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Applications to Real Materials, Extensions and Perspectives
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Metal-insulator transitions in the Hubbard model

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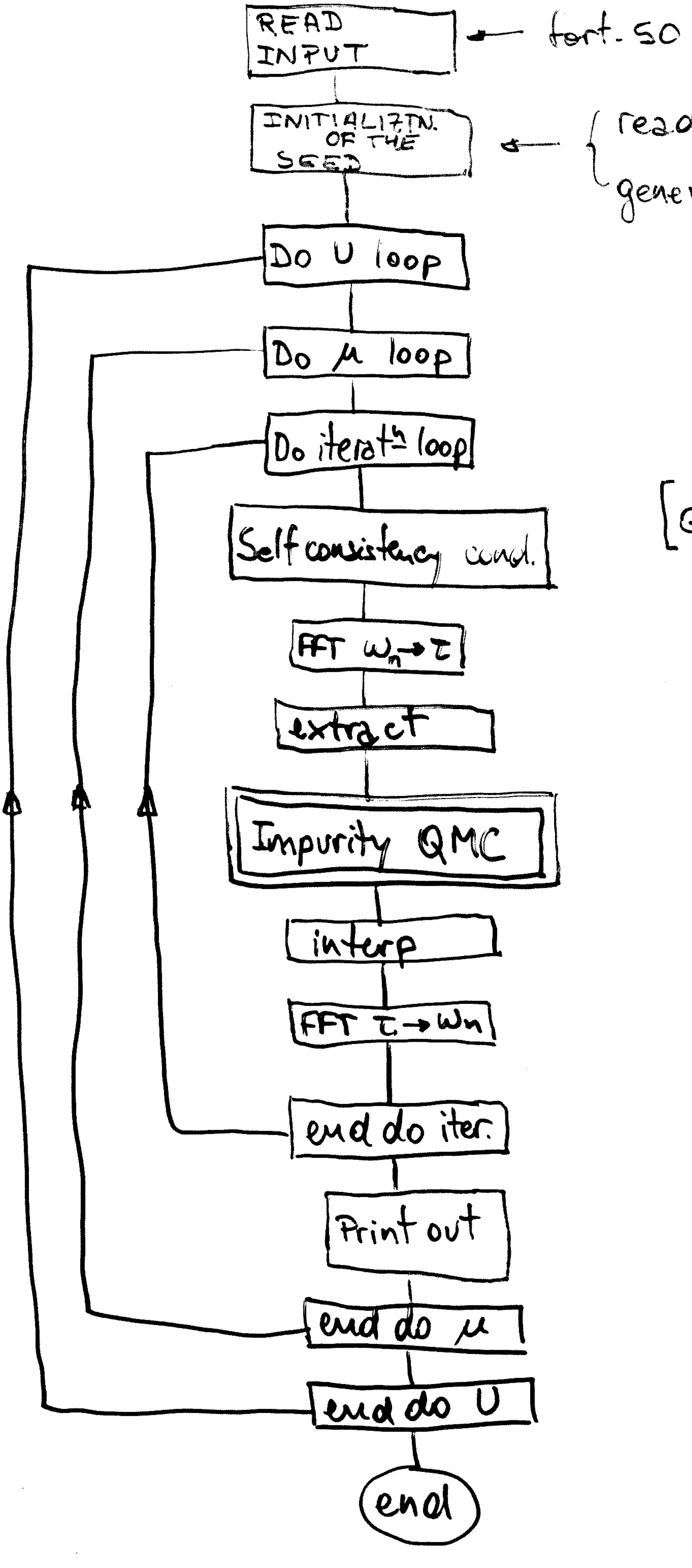
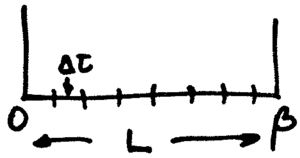
QMC code - Flow diagram



$$\left[G_0^{(n+1)}\right]^{-1} = \left[G^{(n)}\right]^{-1} + \Sigma^{(n)}$$

$$G(\omega) = \int d\epsilon \frac{\rho^0(\epsilon)}{\omega - \epsilon - \Sigma(\omega)}$$

QMC (Blankenbecler, Scalapino, Sugar '81) (Hirsch & Fye '87)



$$Z = e^{-c^{+}_{\sigma}(\tau)\, G_{0\,\tau\tau'}^{-1}\, c_{\sigma}(\tau') + U\, n_{\uparrow}(\tau)\, n_{\downarrow}(\tau)}$$

$$Z = \sum_{S=\pm 1} e^{-c^{+}_{\sigma}(\tau)\, G_{0\,\tau\tau'}^{-1}\, c_{\sigma}(\tau') + \lambda S(\tau)\,(n_{\uparrow}(\tau) - n_{\downarrow}(\tau))}$$

$$\lambda = \lambda(U)$$

$$Z = \sum_{\{s\}} \det[G_{\uparrow}^{-1}[s]]\, \det[G_{\downarrow}^{-1}[s]]$$

$$G^{-1}_{\sigma\,\tau\tau'}[s] = G^{-1}_{0\,\tau\tau'} + \sigma \lambda s\, \delta_{\tau\tau'}$$

$$G_{\sigma} = \frac{1}{Z}\sum_{\{s\}} G_{\sigma}[s]\, \det[G_{\uparrow}^{-1} G_{\downarrow}^{-1}]$$

$$s \to s'$$

$$\langle G_{\sigma}\rangle = \sum_{s} G_{\sigma}[s]\, P(s) \quad ; \quad R = e^{-\Delta S} = \frac{\det[G_{\uparrow}(s)\, G_{\downarrow}(s)]}{\det[G_{\uparrow}(s')\, G_{\downarrow}(s')]}$$

* exact up to the Trotter break-up error $\propto \Delta\tau^2$

rule of thumb $\rightarrow$ $\frac{\Delta\tau\, U}{2} < 1$

$$\beta = \Delta\tau\, L \approx \frac{1}{2}\, 128 = 64$$

$$\boxed{T_{QMC} \gtrsim 10^{-2}}$$

~ 1/2 hour
~~CRAY YMP~~ ('93)
pentium III ('99)

No tricks in the "impurity" routine (QMC

(Fye & Hirsch)

* autocorrelation ~ 2 so store every other sweep

* warm up (thermalization of the $s(\tau)$ pseudo spins) $\sim$ 500 sweeps

* "dirty" vs "clean" inversion

$$G^{-1}_{\tau\tau'} = G^{-1}_{0\,\tau\tau'} + \lambda S(\tau)\,\delta_{\tau\tau'}$$

need to store $G_{\tau\tau}$ (invert matrix)

"dirty" $\to$ Sherman - Morrison formula L^2 operations

"clean" $\to$ direct inversion (Gauss Jordan) L^3 operations

bottle neck !

$\sim$ 500 dirty sweeps every other clean

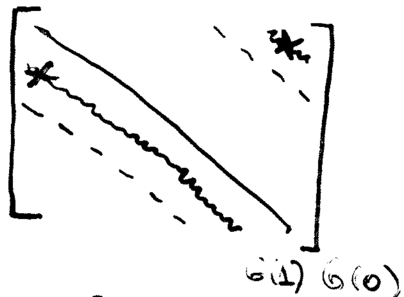
is OK in general.

* "wrap around"

$$G^{i}_{\tau\tau'} \qquad i = 1, \ldots, N_{store}$$

$$G(\tau) = \frac{1}{L \times N_{store}} \sum_{i}^{N_s} \sum_{\tau'}^{L} G^{i}_{\tau'+\tau,\, \tau'}$$

$$G(-\tau) = -G(\beta - \tau)$$



$$\tau' + \tau = \mathrm{mod}'_L(\tau' + \tau)$$

$$1, L = 1 - L \rightarrow -G(1 - \cancel{L} + \cancel{L}) = -G(1)$$

$$2, 1 = 2 - 1 \rightarrow G(1)$$

Very nice but... * $T \rightarrow 0$ is numerically expensive

* imaginary axis results.

$\Rightarrow$ need to analytically continue *noisy* data to the real axis. Is a mathematically ill-posed problem. Something can be done using Maximum-Entropy methods.

Tricks

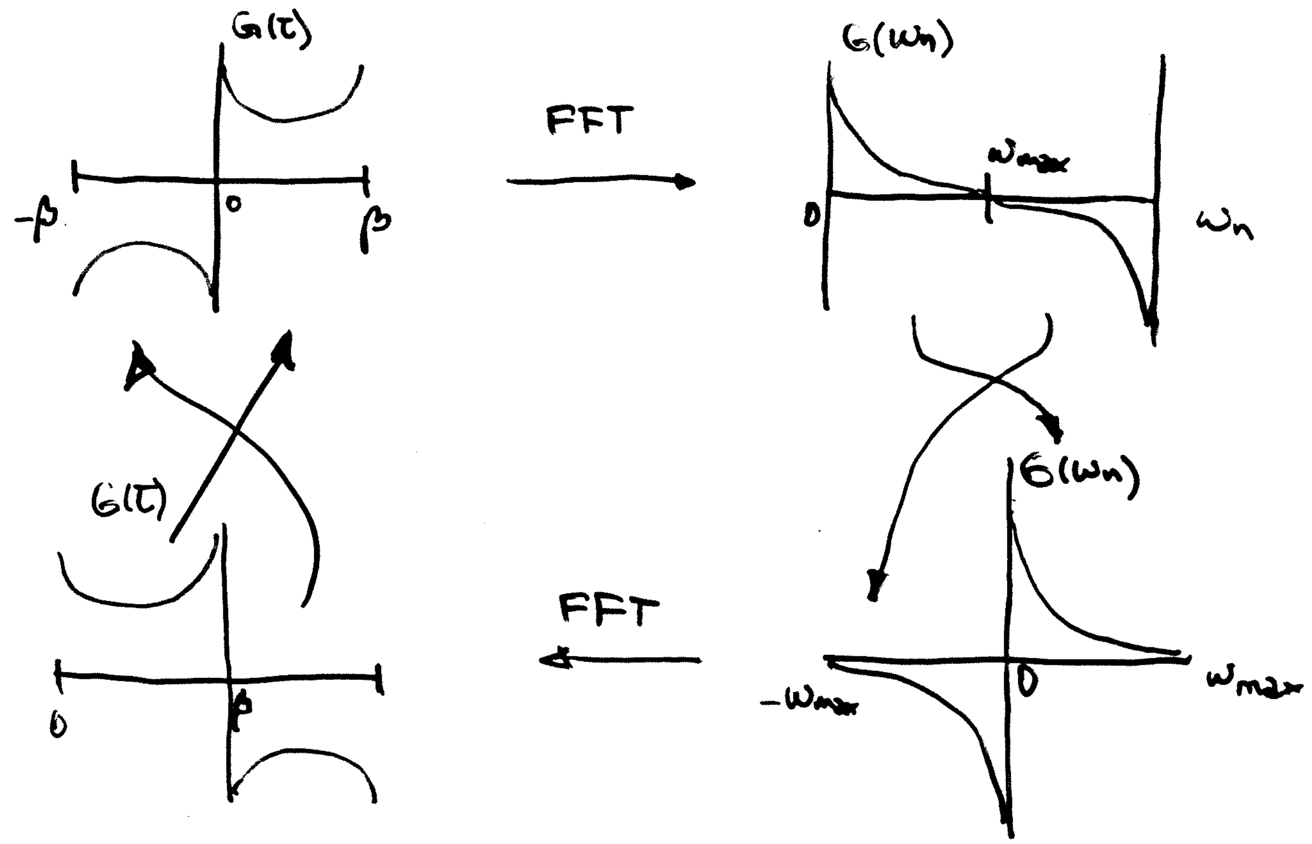
1) Self consistency condition

$$G(\omega_n) = \frac{1}{i\omega_n + sg(\omega_n)\, i\Delta}$$

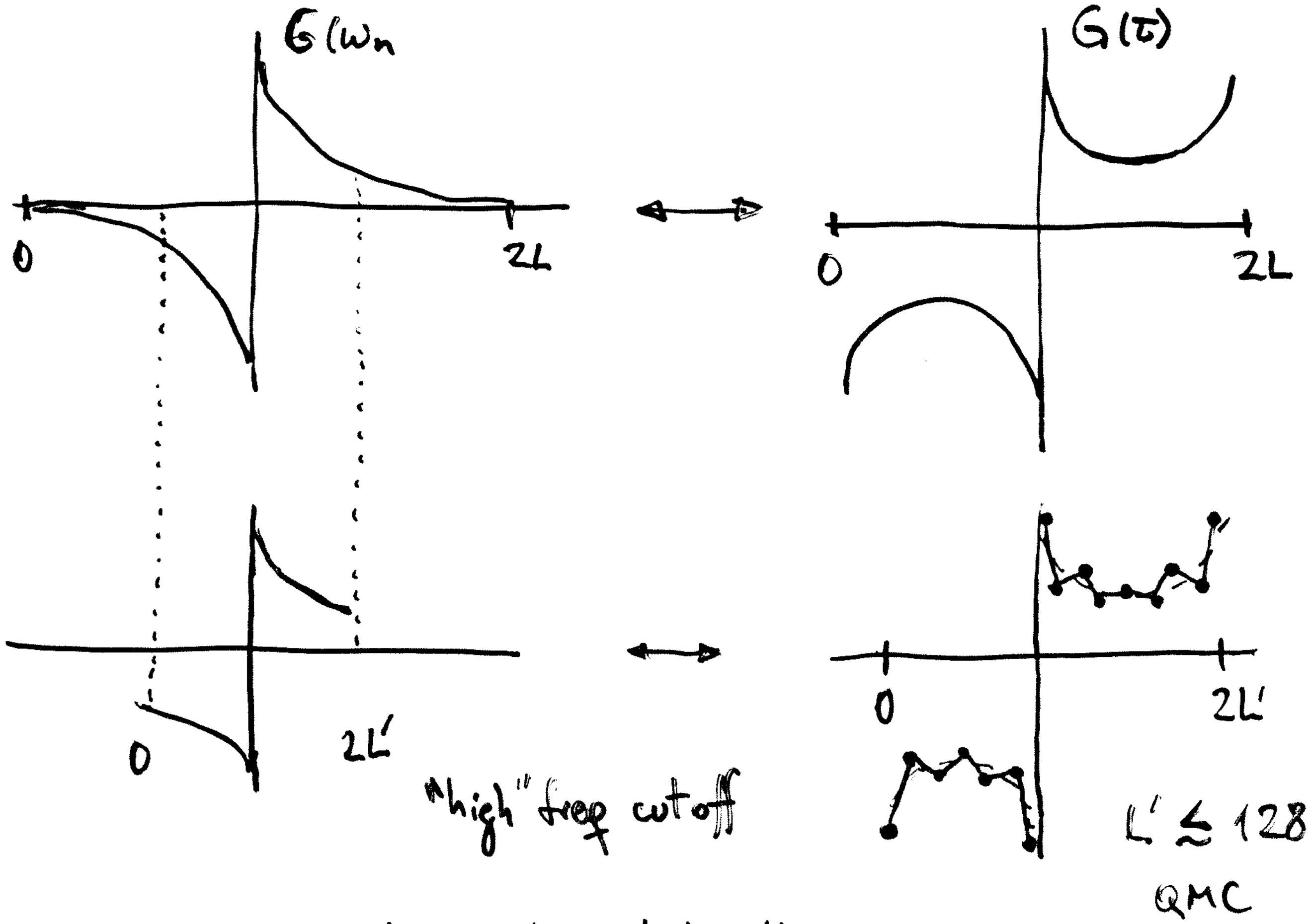
$$\Rightarrow G(\omega_n) = \frac{1}{i\omega_n - \mu - \Sigma(\omega_n) + sg\sqrt{(i\omega_n - \mu - \Sigma(\omega_n))^2 - D^2}}$$

$$sg = sg(\omega_n - \mathrm{Im}[\Sigma]) \cdot sg\left(\mathrm{Im}[\sqrt{(\;)}]\right)$$

2) FFT $\rightarrow$ cycling



3) FFT → extract - interp



The trick is to interpolate the QMC result $G(\tau)$

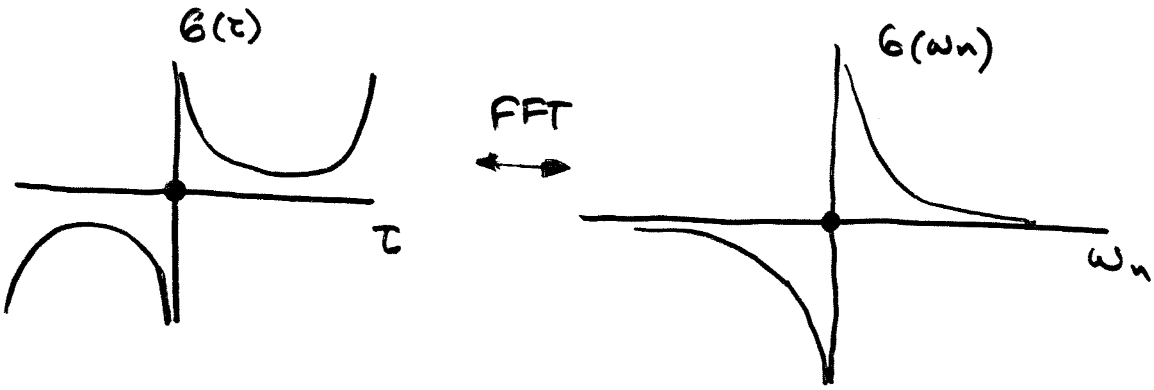
$$G(\tau) = \frac{1}{\beta}\sum_n e^{i\omega_n\tau}\, G(\omega_n) \qquad \text{is continuous } -\beta \le \tau \le \beta$$

$$G(\omega_n) = \int_0^\beta e^{-i\omega_n\tau}\, G(\tau) \qquad \text{is discrete.}$$

$$\begin{array}{ccccc}
\overset{QMC}{G}(\tau) & \xrightarrow{\text{INTERP}} & \overset{SMOOTH}{G}(\tau) & \xrightarrow{\text{FFT}} & \overset{SMOOTH}{G}(\omega_n) \\
L' \lesssim 128 \text{ points} & & L \sim 32K \text{ points} & & \\
\text{QMC} \uparrow & & & & \downarrow \ \omega_{max} \gg \omega_1 = \pi/\beta \\
G_0^{QMC}(\tau) & \xleftarrow{\text{EXTRACT}} & \overset{SMOOTH}{G_0}(\tau) & \xleftarrow{\text{FFT}} & G_0^{-1} = G^{-1} + \overset{SMOOTH}{\Sigma} \\
L' \lesssim 128 \text{ points} & & L \sim 32k \text{ points} & &
\end{array}$$

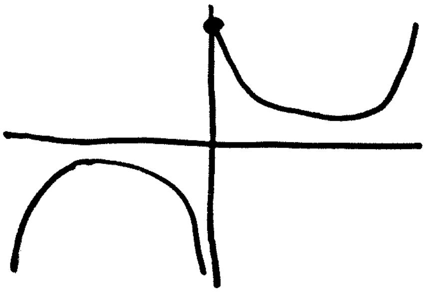
4) FFT $\longleftrightarrow$ QMC $G(0^+)$?

p-h symmetry for the sake of the argument.



$G(0^+) = 1 - n$ $\qquad n$ = part number

$G(0^+) - G(0^-) = 1$



QMC $G(0) \equiv G(0^+)$

<u>Trick</u> $G_0^{QMC}(0^+) \equiv G_0^{QMC}(0) = G_0^{SMOOTH}(0) + \frac{1}{2}$

then

$$G^{SMOOTH}(0) = G^{QMC}(0) - \frac{1}{2}$$

why? FFT for the ω_n or $\tau = 0$ takes the average 0^- & 0^+

$$G^{SMOOTH}(0) = \frac{G(0^+) + G(0^-)}{2} = \frac{G(0^+) + G(0^+) - 1}{2} = G(0^+) - \frac{1}{2}$$

* independent of n

Real systems are usually degenerate

d-band $\rightarrow$ E_g - 2 fold
$\hookrightarrow$ t_{2g} - 3 fold.

$\Rightarrow$ need to implement multy-orbital impurity

<u>Two-band QMC code</u> (2-orbital)

since $t_{\nu\nu'} = t_{\nu\nu}\,\delta_{\nu\nu'}$

$$G_\sigma(\tau) \rightarrow G_{\sigma\nu}(\tau)$$

the generalization is easy.

* Flow diagram is identical
* relevant changes in the impurity routine.

1-orbital case

H-S $$e^{-\Delta\tau U n_\uparrow n_\downarrow + \Delta\tau \frac{U}{2}(n_\uparrow + n_\downarrow)} = \frac{1}{2}\sum_{s=\pm} e^{\lambda s (n_\uparrow - n_\downarrow)}$$

2-orbital

$U n_{1\uparrow} n_{1\downarrow}$; $U n_{2\uparrow} n_{2\downarrow}$; $U n_{1\uparrow} n_{2\uparrow}$; $U n_{1\downarrow} n_{2\downarrow}$; $U n_{1\uparrow} n_{2\downarrow}$; $U n_{1\downarrow} n$

$\Rightarrow$ need to do 6 H-S trafos

$\Rightarrow$ $S_1(\tau)$; $S_2(\tau)$; $S_3(\tau)$; $S_4(\tau)$; $S_5(\tau)$; $S_6(\tau)$

$$e^{\sum'_{\substack{\nu\nu' \\ \sigma\sigma'}} -\Delta\tau U (n_{\nu\sigma}-\frac{1}{2})(n_{\nu'\sigma'}-\frac{1}{2}) - 6\frac{U}{4}}$$

$$= \left(\frac{1}{2}\right)^6 \sum_{s^1,\dots,s^6} e^{\{\lambda s^1(n_{1\uparrow}-n_{1\downarrow}) + \lambda s^2(n_{2\uparrow}-n_{2\downarrow}) + \dots\}}$$

$$= \left(\frac{1}{2}\right)^6 \sum_{s^1,\dots,s^6} e^{\{\lambda(s^1+s^3+s^5)n_{1\uparrow} + \lambda(-s^1+s^4+s^6)n_{1\downarrow} + \lambda(s^2-s^4-s^5)n_{2\uparrow} + \lambda(-s^2-s^3-s^6)n_{2\downarrow}\}}$$

$$G^{-1}_{1\uparrow} = G^{0-1}_{1\uparrow}(\tau,\tau') + \lambda(s^1(\tau)+s^3(\tau)+s^5(\tau))\,\delta_{\tau\tau'}$$

$$G^{-1}_{1\downarrow} = G^{0-1}_{1\downarrow}(\tau,\tau') + \lambda(-s^1(\tau)+s^4(\tau)+s^6(\tau))\,\delta_{\tau\tau'}$$

$$G^{-1}_{2\uparrow} = \quad \vdots \qquad \vdots \qquad \vdots$$

$$G^{-1}_{2\downarrow} = \quad \vdots \qquad \vdots \qquad \vdots$$

$$\Rightarrow \quad xf(4,6) \equiv \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & -1 \end{pmatrix}$$

$$Vn(L,6) \equiv \begin{pmatrix} | & | & | & | & | & | \\ V_1 & V_2 & V_3 & V_4 & V_5 & V_6 \\ | & | & | & | & | & | \end{pmatrix}$$

$$V_\tau = \lambda S_\tau$$

$$G = \begin{bmatrix} G_{1\uparrow} & & & \\ & G_{1\downarrow} & & \\ & & G_{2\uparrow} & \\ & & & G_{2\downarrow} \end{bmatrix}$$

$$Z = \sum \det(G_{1\uparrow}^{-1}) \det(G_{1\downarrow}^{-1}) \det(G_{2\uparrow}^{-1}) \det(G_{2\downarrow}^{-1})$$

$S_\tau^i \to -S_\tau^i$ will affect only 2 G^{-1} : $\nu\sigma$ & $\nu'\sigma'$

$$R \to \frac{\det\left[G_\sigma^\nu(s)\; G_{\sigma'}^{\nu'}(s)\right]}{\det\left[G_\sigma^\nu(s')\; G_{\sigma'}^{\nu'}(s')\right]}$$

3 orbitals (t_{2g}) $\binom{6}{2} = 15$ s^i fields

5 orbitals (full d-band) $\binom{10}{2} = 45$ s^i fields

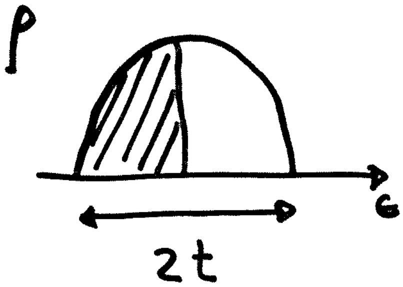
parallelization is easy

Hubbard model has the basic ingredients

$$H = -t \sum_{\substack{\langle ij \rangle \\ \sigma}} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

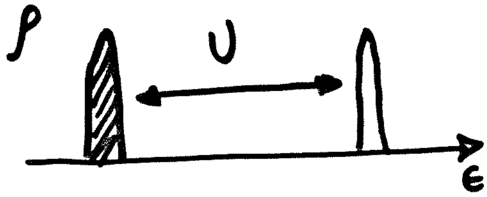
* PM phase , ½ filling

$U=0$



Metal

$t=0$

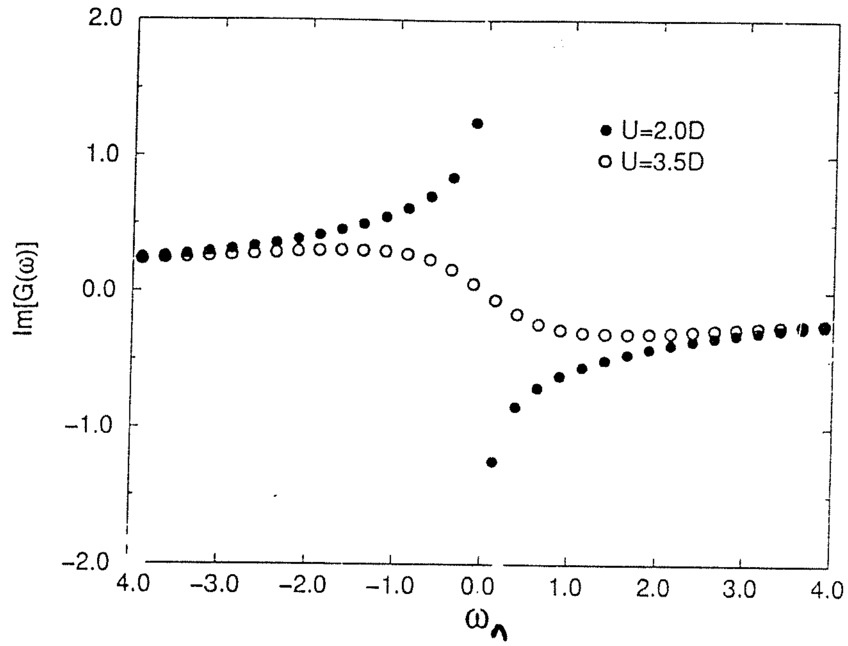


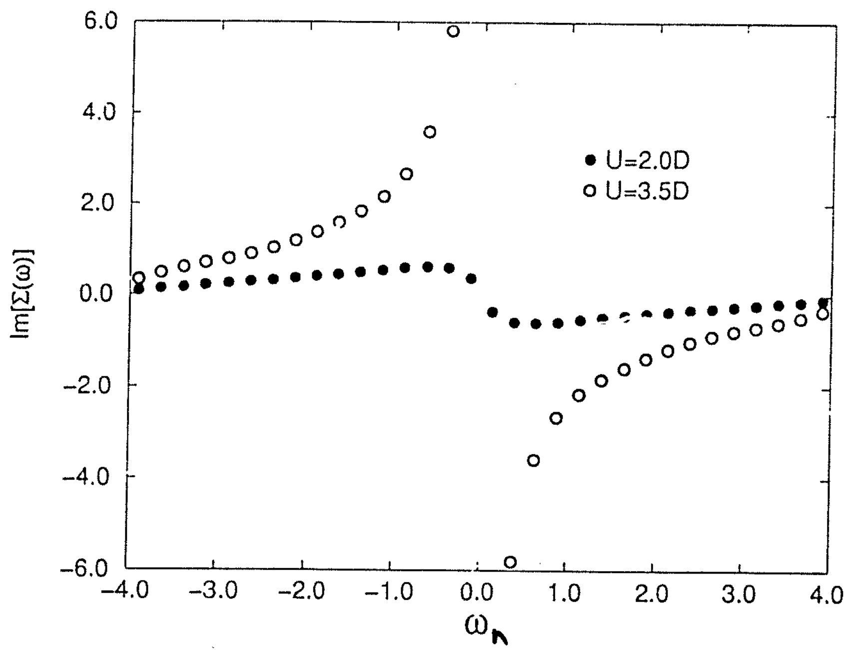
Insulator

* sofar solution exists in $d=1$

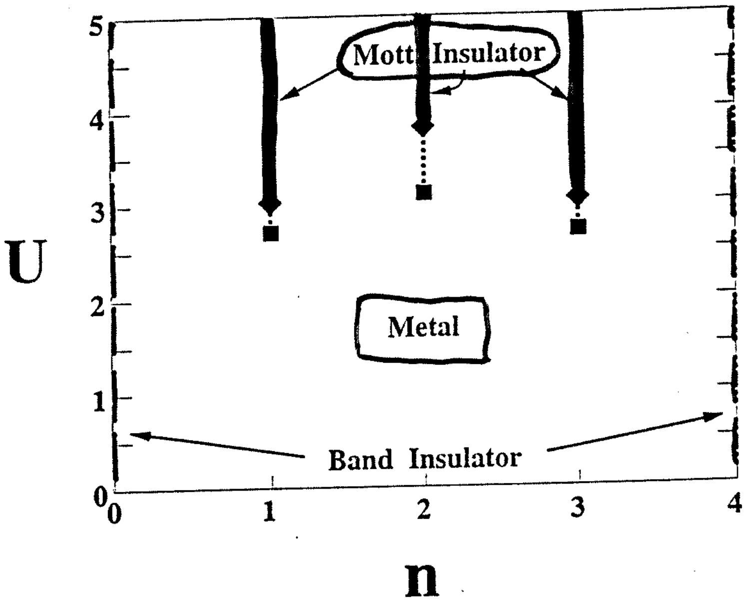
(always insulator , $U \neq 0$)

Metal Insulator Transition (QMC)

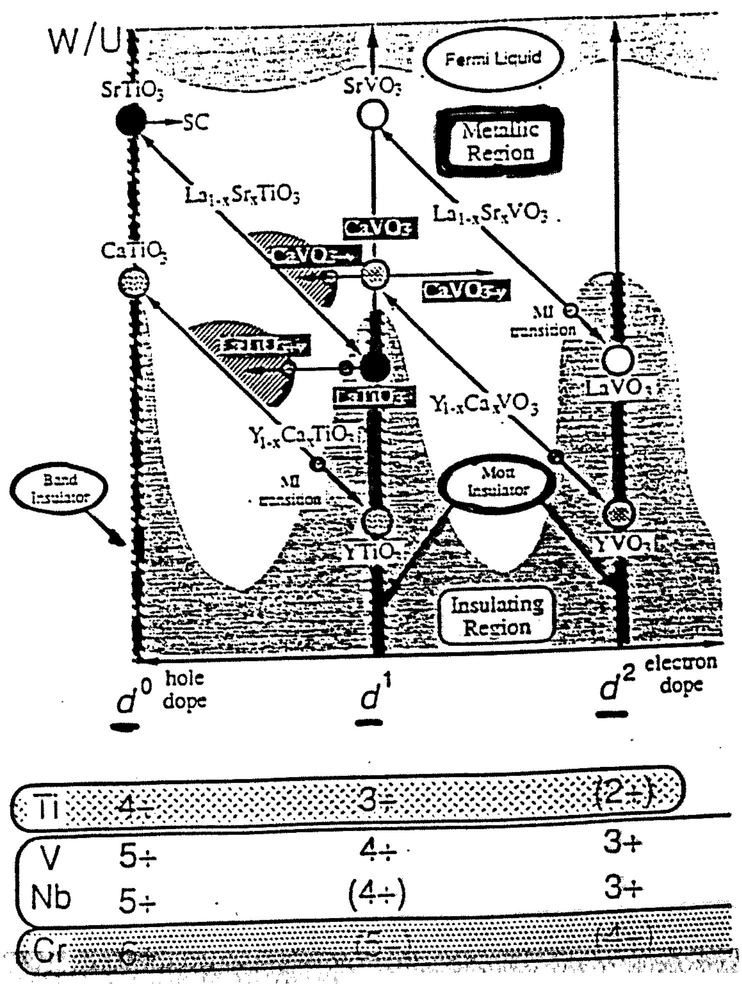




Phase diagram of 2-band degenerate Hubbard model (PM)



Schematic Diagram of
Carrier concentration vs. Electron correlation



Nuts & bolts of the QMC-DMFT code

Input file: fort.50

```
0.5d0,0.0d0,1
1.d0,1,0.1d0,1,0.1d0
2.0d0
2.0d0
2.0d0
2.0d0
2.0d0
2.0d0
1,1
1,1
20000,20000,1000

dtaureal,du,nu
d,nloop,dmu,nmu,xmu0
u(1)
...
u(6)
input,imet
igf,inp
nsweep,nsweep0,ndirty

input=1 reads seed (fort.20)
     =0 generates new seed
imet=1 met seed
    =0 ins seed (use only at 1/2 filling)
igf=1 prints out the gf's
inp=1 prints out the part number
nsweep= number of sweeps
nsweep0= number of sweeps in the last iteration
ndirty= number of dirty updates
```

Output files

```
'fort.12   G (tau)'
'fort.13   Go(tau)'
'fort.60  Im G (w)'
'fort.61  Re G (w)'
'fort.40  Im Go(w)'
'fort.41  Re Go(w)'
'fort.30  Im Se(w)'
'fort.41  Re Se(w)'
'fort.80   <docc>'
'fort.90   <occ>'
'fort.3    seed'
```