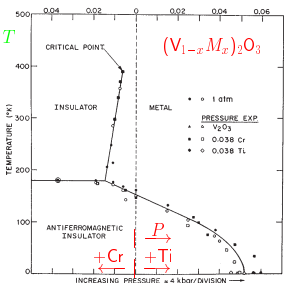
Thermodynamics of the Mott-Hubbard metal-insulator transition in d=∞

N. Blümer[1,2], P. G. J. van Dongen[2], and D. Vollhardt[1], [1]Universität Augsburg, [2]Universität Mainz

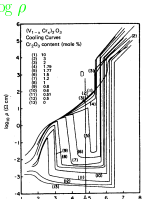
Introduction

Motivation: V_2O_3

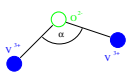


McWhan et al, 1971 ⟵ U/W

log ρ



Kawamoto et al, 1980 $1/T$



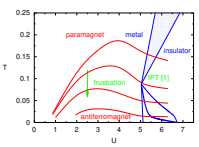
$\alpha_{Cr} < \alpha_V < \alpha_{Ti}$

Doping or external pressure distorts lattice ⟶ changes V-V overlap (effective bandwidth) ⟶ 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 ($W=4$)

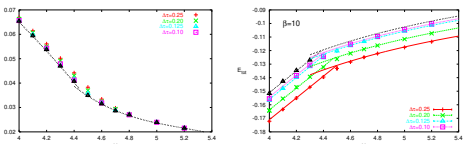
Question: coexistence / order of transition?

Results: crossover and coexistence regions

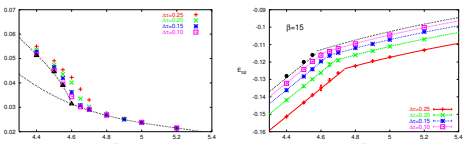
double occupancy D, energy per lattice site $E = E_{kin} + UD$

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

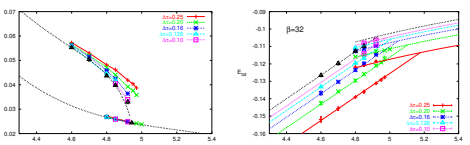
$\beta = 10$: smooth crossover from metal to insulator



$\beta = 15$: 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

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

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

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

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

Fermi liquid properties in metal

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

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

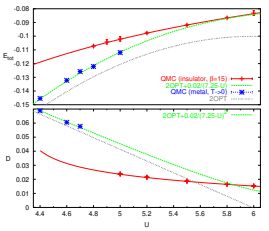
$$E^0_i(U) - E^0_m(U) = \frac{a}{2}(U - U^0_c)^2; \quad \gamma(U) = \frac{\gamma_0}{U^0_c - U};$$

Equate free energie to obtain the low-temperature solution,

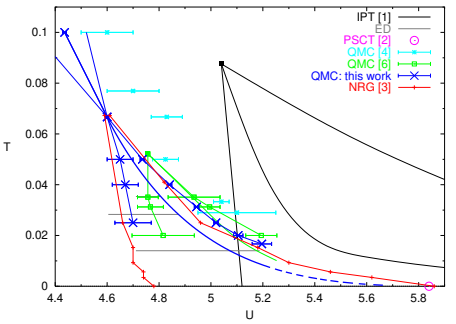
$$U_c(T) = U^0_c - \sqrt{\frac{2S_oT}{a}} + \mathcal{O}(T)$$

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

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

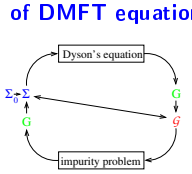


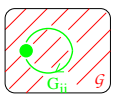
- results from fundamentally different methods now converged towards a reliable phase diagram
- coexistence region at low T → first order transition
- first controlled computation of $U_c(T)$

Work supported by DFG through SFB484

Self-consistent solution of DMFT equations

$$G_n = \int d\epsilon \frac{\rho_0(\epsilon)}{i\omega_n - \epsilon - \Sigma_n}$$
$$G_n = - < \Psi_n \Psi_n{}^* >_{\mathcal{G}_n}$$
$$\mathcal{G}^{-1}_n = G^{-1}_n + \Sigma_n$$

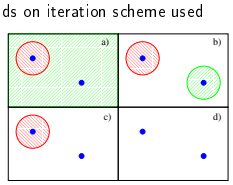




QMC solution of impurity problem:
- discretization $\Delta\tau$ of imaginary time
- Hubbard-Stratonovich trafo
- MC sampling over auxiliary Ising field

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 non-zero radii of convergence for both points (a and b), one point (c), or no fixed point (d).



Connection between physical and numerical stability?

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

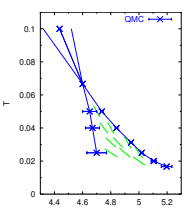
Problems: $F_{m/i}(\beta_0,U_0)$ must be known; different paths of integration introduce different systematic errors (for m/i)

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

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

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

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



References

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