Thermodynamics of the Mott-Hubbard metal-insulator transition in d=∞

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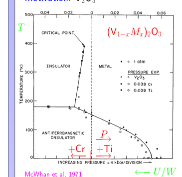
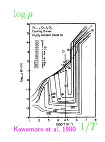
Introduction

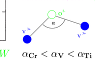
Motivation: V_2O_3



McWhan et al, 1971 $\longleftarrow U/W$



Kawamoto et al, 1980



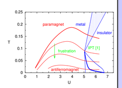
$\alpha_{\rm Cr} < \alpha_{\rm V} < \alpha_{\rm Ti}$

Doping or external pressure distorts lattice $\longrightarrow$ changes V-V overlap (effective bandwidth) $\longrightarrow$ drives metal-insulator transition (MIT) between paramagnetic metal and paramagnetic insulator without long-range order.

Drastically simplified model (no band degeneracy, no lattice degrees of freedom): half-filled one-band Hubbard model

$$\hat H = -t \sum_{\langle ij\rangle\sigma}\left(\hat c^\dagger_{i\sigma}\hat c_{j\sigma} + \hat c^\dagger_{j\sigma}\hat c_{c\sigma}\right) + U\sum_i \hat n_{i\uparrow}\hat n_{i\downarrow}$$

- in unfrustrated model: no MIT, but crossover (AF at low T)
- AF frustrated in many materials
- nonperturbative approach needed
- thermodynamic limit important



Aim: full phase diagram for
- 1-band Hubbard model at half filling
- Dynamical Mean-Field Theory (DMFT)
- no AF order (full frustration)
- semielliptic Bethe DOS ($W=4$)

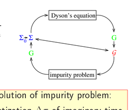
Question: coexistence / order of transition?

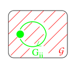
Self-consistent solution of DMFT equations

$$G_n = \int d\epsilon \frac{\rho_0(\epsilon)}{i\omega_n - \epsilon - \Sigma_n}$$

$$G_n = -<\Psi_n \Psi_n{}^*>_{\mathcal{G}_n}$$

$$\mathcal{G}_n^{-1} = G_n^{-1} + \Sigma_n$$

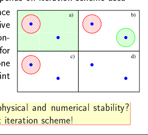




QMC solution of impurity problem:
- discretization $\Delta\tau$ of imaginary time
- Hubbard-Stratonovich trafo
- MC sampling over auxiliary Ising field

abstract view: solution of fixed point problem by iteration stability of fixed point depends on iteration scheme used

scheme: given the existence of 2 fixed points an iterative procedure can have nonzero radii of convergence for both points (a and b), one point (c), or no fixed point (d).



Connection between physical and numerical stability?
Yes: at least for direct iteration scheme!

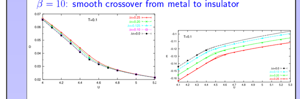
Results: crossover and coexistence regions

double occupancy D, energy per lattice site $E = E_{kin} + UD$

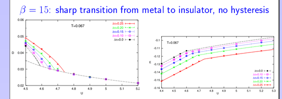
$$E_{kin} = \lim_{\eta\to 0^+} 2T \sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty} d\epsilon \frac{e^{i\omega_n \eta}}{i\omega_n - \epsilon - \Sigma(i\omega_n)}\,\epsilon\rho(\epsilon)\cdot 1$$

$$= 2\int_{-\infty}^{\infty} d\epsilon \frac{\epsilon\rho(\epsilon)}{e^{\beta\epsilon}+1} + 2T \sum_{n=-L/2+1}^{L/2}\int_{-\infty}^{\infty} d\epsilon\, \epsilon\rho(\epsilon)\left(G_\epsilon(i\omega_n) - G^0_\epsilon(i\omega_n)\right)$$

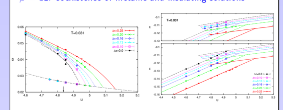
$\beta = 10$: smooth crossover from metal to insulator



$\beta = 15$: sharp transition from metal to insulator, no hysteresis



$\beta = 32$: coexistence of metallic and insulating solutions



- significant shift of U_c with $\Delta\tau \to 0$
- double occupancy D: curvature, irregular $\Delta\tau$ dependence
- energy E: almost (piecewise) linear in U, quadratic in $\Delta\tau$
- no significant T dependence of D, E in insulator

Comparing free energies

$F(U,T)$ cannot be directly computed from QMC, NRG but differential known:

$$d(\beta F_{m/i}(\beta,U)) = E_{m/i}(\beta,U)d\beta + \beta D_{m/i}(\beta,U)dU$$

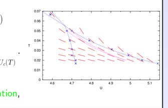
Naive solution: $F(\beta,U) = F(\beta_0,U_0) + \int_{\beta_0,U_0}^{\beta,U} d(\beta' F_{m/i}(\beta',U'))$

Problems: $F_{m/i}(\beta_0,U_0)$ must be known; different paths of integration introduce different systematic errors (for m/i)

local criterion at transition line ($\Delta F := F_m - F_i$):

$$\Delta F(\beta,U)|_{U=U_c(\beta)} = 0; \quad d(\beta\Delta F(\beta,U))|_{U=U_c(\beta)} = 0$$

$$\frac{dU_c(T)}{dT} = f(T,U_c(T)) := \left.\frac{\Delta E(T,U)}{T\Delta D(T,U)}\right|_{U=U_c(T)}.$$



$U_c(T^*) = U^*$, integrate Clausius-Clapeyron equation,

$$U_c(T) = U^* + \int_{T^*}^{T} dT' f(T',U_c(T')); \quad T < T^*.$$

$f(T,U) \approx \tilde f(T)(A+BU)$ fit parameters A, B

supplement QMC results with low-T information:
entropy of insulator (almost) independent of U

$$E_i(U,T) = E_i^0(U); \quad S_i(U,T) = S_0\,.$$

Fermi liquid properties in metal

$$E_m(U,T) = E_m^0(U) + \frac{1}{2}\gamma(U)T^2; \quad S_i(U,T) = \gamma(U)T$$

$T=0$ numerics [2,3] ($U_c^0 := U_c(T=0) = U_{c2}(T=0)$):

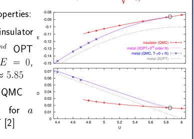
$$E_i^0(U) - E_m^0(U) = \frac{a}{2}(U-U_c^0)^2; \quad \gamma(U) = \frac{\gamma_0}{U_c^0 - U}.$$

Equate free energies to obtain the low-temperature solution,

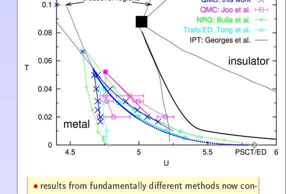
$$U_c(T) = U_c^0 - \sqrt{\frac{2S_oT}{a}} + \mathcal{O}(T)$$

$$\longrightarrow \tilde f(T) = CT^{-1/2} + D + ET^{1/2}; \quad C \approx -\sqrt{S_o/2a}$$

Ground state properties:
E,D known for insulator
fit based on 2^{nd} OPT for metal $\to \Delta E = 0$, $\Delta D = 0$ at $U_c \approx 5.85$
agrees well with QMC
better estimate for a than from PSCT [2]



Full phase diagram: Comparison



- results from fundamentally different methods now converged towards a reliable phase diagram
- coexistence region at low T $\to$ first order transition
- first controlled computation of $U_c(T)$

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