xi(k)t}\, c^\dagger_{k\sigma}$$

$$c_{k\sigma}(t) = e^{-i\xi(k)t}\, c_{k\sigma}$$

With this

$$G_{\vec{k}\sigma,\vec{k}'\sigma'}(t-t') = -i\,\theta(t-t')\, e^{-i\xi(k)t}\, e^{i\xi(k')t'} \left\langle\left\{ c_{\vec{k}\sigma}, c^\dagger_{\vec{k}'\sigma'}\right\}\right\rangle$$

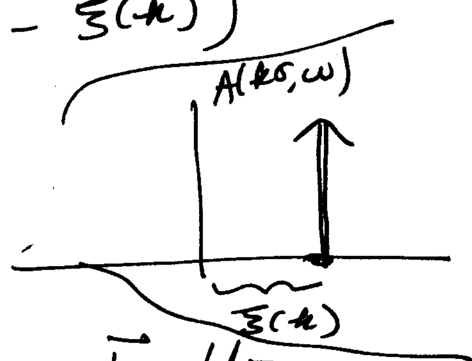
$$G_{\vec{k}'\sigma',\vec{k}'\sigma'}(t-t') = -i\theta(t-t')\, e^{-i\xi(\vec{k})t}\, e^{-i\xi(\vec{k})t'}\, \delta_{\vec{k}\vec{k}'}\,\delta_{\sigma\sigma'}$$

$$= -i\theta(t-t')\, e^{-i\xi(\vec{k})(t-t')}.$$

Thus
$$G_{\vec{k}\sigma,\vec{k}'\sigma'}(\omega^+) = \frac{\delta_{\vec{k},\vec{k}'}\,\delta_{\sigma\sigma'}}{\omega^+ - \xi(\vec{k})}$$

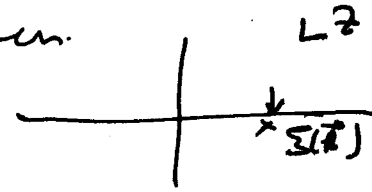
~~[illegible]~~ Note that the δ functions in momentum and spin σ appear since the free gas does not break translation ~~or~~ spin rotation symmetry. We ~~not~~ write
$$G_{\vec{k}\sigma}(\omega^+) = \frac{1}{\omega^+ - \xi(\vec{k})}$$

We get
$$A(\vec{k}\sigma,\omega) = \delta(\omega - \xi(\vec{k}))$$



Note that this A satisfies the sum rule, and also note that A~~[illegible]~~ for a given $\vec{k}$ there excitation can ~~[illegible]~~ has a precise energy.
~~[illegible]~~

We say that the presence of particle like excitations is characterized by a pole in the Greens' function.



$$G_{\vec{k}\sigma}(z) = \frac{1}{z - \xi(k)}$$

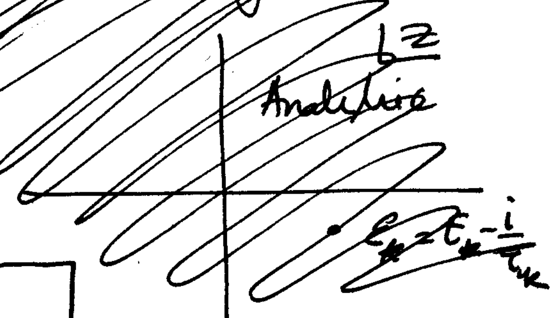
and there is a pole at $z = \xi(\bar{k})$

$\boxed{\text{DISCUSS } G_{i\sigma, i\sigma}}$

What happens if there are interactions? Generically, we cannot find the Green's function exactly. Let us assume that the system does not break any symmetry. We can then discuss

$$G_{\vec{k}\sigma}(z) = \sum_{n,m}{}' (P_n + P_m) \frac{|\langle m | c^{\dagger}_{k\sigma} | n \rangle|^2}{z - \omega_{mn}}$$

This is a function that is analytic in the upper half space. ~~It may have a pole in the lower half plane. Suppose it does,~~



We will come back to this later in the course.

We now know that calculation of correlation functions such as χ and G etc are important for understanding experiments and even making predictions. How do we calculate these things? Here is where further development is needed. The idea is to use field theoretic techniques formulated via the Feynman path integral

Feynman Path Integral

Consider a particle ~~in~~ at state $|\vec{r}_I\rangle$, the initial state at time $t=0$. What is the amplitude that at time $t=t_F$ (the final time) the particle is in the state $|\vec{r}_F\rangle$. If we know the Hamiltonian

$$\mathcal{H} = \frac{P^2}{2} + V(\vec{r}),$$

then we know

$$\longrightarrow K(\vec{r}_F, t_F; \vec{r}_I, 0)$$

$$= \langle \vec{r}_F | e^{-i \int_0^{t_F} dt\, H} | \vec{r}_I \rangle .$$

Feynmann gave a diffrent prescription for the ~~calculation of~~ amplitude.

Feynman thought about how the particle reaches from $\vec{r}_I$ to $\vec{r}_F$ ~~via~~

He said that

① The particle is allowed to choose any path P such that $\vec{r}(0)=\vec{r}_I$ and $\vec{r}(t_F)=\vec{r}_F$. ; $P \equiv \left\{ \vec{r}(t) ; \begin{array}{l} \vec{r}(0)=\vec{r}_I \\ \vec{r}(t_F)=\vec{r}_F \end{array} \right\}$

② Associated with very path P there is an amplitude $K(P)$.

③ The amplitude $K(\vec{r}_F t_F ; \vec{r}_I 0)$ is a sum ~~over all paths~~ over all ~~paths~~ such amplitudes

$$K(\vec{r}_F t_F ; \vec{r}_I 0) = {\sum_P}' K(P).$$

But what is $K(P)$? Here, Feynman, possibly motivated by comments from Dirac

$$K(P) = e^{i S_{class}[\vec{r}(t)]}.$$

S_{class} is the classical action associated with this path P.

In other words,

$$S_{class}[P] = \int_0^{t_F} dt \, \underbrace{\mathcal{L}(\vec{r}, \dot{\vec{r}})}_{\text{Lagrangian.}}$$
$$S_{class}[\vec{r}(t)]$$

The amplitude now is written as a path integral.

$$K(F, I) = \int \mathcal{D}[\vec{r}(t)] \, e^{i S_{class}[\vec{r}(t)]}$$

It turns out that all of the other postulates of quantum mechanics, such as the uncertainty principle etc follow from these postulates of Feynman.

Keep all of this in mind. I will now change gears and work with ~~something~~ ~~Keep~~ discuss something else.

Back to our problem of calculation of response functions. We know that this is the correlation of A and B operators.

Let us play a little game, ~~at~~ and at the end of this we will see a rather neat thing.

Consider the Schrödinger propagator of our system $U_s(t) = e^{-i\mathcal{H}t}$

Now consider the partition function

$$Z = \mathrm{tr}\, e^{-\beta \mathcal{H}} = \mathrm{tr} e^{-\beta \mathcal{H}}$$

$$= \mathrm{tr}\, e^{-(-i^2)\beta \mathcal{H}}$$

$$= \mathrm{tr}\, e^{-i(-i\beta)\mathcal{H}}$$

$$= \mathrm{tr}\, U_s(-i\beta)$$

We see that the partition function is related to propagation in imaginary time! Buoyed by this realization, we get carried away and define an imaginary time τ (which is a real quantity) and define

$$U_s(\tau) = e^{-\tau \mathcal{H}} \quad ; \quad \boxed{\frac{\partial U_s}{\partial \tau} = -\mathcal{H} U_s \,!}$$

For any operator A, we now <u>define</u> a Heisenberg version, now in imaginary time

$$A(\tau) = e^{\tau \mathcal{H}} A e^{-\tau \mathcal{H}}$$

Now <u>define</u>

$$\chi_{AB}(\tau - \tau') = -\langle T_\tau A(\tau) B(\tau') \rangle \quad \left.\begin{matrix} \tau \in [0,\beta] \\ \tau' \in [0,\beta] \end{matrix}\right\}$$

$$\Rightarrow \tau - \tau' \in [-\beta, \beta]$$

where A and B can be either ~~f~~ bosonic (quadratic in $c^\dagger, c$) or fermionic (say linear in $c, c^\dagger$) T_τ denotes the ~~time~~ imaginary time ordering.

T_τ is defined as

$$T_\tau A(\tau) B(\tau') = \begin{cases} A(\tau) B(\tau') & \tau > \tau' \\ \pm B(\tau') A(\tau) & \tau' > \tau \end{cases}$$

Bosonic ← ± → Fermionic.

Note the + sign is for bosons, and − for fermions. We immediately see that $\tau - \tau'$ variable can be ~~$\chi_{AB}(\tau)$~~ replaced by a single variable $\tau \in [-\beta, \beta]$

$$\chi_{AB}(\tau) = -\langle T_\tau A(\tau) B(0) \rangle ; \tau \in [-\beta, \beta]$$

Now consider $\tau > 0$, and ask what is

$$\chi_{AB}(\underbrace{\tau - \beta}_{\tilde{\tau}}) = -\langle T_\tau A(\tilde{\tau}) B(0) \rangle$$

Since $\tilde{\tau} < 0$, we have

$$\chi_{AB}(\tau - \beta) = \mp \langle B(0) A(\tau - \beta) \rangle$$

$$= \mp \, \mathrm{tr}\left(e^{-\beta \mathcal{H}} B \, e^{(\tau-\beta)\mathcal{H}} A \, e^{-(\tau-\beta)\mathcal{H}}\right)$$

By cyclic invariance of the trace we see that

$$\chi_{AB}(\tau-\beta) = \pm\, \chi_{AB}(\tau)$$

+ . "Bosonic" operators, − Fermionic operators.

Now, since $\chi_{AB}(\tau)$ is a function defined in the interval $[-\beta,\beta]$, we can write this down as a Fourier series.

$$\chi_{AB}(\tau) = \sum_{\ell}{}^{'} e^{-i\omega_{\cancel{\ell}}\tau}\, \underbrace{\chi_{AB}(i\omega_{\cancel{\ell}})}_{\text{Fourier coefficient}}$$

where $i\omega_n = \dfrac{2\pi \cancel{k}}{(2\beta)}$, ($\cancel{k}$ n ~~is~~ integer).

~~For~~ Since

$$\chi_{AB}(\tau-\beta) = \pm\, \chi_{AB}(\tau)$$

We see that

$$e^{+i\omega_{\cancel{\ell}}\beta} = \pm\, 1 \quad \text{for}$$

all n.

$$e^{i\frac{2\pi \cancel{k}\beta}{2\beta}} = \pm 1$$

$$\Rightarrow \quad e^{i\pi \cancel{k}} = \pm 1.$$

This means that for Bosonic operators n must be even, and for fermionic operators ~~k~~ must be odd. We will use notation to distinguish this. ~~These~~ ~~iq_e for Bosonic~~ ~~For~~ (bosonic)

$$iq_e = \frac{2\pi}{\beta}(\cancel{2e})(e) \qquad e \text{ even}$$

$$ik_k = \frac{\pi}{\beta} k \qquad k \text{ odd.}$$

These are called ~~[illegible]~~ Bosonic and fermionic Matsubara frequencies.

We write

$$\chi_{AB}(\tau) = \frac{1}{\beta} \sum_{iq_e}{}' e^{-iq_e\tau} \chi_{AB}(iq_e) \quad \text{(Bosonic)}$$

$$\frac{1}{\beta} \sum_{ik_k}{}' e^{-ik_k\tau} \chi_{AB}(ik_k) \quad \text{(Fermionic)}$$

$$\chi_{AB}(iq_e) = \int_0^\beta d\tau\, e^{iq_e\tau} \chi_{AB}(\tau).$$

$$\chi_{AB}(ik_k) = \int_0^\beta d\tau\, e^{ik_k\tau} \chi_{AB}(\tau)$$

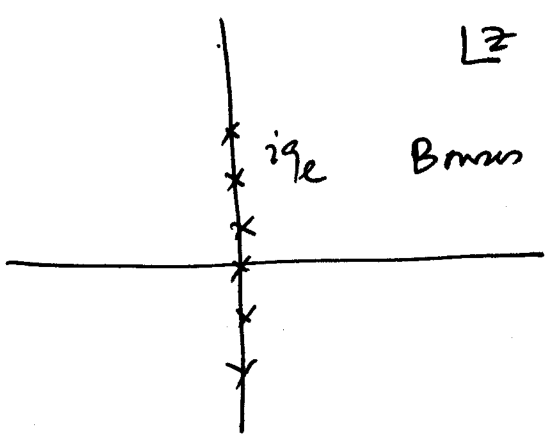
~~[illegible]~~

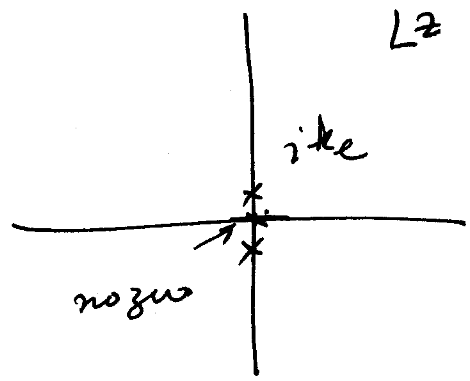
Now, we can write a Lehmann representation of ~~that~~ $\chi_{AB}(iq_l)$

$$\underset{\text{(Bosonic)}}{\chi_{AB}(iq_l)} = \sum_{m,n}{}' (p_n - p_m) \frac{\langle n|A|m\rangle\langle m|B|n\rangle}{iq_l - \omega_{mn}}$$

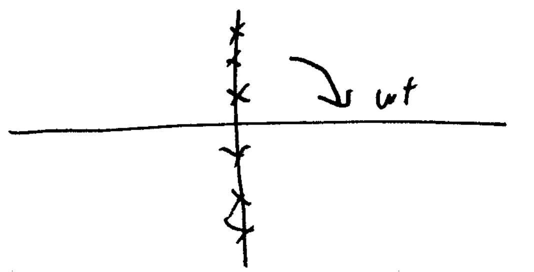
$$\underset{\text{(Fermi)}}{\chi_{AB}(ik_l)} = \sum_{m,n}{}' (p_n + p_m) \frac{\langle n|A|m\rangle\langle m|B|n\rangle}{ik_l - \omega_{mn}}$$

Note that these are <u>exactly the same</u> function we obtained before





Thus if we calculate $\chi_{AB}(iq_l)$ or $\chi_{AB}(ik_l)$ we can analytically continue this to obtain $\chi_{AB}(\omega^+)$



What is quite remarkable is that we can use field theoretic techniques to calculate $\chi_{AB}(\tau) \to \chi_{AB}(i\varsigma_{2\pi i/\beta}) \to \chi_{AB}(\omega^+)$.

~~We know about the the calculation~~ We now see that $\chi_{AB}(t-t')$ and $\chi_{AB}(\tau)$ are really the same thing.

We will see how to calculate $\chi_{AB}(\tau)$, but before that let us understand

$$\mathcal{G}_{ab}(\tau) = -\langle T_\tau\, c_a(\tau)\, c_b^{\dagger}(0)\rangle.$$

(temporal Green's function)

For simplicity, let us assume that the state does not break translational invariance and hence momentum is a good quantum number.

Let us take the Hamiltonian to be of the form

$$\mathcal{H} = \underbrace{\sum_{k\sigma}{}' \xi(k)\, c^{\dagger}_{k\sigma} c_{k\sigma}}_{\mathcal{H}_0} + \overbrace{\frac{U}{N}\sum_{\substack{k\\ k'\\ q}}{}' c^{\dagger}_{\frac{q}{2}+k\uparrow} c^{\dagger}_{\frac{q}{2}-k\downarrow} c_{\frac{q}{2}-k'\downarrow} c_{\frac{q}{2}+k'\uparrow}}^{\mathcal{H}_{\text{int}}}$$

Consider free fermions

$$\mathcal{H} = \sum_{k}{}' \xi(k)\, c^{\dagger}_{k\sigma} c_{k\sigma}$$

Let us obtain

$$\mathcal{G}_{k\sigma, k'\sigma'}(\tau-\tau')$$

$$= -\theta(\tau-\tau') \langle c_{k\sigma}(\tau) c^{\dagger}_{k'\sigma'}(\tau') \rangle$$

$$+ \theta[-(\tau-\tau')] \langle c^{\dagger}_{k'\sigma'}(\tau') c_{k\sigma}(\tau) \rangle$$

By the same arguments we have seen before

$$c_{k\sigma}(\tau) \underset{\text{free fermions}}{=} e^{-\tau\xi(k)} c_{k\sigma}$$

$$c^{\dagger}_{k\sigma}(\tau) = e^{\tau\xi(k)} c^{\dagger}_{k\sigma}$$

$$\mathcal{G}_{k\sigma,k'\sigma'}(\tau-\tau') = -\cancel{\theta(\tau-\tau') e^{-\tau\xi(k)} e^{-\tau'\xi(k')}}$$

$$= \Big[-\theta(\tau-\tau') \langle c_{k\sigma} c^{\dagger}_{k'\sigma'} \rangle + \theta(-(\tau-\tau')) \langle c^{\dagger}_{k'\sigma'} c_{k\sigma} \rangle \Big] e^{-\tau\xi(k)} e^{\tau'\xi(k')}$$

$$\langle c_{k\sigma} c^{\dagger}_{k'\sigma'} \rangle = (1 - n_F(\xi_k))\, \delta_{kk'} \delta_{\sigma\sigma'}$$

$$\langle c^{\dagger}_{k'\sigma} c_{k\sigma} \rangle = n_F(\xi_k)\, \delta_{kk'} \delta_{\sigma\sigma'}$$

$$n_F(x) = \frac{1}{e^{\beta x}+1}$$

$$\mathcal{G}_{k\sigma, k'\sigma'}(\tau-\tau')$$
$$= \Big(-\theta(\tau-\tau')\,(1-n_F(\xi_k))$$
$$+\theta(-(\tau-\tau'))\, n_F(\xi_k)\Big)\, e^{-\xi(k)(\tau-\tau')}\,\delta_{kk'}\delta_{\sigma\sigma'}$$

$$\frac{\partial}{\partial\tau}\mathcal{G}_{k,\ }(\tau-\tau')$$
$$= \Big(-\delta(\tau-\tau')\,(1-n_F(\xi_k))$$
$$-\delta(\tau-\tau')\, n_F(\xi_k)\Big)\,\delta_{kk'}\delta_{\sigma\sigma'}$$
$$-\xi(k)\,\mathcal{G}$$

$$-\left(\frac{\partial}{\partial\tau}+\xi(k)\right)\mathcal{G}_{k\sigma,k'\sigma'}(\tau-\tau') = \delta(\tau-\tau')\,\delta_{kk'}\delta_{\sigma\sigma'}$$

$$=\sum_{k_1\sigma_1}\int_0^\beta d\tau_1\; -\left(\frac{\partial}{\partial\tau}+\xi(k)\right)\delta(\tau-\tau_1)\,\delta_{kk_1}\delta_{\sigma\sigma_1}\,\mathcal{G}_{k_1\sigma_1,\,k'\sigma'}(\tau_1-\tau')$$
$$= \delta(\tau-\tau')\,\delta_{kk'}\delta_{\sigma\sigma'}$$

$$\Rightarrow \sum_{k_1\sigma_1}\int_0^{\beta} d\tau_1\; \mathcal{G}^{-1}_{k\sigma,k_1\sigma_1}(\tau-\tau_1)\,\mathcal{G}_{k_1\sigma_1,k'}(\tau_1-\tau') = \delta(\tau-\tau')\,\delta_{kk'}\delta_{\sigma\sigma'}$$

$$\mathcal{G}^{-1}_{k\sigma, k'\sigma'}(\tau-\tau')$$

$$= -\left(\frac{\partial}{\partial\tau} + \xi(k)\right)\delta(\tau-\tau')\,\delta_{k\sigma,k'\sigma'}$$

(This is <u>ONLY for free particles</u>).

What happens ~~we~~ if we have interactions?
Then one can show that ~~ff~~

$$\mathcal{G}^{-1}_{k\sigma, k'\sigma'}(\tau-\tau') = -\left(\frac{\partial}{\partial\tau} + \xi(\vec{k})\right)\delta(\tau-\tau')\,\delta_{\vec{k}\sigma,\vec{k}'\sigma'} - \Sigma_{k\sigma;k'\sigma'}(\tau-\tau')$$

with interactions

where Σ is called the <u>self Energy</u> or mass operator. If the state ~~M~~ retains traslational and spin rotation invariance then Σ will have the form $\Sigma_{k}(\tau-\tau')\,\delta_{\vec{k}\vec{k}'}\,\delta_{\sigma\sigma'}$.

Rather than derive this result, let us understand the meaning of Self Energy. Recall that $G^{t}_{k\sigma,k'\sigma'}(t-t')$ is the amplitude of propagation for an ~~do~~ added particle. Assuming that no symmetries are broken, we can write the real time ~~ф~~ evolution equation for the retarded Green's function

$$\left(i\frac{\partial}{\partial t} - \xi_k\right)G - \int_{-\infty}^{\infty} dt'\, \Sigma'(k\sigma, t-t')\, G_{k\sigma}(t-t') = \delta(t-t')$$

Thus $\Sigma(k\sigma, t-t')$ is the effective, retarded time dependent potential seen by the particle. This arises due to the interaction with other particles. ~~Nothing this exp~~

Going back to the imaginary time domain.

$$\mathcal{G}^{-1}_{k\sigma}(\tau-\tau') = -\left(\left(\frac{\partial}{\partial\tau} + \xi(k)\right)\delta(\tau-\tau') + \Sigma'_{k\sigma}(\tau-\tau')\right)$$

$\delta_{kk'}\delta_{\sigma\sigma'}$

~~Writing~~ writing $\int \mathcal{G}^{-1}(\tau-\tau_1)\,\mathcal{G}(\tau-\tau') = 1$.

we get $\left(ik_l - \xi(\vec{k}) - \Sigma_{k\sigma}(ik_l)\right)\mathcal{G}_{k\sigma}(ik_l) = 1$.

$$\mathcal{G}_{k\sigma}(ik_l) = \frac{1}{ik_l - \xi(\vec{k}) - \Sigma_{k\sigma}(ik_l)}$$

Thus

$$G_{k\sigma}(\omega^+) = \frac{1}{\omega^+ - \xi(k) - \Sigma_{k\sigma}(\omega^+)}$$

$$\Rightarrow \quad A_{k\sigma}(\omega) = -\frac{1}{\pi} \frac{\Sigma''^{i}_{k\sigma}(\omega)}{(\omega - \xi(k) - \Sigma^{r}_{k\sigma}(\omega))^2 + (\Sigma^{i}_{k}(\omega))^2}$$

Note that $\Sigma^{i}_{k\sigma}(\omega)$ has to be ~~neg~~ non positive for all ω!

The key question now is how to calculate $\Sigma_{k\sigma}(ik_l)$?

<u>Path Integral Representation of the partition function</u>:

It turns out that the calculation of Σ can be ~~written~~ formulated in terms of ~~partition function~~ path interal formulation. The idea is this: The partition function

$$\mathrm{tr}\, e^{-\beta\mathcal{H}} = \sum_n \langle n | e^{-\beta\mathcal{H}} | n \rangle$$

Now $\langle n | e^{-\beta\mathcal{H}} | n \rangle$ is the amplitutde of propagation in imagiary time starting from the state $|n\rangle$ and ending up at the state $|n\rangle$ again. Except that the propagation is in imaginary time nothing is particularly different here. Thus one must be able to write $\langle n| e^{-\beta H} |n\rangle$ as a path integral. i.e $\int \mathcal{D}(\text{classical paths}) \, e^{iS_{class}}$

But here is key question? Suppose we have many particles. We know that there is indistinguishability and associated statistics. How do we ensure that we deal with bosons and fermions correctly in ~~statistics~~ the classical mechanics. ~~Pass it to~~ Clearly we must build up a classical mechanics of fermions. To motivate the idea, consider a ~~classical~~ harmonic oscillator

$$\mathcal{H} = \frac{p^2}{2} + \frac{\omega^2 x^2}{2}.$$

Up to a constant

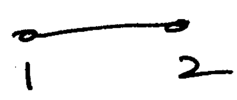
$$\mathcal{H} = \omega \underbrace{a^+ a}$$

$\hookrightarrow$ bosonic creation annihilation operators what are the states of the oscillator that are "most classical". These are the so called coherent states

$$a|\phi\rangle = \phi|\phi\rangle.$$

are the right eigenstates of the annihilation operator. ~~here~~ ~~so~~ ϕ can be any complex number. The key this is that $\Delta p \Delta x = \hbar$ in any coherent state and is therefore the minimum uncertainty state.

Let us try to do the same thing with fermions. The simplest ~~way~~ ~~to the~~ situation to describe this would be ~~the~~ two sites 1 and t (S



with a hopping between them

say $H = -t\,(c_1^\dagger c_2 + c_2^\dagger c_1)$

Now let us ask: does c_1 and c_2 have coherent states? Let us say there $\boxed{\text{to show immediately with } c^2}$ are. call them

$$c_1|\phi_1,\phi_2\rangle = \phi_1|\phi_1,\phi_2\rangle$$

$$c_2|\phi_1,\phi_2\rangle = \phi_2|\phi_1,\phi_2\rangle$$

Now $$c_2 c_1 |\phi_1, \phi_2\rangle = \phi_1 \, c_2 |\phi_1, \phi_2\rangle$$
$$= \phi_1 \, \phi_2 |\phi_1, \phi_2\rangle .$$

$$c_1 c_2 |\phi_1, \phi_2\rangle = \phi_2 \, c_1 |\phi_1, \phi_2\rangle$$
$$= \phi_2 \, \phi_1 |\phi_1 \, \phi_2\rangle$$

$$(c_2 c_1 + c_1 c_2) |\phi_1, \phi_2\rangle = (\phi_1 \phi_2 + \phi_2 \phi_1) |\phi_1, \phi_2\rangle$$
$$= 0 \qquad\qquad = (\phi_1 \phi_2 + \phi_2 \phi_1) |\phi_1, \phi_2\rangle$$

We need $$\phi_1 \phi_2 + \phi_2 \phi_1 = 0 \,!!$$

clearly ϕ_1 and ϕ_2 cannot be c-numbers.

Thus to make "classical" states of fermions we have to expand our "number system" to include anti commuting numbers. Fortunately for us some mathematicians were at this infact awhile ago! Infact this is also not so puzzling since $i = \sqrt{-1}$. Now I have two Grassman numbers called generators. They satisfy the algebra

$$\phi_1 \phi_2 + \phi_2 \phi_1 = 0$$
$$\phi_1^2 = 0 \quad \text{and} \quad \phi_2^2 = 0$$

Now associated with this we have two other generators ϕ_1^* and ϕ_2^*, these are Grassmann conjugates the algebra has $\{\phi_1, \phi_2, \phi_1^*, \phi_2^*\}$

it follows that $\phi_i^*\phi_j + \phi_j\phi_i^* = 0$

$\phi_i^*\phi_j^* + \phi_j^*\phi_i^* = 0$. Now define $a\phi_i$: (alike $3i$) complex multiplication and etc. One can define composite numbers $a\phi_1 + b\phi_2\phi_1 + c\phi_2^*\phi_1^*\phi_2\phi$ . .

etc. $(a\phi_1)^* = a^*\phi_1^*$

~~Let us then construct a coherent state for one state~~

~~$c_1|\phi_1\rangle = \phi_1|\phi_1\rangle$~~ ~~we need to here~~

~~$|\phi_1\rangle = |0\rangle - \phi_1|1\rangle$.~~

~~$c_1\phi_1 = -\phi_2\phi_1$~~

Consider a simple Grassmann variable complex numbers

$$f(\phi) = a_0 + a_1\phi$$

$$f(\phi^*,\phi) = a_0 + a_1\phi + a_2\phi^* + a_3\phi^*\phi$$

Calculus of Grassmann numbers.

$$\frac{\partial f(\phi)}{\partial \phi} = a_1 \quad \text{in a natural way.}$$

How do we do the integration

$$\int d\phi \; f(\phi) = \int d\phi \; (a_0 + a_1 \phi)$$

A consistent way to define this:

$$\int d\phi \; 1 = 0 \quad \text{and} \quad \int d\phi \; \phi = 1.$$

Thus $\int d\phi \; f(\phi) = a_1$.

We see that Grassmann integration is same as differentiation!

~~Armed with this mathematics we are ready to define a fermionic coherent states. Consider a single fermionic state such as a single orbital one (case (say the Hamiltonian is $H = \varepsilon_0 c^\dagger c$)~~

$$\int d\phi^* d\phi \; e^{-\phi^*\phi} = \int d\phi^* d\phi \, (1 - \phi^*\phi)$$

$$= 1.$$

We need one more ~~piece~~ property to do everything consistently. Grassmann numbers anticommute with fermionic operators

$$\phi c + c\phi = 0.$$

We are now ready to define a fermionic coherent state (think of a single state system $\varepsilon_0 c^\dagger c$ Hilbert space is spanned by $|0\rangle, |1\rangle$)

$$c|\phi\rangle = \phi|\phi\rangle$$

Claim $\quad |\phi\rangle = |0\rangle - \phi|1\rangle$

$$\begin{aligned} c|\phi\rangle &= c|0\rangle - c\phi|1\rangle \\ &= 0 + \phi\, c|1\rangle = \phi|0\rangle \\ &= \phi(|0\rangle - \phi|1\rangle) \\ &= \phi|\phi\rangle \;! \end{aligned}$$

$$\begin{aligned} |\phi\rangle = e^{-\phi c^\dagger}|0\rangle &= (1 - \phi c^\dagger)|0\rangle \\ &= |0\rangle - \phi|1\rangle. \end{aligned}$$

Now $\quad \langle\phi| = \langle 0| e^{-c\phi^*} = \langle 0| - \langle 1|\phi^*$

or $\quad \langle\phi|c^\dagger = \langle\phi|\phi^*$

~~Now~~

Now what is

$$\langle \psi | \phi \rangle = \left(\langle 0| - \langle 1| \cancel{\phi}\psi^* \right)\left(|0\rangle - \phi |1\rangle \right)$$

$$= \left(1 + \cancel{\phi}\,\psi^* \phi \right)$$

$$= e^{\psi^* \phi} \quad !$$

With this we are ready to ~~define~~ obtain the all important relationship

$$\int d\phi^* d\phi \; e^{-\phi^* \phi} \; |\phi\rangle\langle\phi| = \mathbb{1}$$

$$= |0\rangle\langle 0| + |1\rangle\langle 1| .$$

Similarly, the ~~te~~ ~~exp~~ trace of an operator

$$\mathrm{tr}\,(A) = \langle 0|A|0\rangle + \langle 1|A|1\rangle$$

$$= \int d\phi^* d\phi \; e^{-\phi^* \phi} \langle -\phi | A | \phi \rangle$$

$\uparrow$

NOTE!

We can immediately make sure that all this makes sense. The partition function of ~~the~~ our single site is

$$\mathrm{tr}\; e^{-\beta \varepsilon_0 c^\dagger c} = 1 + e^{-\beta \varepsilon_0} .$$

Now we obtain this result using the "classical" states

$$Z = \int d\phi^* d\phi \; e^{-\phi^*\phi} \langle -\phi | \underbrace{e^{-\beta \varepsilon_0 c^\dagger c}}_{1 + (e^{-\beta\varepsilon_0} - 1) c^\dagger c} | \phi \rangle .$$

$$= \int d\phi^* d\phi \; e^{-\phi^*\phi} \langle -\phi | \phi \rangle \left(1 - (e^{-\beta\varepsilon_0} - 1)\phi^*\phi\right)$$

$$= \int d\phi^* d\phi \; e^{-\phi^*\phi} \, e^{-\phi^*\phi} \, e^{-(e^{-\beta\varepsilon_0} - 1)\phi^*\phi}$$

$$= \int d\phi^* d\phi \; e^{-(e^{-\beta\varepsilon_0} + 1)\phi^*\phi}$$

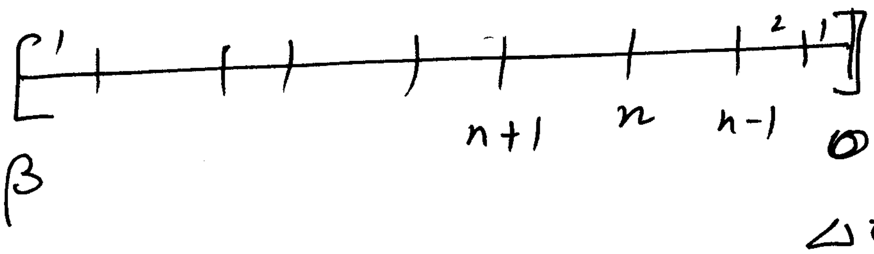
$$= 1 + e^{-\beta\varepsilon_0} \quad !$$

We are now very encouraged by all of this and are ready to derive the path integral formula of the partition function.

$$Z = \int d\phi^* d\phi \; e^{-\phi^*\phi} \langle -\phi | e^{-\beta\varepsilon_0 c^\dagger c} | \phi \rangle$$

Now visualize the interval from

$[0, \beta)$ as



$\Delta\tau = \frac{\beta}{N}$

$$e^{-\beta\mathcal{H}} = \prod_{n=1} e^{-\Delta\tau\mathcal{H}}$$

$\phi_0 = \phi$ and $\phi_N = \xi\phi$

$$\langle -\phi | e^{-\beta\mathcal{H}} | \phi \rangle$$

$$\prod_{n=0}^{N-1} d\phi_n^* d\phi_n \, e^{-\phi_n^*\phi_n} \langle \phi_N | e^{\Delta\tau\varepsilon_0 c^\dagger c} | \phi_{N-1} \rangle \langle \phi_{N-1} |$$

$$\cancel{\prod_{n=0}^{N-1}} \int \prod_{n=1}^{N} e^{-\phi_n^*\phi_n} \langle \phi_{n+1} | e^{-\Delta\tau\varepsilon_0 c^\dagger c} | \phi_{n-1} \rangle .$$

$(1 - \Delta\tau\,\varepsilon_0 c^\dagger c)$

$(1 - \Delta\tau\,\varepsilon_0 \phi_{n+1}^* \phi_n)$

$\langle \phi_{n+1} | \phi_n \rangle e^{-\Delta\tau\varepsilon_0 \phi_{n+1}^* \phi_n}.$

$$\int \prod_{n=} d\phi_n^* \prod e^{-\phi_n^*\phi_n} \, e^{+\phi_n^*\phi_{n-1}} \, e^{-\Delta\tau\varepsilon_0 \phi_n^* \phi_{n-1}}$$

$$\int \prod_n d\phi_n^* d\phi_n \; e^{-\sum_n \Delta\tau\left(\phi_n^* \frac{(\phi_n - \phi_{n-1})}{\Delta\tau} + \varepsilon_0 \phi_n^* \phi_n\right)}$$

Now take limit $N \to \infty$. We will get S

$$Z = \int_{\phi(\beta) = -\phi(\beta)} \mathcal{D}[\phi^*, \phi] \, e^{-\overbrace{\int_0^\beta d\tau \, \underbrace{\phi^*(\tau) \frac{\partial \phi(\tau)}{\partial \tau} + \epsilon_0 \phi^*(\tau)\phi(\tau)}_{\mathcal{L}(\phi^*, \phi)}}^{S}}$$

$\phi(\beta) = -\phi(\beta)$

anti periodic

Classical lagrangian of fermions

~~We have~~

We have thus extracted the classical lagrangian. One can go on to show that this is fully consistent with classical mechanics etc. (See my notes on the web).

We are now ready to see Antoine's formulation of the Hubbard model.

One defines a coherent state

$|\{\phi_{i\sigma}\}\rangle$

on the lattice. There is a completeness relation

$$\mathbb{1} = \int \prod_i d\phi^*_{i\sigma} d\phi_{i\sigma} \, e^{-\sum_{i\sigma} \phi^*_{i\sigma} \phi_{i\sigma}} |\{\phi_{i\sigma}\}\rangle\langle\{\phi_{i\sigma}\}|.$$

$$Z = \int \mathcal{D}[\phi^*, \phi] \, e^{-\int_0^\beta d\tau \int_0^\beta d\tau' \, \phi^*(\tau) \left[-\mathcal{G}^{-1}(\tau-\tau')\right] \phi(\tau')}$$

$$S = \boxed{\cancel{\phi^*}} \int_0^\beta d\tau \int_0^\beta d\tau' \, \phi^*(\tau) \left[-\mathcal{G}^{-1}(\tau-\tau')\right] \phi(\tau')$$

We are now ready to formulate the partition function of the Hubbard model ~~[illegible]~~ as a path integral.

Define Grassmann generators $\phi_{i\sigma}$ at each site along with their conjugates $\phi^*_{i\sigma}$.

We have the completeness relation

$$\int \prod d\phi^*_{i\sigma} \, d\phi_{i\sigma} \, e^{-\sum_{i\sigma}' \phi^*_{i\sigma}\phi_{i\sigma}} \, |\{\phi_{i\sigma}\}\rangle\langle\{\phi_{i\sigma}\}|$$

where $|\{\phi_{i\sigma}\}\rangle$ are the "classical" states of the system. The partition function is

$$Z = \int \prod d\phi^*_{i\sigma} \, d\phi_{i\sigma} \, e^{-\sum_{i\sigma}' \phi^*_{i\sigma}\phi_{i\sigma}} \langle -\{\phi_{i\sigma}\}| e^{-\beta H} |\{\phi_{i\sigma}\}\rangle.$$

Again going through the same process we get

$$[\,\underset{\beta}{|}\,\cdots\,\underset{n+1}{|}\,\underset{n}{|}\,\underset{n-1}{|}\,\cdots\,\underset{0}{]}$$

$$Z = \int \prod_{n=1}^{N} \prod_{i} d^*\phi^n_{i\sigma}\, d^*\phi^n_{i\sigma}$$

$$e^{-\sum' \phi^{*(n)}_{i\sigma}\phi^{(n)}_{i\sigma}} \langle \{\phi^{(n)}_{i\sigma}\} | \underbrace{e^{-\Delta\tau \mathcal{H}}} | \{\phi^{(n+1)}_{i\sigma}\} \rangle$$

$$\approx :e^{-\Delta\tau\mathcal{H}}:$$

$$= \int \prod_{n=1}^{N} \prod_{i} d\phi^{*(n)}_{i\sigma}\, d\phi^{n}_{i\sigma}\; e^{-\sum' \phi^{*(n)}_{i\sigma}\phi^{(n)}_{i\sigma} + \sum' \phi^{*(n)}_{i\sigma}\phi^{(n-1)}_{i\sigma}}$$

$$\times\, e^{-\Delta\tau\, \mathcal{H}(\{\phi^{*(n)}, \phi^{n}\})}$$

$$= \int \mathcal{D}[\phi^*_{i\sigma}, \phi]\; e^{-S}$$

$$\{\phi_{i\sigma}(\beta)\} = -\{\phi_{i\sigma}(0)\}$$

$$S = \int_0^\beta d\tau \Big(\sum'_{i\sigma} \phi^*_{i\sigma} \frac{\partial}{\partial\tau}\phi_{i\sigma} + \big(-t\sum'_{\langle ij\rangle}(\phi^*_{i\sigma}\phi_{j\sigma} + h.c.)$$

$$- U\sum'_{i} \phi^*_{i\uparrow}\phi^*_{i\downarrow}\phi_{i\downarrow}\phi_{i\uparrow} - \mu\sum'_{i}\phi^*_{i\sigma}\phi_{i\sigma}\big)$$

There are a couple of more things to remember. ~~Q~~ The path integral formulation allows for the calculation of correlation or response function.

$$-\langle T_\tau A(\tau) B(\tau') \rangle$$

$$= \frac{\int \mathcal{D}[\psi^* \psi]\, e^{-S[\psi^*, \psi]} A(\tau) B(\tau')}{\int \mathcal{D}[\psi^*, \psi]\, e^{-S[\psi^*, \psi]}}$$

The remarkable thing about this is that we do not need to worry about the imaginary time ordering. It is automatic! - path integrals always produce time orderd answers.

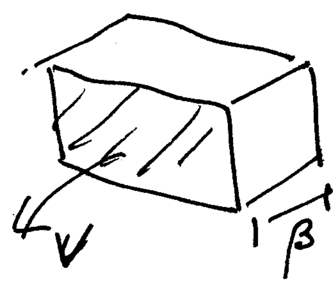
Finally, we see that QM statmech problem in d dimensions can be treated as a classical statmech problem in $d+1$

To see this explicitly, consider the action for the short range interacting fermions that we see in cold atoms.

The action

$$S = \int_0^\beta d\tau \int_V d^d r \Big[c^*_\sigma(\vec{r},\tau) \frac{\partial}{\partial \tau} c_\sigma(\vec{r},\tau) + c^*_\sigma(\vec{r},\tau)\left(-\frac{\nabla^2}{2}\right) c_\sigma(\vec{r},\tau) + U\, c^\dagger_\uparrow(\vec{r},\tau)\, c^\dagger_\downarrow(\vec{r},\tau)\, c_\downarrow(\vec{r},\tau)\, c_\uparrow(\vec{r},\tau)$$

This. ~~tt~~ is the action of a field in $d+1$ dimensional space of volume βV!



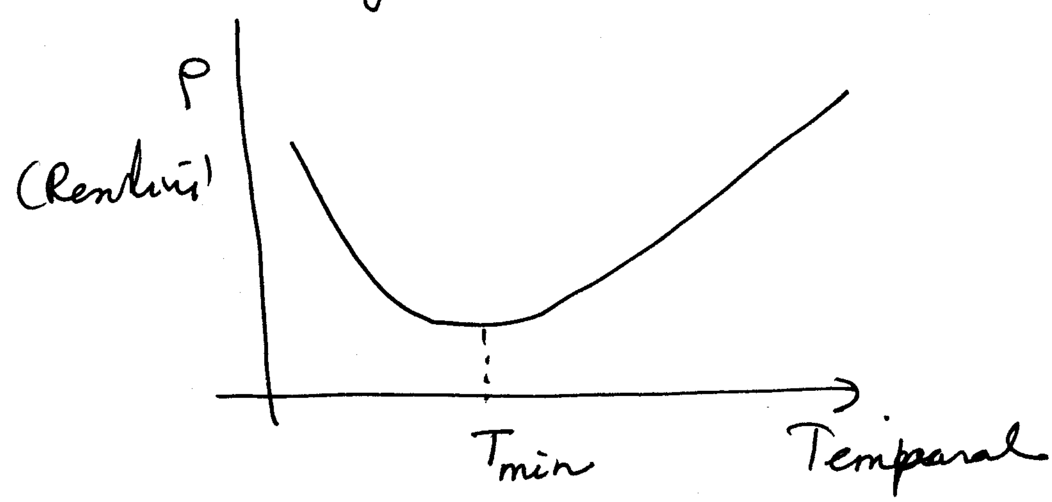
$$Z = \int \mathcal{D}[c^+ c]\, e^{-S} \; !$$

Indeed this ~~....~~ ~~tt~~ point is not just a curiosity, but can actually be gainfully used to simulate quantum systems.

Much of what we have discussed so far is formulation. Lets now do some real physics.

The Anderson Impurity Problem

Back in the 50s and 60s folks were intrigued by the following phenomenon. When Fe was "dissolved" in ~~cu~~ Cu (small % Fe in Cu crystal), the resistivity of the system showed a rather strange behaviour



$T_m \sim c^{1/5}$ where c ~~[illegible]~~ is the concentration of Fe. $T_{min} \sim 10$-$20\,K$.

Interesting at $T \gg T_{min}$, such systems also show a Curie like susceptibility ~~do~~ showing that the magnetic impurities form "permanent" moments. However, no "divergent" susceptibility is found at low temperatures. Suggesting that the moment "disappear" at low temperatures, ~~roughly~~ below where there is the resistivity minimum!-

Yet other systems (~~such~~ as Fe in Al, check this) do not show local moment formation - i.e, a magnetic ion does not remain a magnetic ion in these systems.

$\boxed{\cancel{\text{Kkkey}}}$ Let us think of Fe in Cu.

The host metal has an s-band (conduction band) and the Fe ~~ba~~ atom has localized d-orbitals. We can write out the individual Hamiltonian, as

$$\sum_{k}' \xi(\vec{k})\, c^{\dagger}_{k\sigma} c_{k\sigma}$$

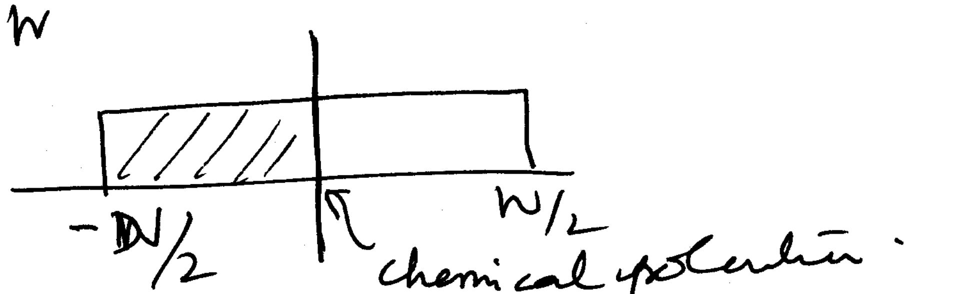
and $\xi_d\, d^{\dagger}_{\sigma} d_{\sigma}$. (Sum over repeated indices is implied).

When we place this in the ion, it hybridizes with the conduction band. We ~~will as~~ and this we take to be of the form

$$\frac{\gamma}{\sqrt{N}} \sum_{k}' \left(c^{\dagger}_{k\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{k\sigma}\right)$$

where N is the number of sites in the lattice. The hamiltonian has ~~No translation invariance~~, but has spin rotation invariance as a symmetry.

~~There~~ We will assume that the band is flat in that $\rho(\omega) = \rho_0 = \frac{1}{W}$ (W is the band width)



Thus we have three scales in the problem, ① bandwidth W, ② ξ_d - Energy of the impurity ③ γ - the hybridization.

When will the impurity be magnetic, say, when does it pick up a permanent moment? If this happens the $m = \langle d^\dagger_\uparrow d_\downarrow \rangle - \langle d^\dagger_\downarrow d_\uparrow \rangle \neq 0$ and we will pick up a moment!

Let us see, if this happens. And in doing

We now Fourier expand

$$c^*_{k\sigma}(\tau) = \frac{1}{\sqrt{\beta}} \sum_{ik_e}{}' e^{-ik_e\tau}\, c_{\vec{k}\sigma}(ik_e)$$

After a bit of algebra, we get

$S[c_{k\sigma}(ik_e), d_{k\sigma}(ik_e)]$

$$= \sum_{ik_e}{}' \Big[\Big(\sum_{k\sigma}{}' c^*_{k\sigma}(ik_e)(-ik_e + \xi(\vec{k}))\, c_{k\sigma}(ik_e) \Big) + (-ik_e + \xi_d)\, d^*_\sigma(ik_e)\, d_\sigma(ik_e) \Big) + \frac{\gamma}{\sqrt{N}} \sum_k{}' \big(c^*_{k\sigma}(ik_e)\, d_\sigma(ik_e) + d^*_\sigma(ik_e)\, c_{k\sigma}(ik_e) \big) \Big]$$

$$Z = \int \prod_{\substack{k\sigma \\ ik_e}} d c^*_{k\sigma}(ik_e)\, d c_{k\sigma}(ik_e)\, d(d^*(ik_e))\, d(d(ik_e))\; e^{-S[c,d]}$$

~~One can easily see that the integral for each ik_e and $k\sigma$ can be done separately, let us perform~~ Let us now perform the integration over the $c^*_{k\sigma}(ik_e)$ and $c_{k\sigma}(ik_e)$ variables.

We will also ~~ex~~ flex our just acquired technical muscle..
We notice that we can calculate
m by the following ~~trick~~ trick.
Consider
$$\mathcal{G}_{d\sigma}(\tau) = -\langle T_\tau d_\sigma(\tau) d_0^\dagger(0)\rangle$$

clearly $$\sum_\sigma{}' \sigma \mathcal{G}_{d\sigma}(0^-) = m!$$
How do we obtain $\mathcal{G}_{d\sigma}(\tau)$? Well
We can equivalently obtain $\mathcal{G}_{d\sigma}(ik_e)$
an then
$$m = \sum_\sigma{}' \frac{1}{\beta} \sum_z{}' e^{ik_e 0^+} \sigma \mathcal{G}_{d\sigma}(ik_e).$$
~~Let us obtain~~ To obtain this, let us
Write the action
$$S[c,d] = \int_0^\beta d\tau \Big(\sum_{\vec{k}\sigma}{}' c^*_{k\sigma}(\tau) \frac{\partial}{\partial\tau} c_{k\sigma} + \xi(\vec{k}) c^*_{k\sigma}(\tau) c_{k\sigma}$$
$$+ d^*_\sigma\Big(\frac{\partial}{\partial\tau} + \xi_d\Big) d_\sigma$$
$$+ \frac{\gamma}{\sqrt{N}} \sum_{k\sigma}{}' \big(c^*_{k\sigma}(\tau) d_{\sigma}(\tau) + d^*_\sigma(\tau) c_{k\sigma}(\tau)\big)\Big)$$
With $c_{k\sigma}(\beta) = -c_{k\sigma}(\tau)$ and same for d.

Now we can integrate out the c variables using the following trick. Consider

$$\int d\phi^* d\phi \, d\psi^* d\psi \; e^{-(A\psi^*\psi + B(\psi^*\phi + \phi^*\psi) + D(\phi^*\phi))}$$

$$= \int d\phi^* d\phi \, d\psi^* d\psi \Big(1 - (A\psi^*\psi + B(\psi^*\phi + \phi^*\psi) + D\phi^*\phi) + \frac{1}{2}(A\psi^*\psi + B(\psi^*\phi + \phi^*\psi) + D\phi^*\phi)^2 .$$

$$= \int d\phi^* d\phi \, d\psi^* d\psi \, (AD\psi^*\psi \, \phi^*\phi - B^2 \psi\psi^* \phi^*\phi)$$

$$= \cancel{-A\int d\phi^* d\phi \quad \phi^*}$$

$$- A\int d\phi^* d\phi \Big[\underbrace{\int d\psi^* d\psi \;\; \psi^*\psi}_{1}\Big] \Big(-(D - \frac{B^2}{A}) \phi^*\phi$$

$$- A\int d\phi^* d\phi \; \Big[1 - \phi^* ((D - \frac{B}{A^2})\phi \Big)$$

$$- A\int d\phi^* d\phi \; e^{-\phi^*(D - \frac{B}{A^2})\phi} .$$

By using this, we get

$S[d^*_\sigma, d_\sigma]$

$$= \sum_{\substack{ik_l \\ \sigma}}' d^*_\sigma(ik_l)\left[-ik_l + \xi_d - \left[\frac{\gamma^2}{N}\sum_k' \frac{1}{-ik_l+\xi_k}\right]\right] d_\sigma(ik_l)$$

or $S[d^*_\sigma(\tau), d_\sigma(\tau')]$

$$= \int_0^\beta d\tau \int_0^\beta d\tau' \, d^*_\sigma(\tau)\left[-\mathcal{G}^{-1}_{\sigma\sigma'}(\tau-\tau')\right] d_{\sigma'}(\tau)$$

where

$$\mathcal{G}^{-1}_{\sigma\sigma'}(\tau-\tau') = \frac{1}{\beta}\left(\sum' e^{i(\tau-\tau')}\mathcal{G}^{-1}(ik_l)\right)\delta_{\sigma\sigma'}$$

$$\mathcal{G}^{-1}(ik_l) = ik_l - \xi_d - \frac{\gamma^2}{N}\sum' \frac{1}{ik_l - \xi_k}$$

Thus

$$\mathcal{G}_{d\sigma}(ik_l) = \frac{1}{ik_l - \xi_d - \frac{\gamma^2}{N}\sum_k' \frac{1}{ik_l - \xi_k}}$$

$$\mathcal{G}_{d\sigma}(\omega^+) = \frac{1}{\omega^+ - \xi_d - \frac{\gamma^2}{N}\sum_k' \frac{1}{\omega^+ - \xi_k}}$$

Look at

$$\frac{1}{N}\sum_k{}' \frac{1}{\omega^+ - \xi_k} = \frac{1}{N}\, \mathcal{P}\sum_k{}' \frac{1}{\omega - \xi_k} \underbrace{- i\pi \frac{1}{N}\sum_k{}' \delta(\omega - \xi_k)}_{\rho_0}$$

Some infero

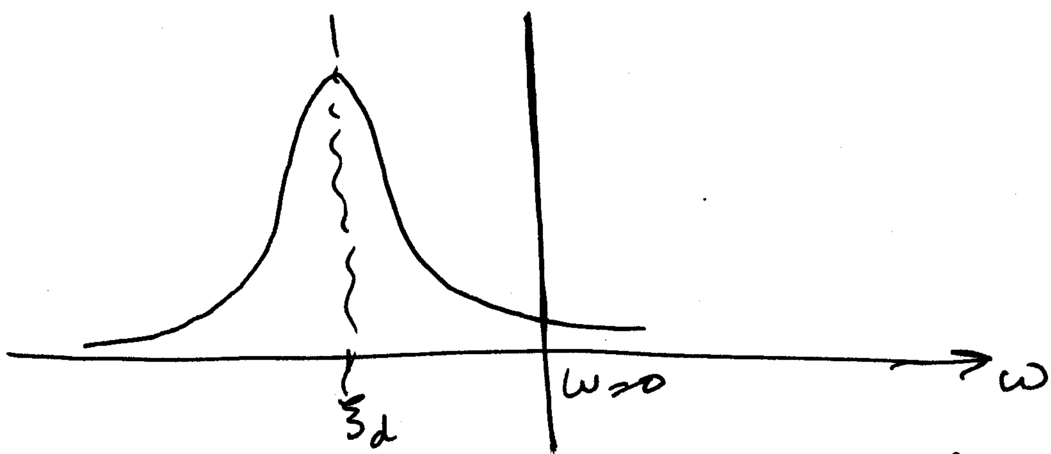
Absolb this in the defintn of ξ_d.

$$\Rightarrow \quad \mathcal{G}_{d\sigma}(\omega^+) = \frac{1}{\omega - (\xi_d - i\Delta)}$$

Wher $\Delta = \pi \gamma^2 \rho_0$ or $\dfrac{\pi\gamma^2}{W}$

$$\Rightarrow \quad A_{d\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, \mathcal{G}_{d\sigma}(\omega^+)$$

$$= \frac{1}{\pi}\frac{\Delta}{(\omega - \xi_d)^2 + \Delta^2}$$

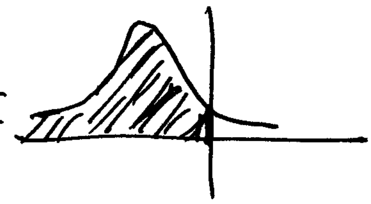


Make a comment about spectral function and quasi particles.

Note that

$$\frac{1}{\beta}\sum_{n} e^{ik_n 0^+}\, \mathcal{G}_{d\sigma}(ik_n) \longrightarrow \text{(Show this)}.$$

$$\langle d^\dagger_\sigma d_\sigma\rangle = \int_{-\infty}^{\infty} d\omega \; n_F(\omega)\, A_{d\sigma}(\omega)$$

$$\langle d^\dagger_\sigma d_\sigma\rangle \overset{T=0}{=} \frac{1}{2} - \tan^{-1}\left(\frac{\xi_d}{\Delta}\right) =$$ 

~~But~~ ~~now~~ We are now ready to obtain m

$$m = \langle d^\dagger_\uparrow d_\uparrow\rangle - \langle d^\dagger_\downarrow d_\downarrow\rangle = 0!$$

Infact this will be the case at any temperature! This is an unhappy simulation since we find that the added impurity never picks up a moment. ~~[illegible]~~ We are clearly missing something crucial!

This the ~~elec~~ repulsive interaction between the fermions at the d-orbital! We need to add a new term to our Hamiltonian and this is

$$U \equiv n_{d\uparrow} n_{d\downarrow}$$
$$= U\, d^\dagger_\uparrow d^\dagger_\downarrow d_\downarrow d_\uparrow$$

First thing we need to ask is why would an ~~onsite~~ "Hubbard U" at the ~~d~~ d site give a moment? Here is simple, but very crucial point.

Take the d state spin operator

~~the~~ $$\vec{S}_d = \frac{1}{2} \sum'_{\sigma\sigma'} d^+_\sigma \vec{\tau}_{\sigma\sigma'} d_{\sigma'} \qquad \vec{\tau} \text{ (Pauli matrices)}$$

$$\vec{S}_d \cdot \vec{S}_d = \frac{3}{4} (d^+_\uparrow d_\uparrow + d^+_\downarrow d_\downarrow) - \frac{3}{2} n_{d\uparrow} n_{d\downarrow}$$

or $$n_{d\uparrow} n_{d\downarrow} = \frac{1}{2}(n_\uparrow + n_\downarrow) - \frac{2}{3} \vec{S}_d \cdot \vec{S}_d .$$

Thus We ~~c~~ can

Thus We can define

$$U n_{d\uparrow} n_{d\downarrow} = \frac{U}{2}(n_\uparrow + n_\downarrow) - \frac{2U}{3} \vec{S}_d \cdot \vec{S}_d .$$

Now the linear term can be absorbed in the definition of ξ_d. Now if ξ_d is negative ~~it will be~~ and $\gamma = 0$ then we will like to have exactly one eleron on the d site maxing the correlation energy. So this makes the formation of a moment plausible.

If we had written the action of the impurity prior to changing over to the spin ~~would~~ $\vec{S}_d$, we would obtain

$$S[d^*_\sigma, d_\sigma] = -\int_0^\beta d\tau \int_0^\beta d\tau' \, d^*_\sigma(\tau)\left(-\mathcal{G}^{-1}_{\sigma\sigma'}(\tau-\tau')\right) d_\sigma(\tau)$$

$$+ \int_0^\beta d\tau \, d^*_\uparrow(\tau) d^*_\downarrow(\tau) d_\downarrow(\tau) d_\uparrow(\tau).$$

This is exactly like the action in the RMP of Georges et al. !

Now let me go back to the redefined $\vec{S}_d$ and we write the action as

~~and~~

$$S[d^\dagger_\sigma, d_\sigma] = -\int\int d^*(-\mathcal{G}^{-1})\, d$$

$$\frac{2U}{3}\int_0^\beta d\tau \, \vec{S}_d(\tau)\cdot\vec{S}(\tau)$$

Note that $\vec{S}_d(\tau)$ ~~is a classical field~~ is a "bosonic" field.

$$\left[\begin{array}{l} \int e^{\frac{b^* b}{a}} \\ = \int e \end{array}\right.$$

$$\cancel{e^{\frac{\vec{M}(\tau)}{a}}} \quad e^{\frac{2U}{3}\vec{S}_d(\tau)\cdot\vec{S}_d(\tau)}$$

$$= \int d\vec{M}^* dM \; e^{-\left(\frac{3}{2U}\vec{M}(\tau)\cdot\vec{M}(\tau) - \vec{M}(\tau)\vec{S}(\tau)\right)}$$

and thus

$$\cancel{Z} = \int \mathcal{D}[d^*, d, \vec{M}] \; e^{-S[d^*, d, \vec{M}]}$$

Now $\quad S[d^* d, M] = \int_0^\beta d\tau \, \frac{3\vec{M}^2(\tau)}{2U} + \int_0^\beta d\tau \int_0^\beta d\tau'$
$$d^*_\sigma \left[-\mathcal{G}^{-1}_{\sigma\sigma'} [\tau - \tau'; \vec{M}(\tau)] \right] d_\sigma(\tau')$$

Integrate out the fermions to get

$$Z = \int \mathcal{D}[\vec{M}(\tau)] \; e^{-S[\vec{M}]}$$

$$S(\vec{M}) = \int_0^\beta d\tau \, \frac{3|\vec{M}(\tau)|^2}{2U} - \ln \det[-\mathcal{G}^{-1}[\vec{M}]]$$

Now we look for extremal, saddle pt solutions of $\vec{M}(\tau)$, i.e. and look for solution of the type $\vec{M}(\tau)_{saddle} = m\vec{e}_z$ (static solution).

We simply substitute

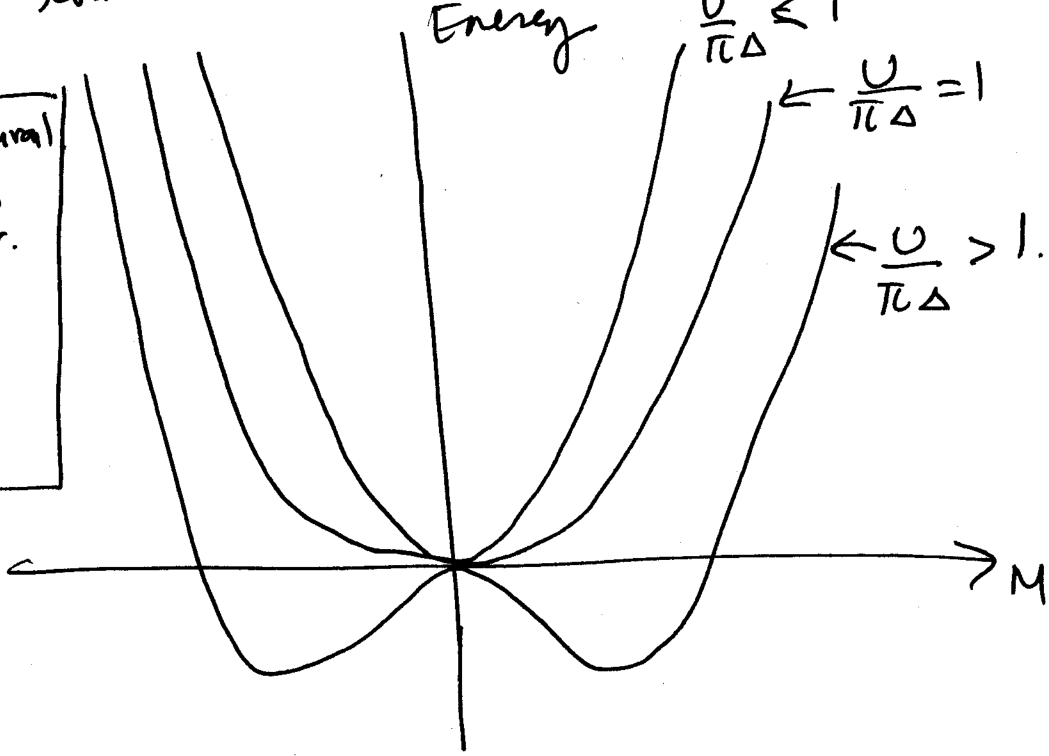
$M(\tau) = m e_z$.

For the symmetric Anderson model

$$\xi_d + U = -\xi_d \quad \text{or} \quad \xi_d = -\frac{U}{2}$$

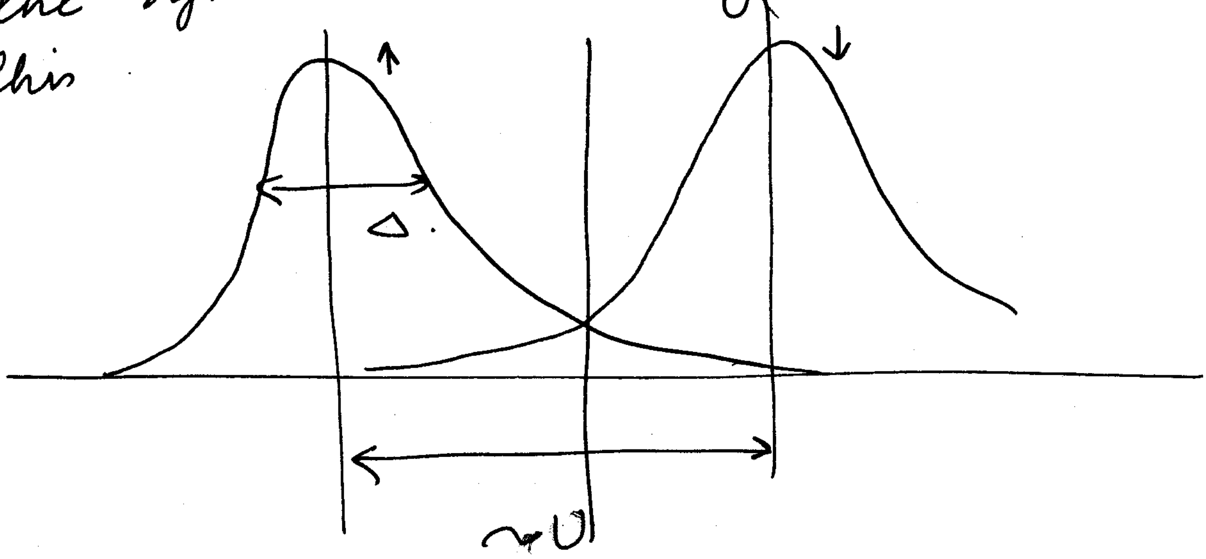
One can work this out exactly.
The energy state as a function of M
will look like

Anderson/Yuval
Wang, Evenson, Schreiffer.
Hamann
PRL 1969
(July)



$\mathcal{E}(M) = \lim_{T \to 0} -T \ln Z[M]$

We see that when $U > \pi\Delta$ then
the system picks up a moment. Physics is
say $m > 0$
this.



~~But~~ This is excellent. We see that for large ~~enough~~ enough U, the system picks up a moment.

How good is the HF solution? ~~Once clarified~~ Anderson himself had an interesting comment in ~~the~~ his paper.

There are two issues: One a real one, ~~and another an~~

(A) The ground state obtained by the saddle point analysis is not a ground state of the system.

Reason, the ↑ spin electron ~~to~~ can hop into the conduction band and come back as a down spin

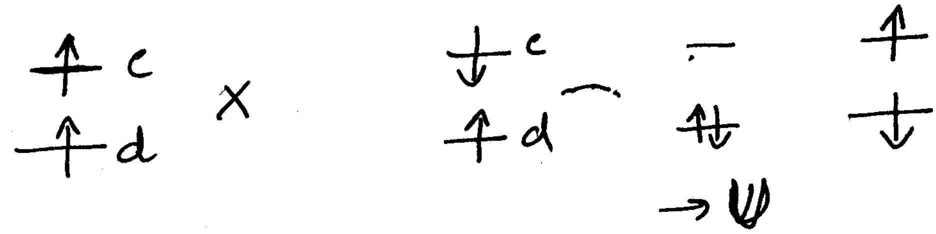
(B) This is a symmetry breaking in a "small" quantum system which is not so nice.

How do we describe the fluctuation of spin, but no charge? The idea is to "integrate out" charge fluctuation and obtain the effective ~~~~ sd Hamiltonian.

$$\mathcal{H}_{sd} = \sum_{k}' \xi(\vec{k})\, c^{\dagger}_{k\sigma} c_{k\sigma} + J\, \vec{S}(0)\cdot\vec{S}_d \qquad J \sim \frac{\gamma^2}{U}$$

$$\vec{S}(\vec{0}) = \frac{1}{N} \sum_{k,k'} c^{\dagger}_{k\sigma}\, \vec{\tau}_{\sigma\sigma'}\, c_{\sigma' k'}$$

Note that $J > 0$ antiferro magnetic.
Where does this come from?



$\sim \frac{\gamma^2}{U}$ Energy gain

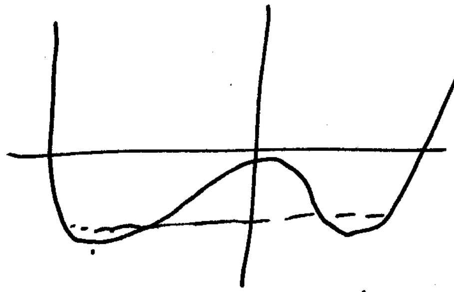
process occurs only if c spin is antiferro magnetically aligned with the d spin.

What is the Ground state of the s-d Hamiltonian?
It turns out that the system ~~is a singlet~~ forms a singlet which gains an energy. Now to form the screening singlet some states have to be localized around the impurity, and this ~~causes~~ costs kinetic energy. The key thing is that the gain in energy is exponentially small. In fact it is $e^{-\frac{W}{J}}$

$$T_K \sim \sqrt{U\Delta}\, e^{-\frac{\pi U}{\Delta}}$$ (Some factors may be wrong)

This is the Kondo scale.

This entire singlet formation can also be viewed as a tunning process across the classical potential



and the exponentially small scale can be understood in this way.

~~Bottom~~
This explains the Kondo effect.

One can summarize this by saying that for $\frac{U}{\pi\Delta} \gtrsim 1$, there are two key scal