Hubbard model with spin disorder

Karol Makuch

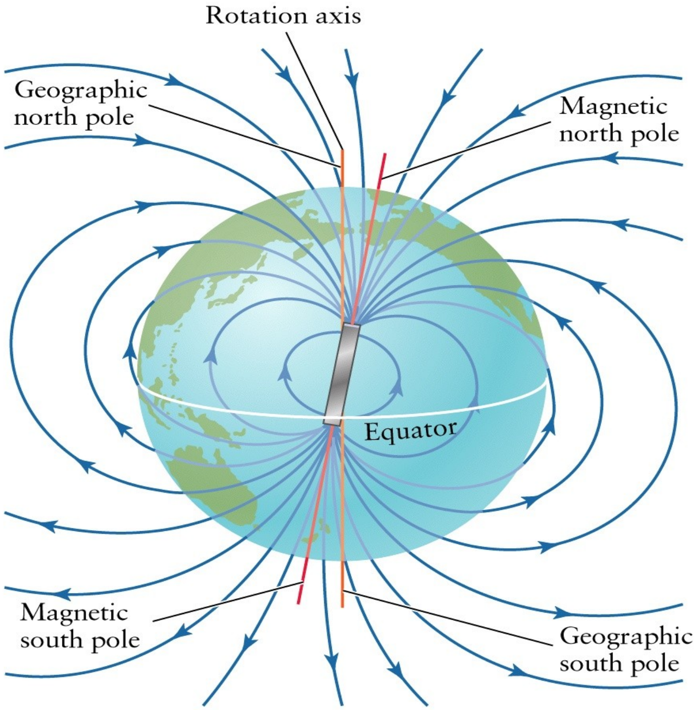
21.06.2012

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

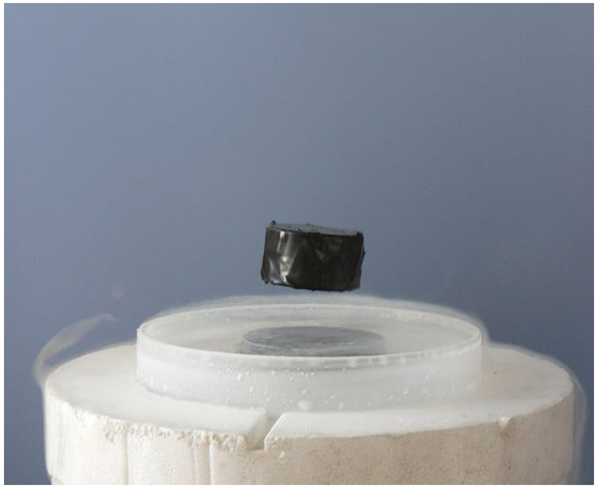
FNP
Foundation for Polish Science

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

Hubbard model



Magnetism (itinerant moment metals)



High-temperature superconductivity

Electrons in crystal

Hamiltonian

$$H = \sum_{i=1}^{N} \frac{(-\hbar \nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{j<i}^{N} \sum_{i=1}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

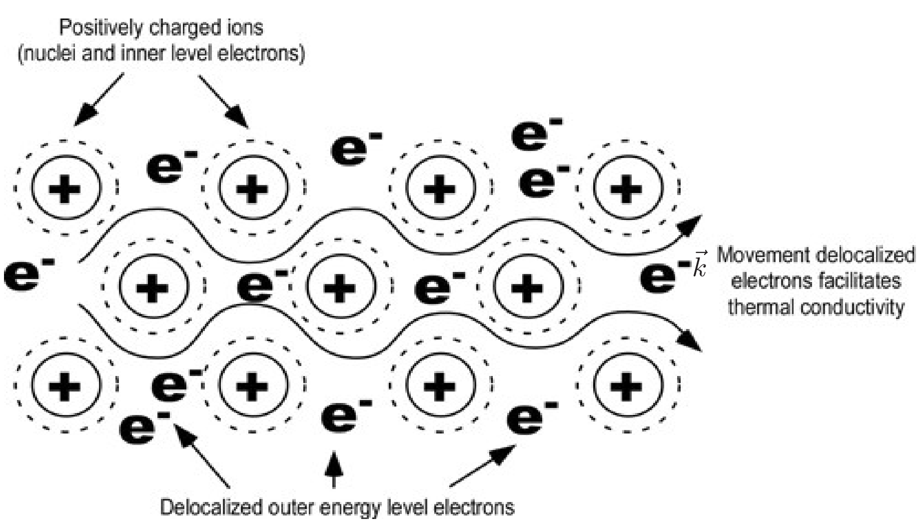
Kinetic energy

Periodic potential from ions

Coulomb interactions between electrons

Hamiltonian (second quantization)

$$H = \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \sum_{\alpha\beta} V_{\alpha\beta} a_\alpha^\dagger a_\beta + \sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger U_{\alpha\beta\gamma\delta} a_\delta a_\gamma$$



One-particle states

α ← $n = 0, 1, \ldots$

α ← $\vec{R}_i$ lattice site

α ← spin

Hubbard model

From full Hamiltonian only some terms taken into consideration
-single band; local Coulomb interaction, kinetic energy term (including potential from ions):

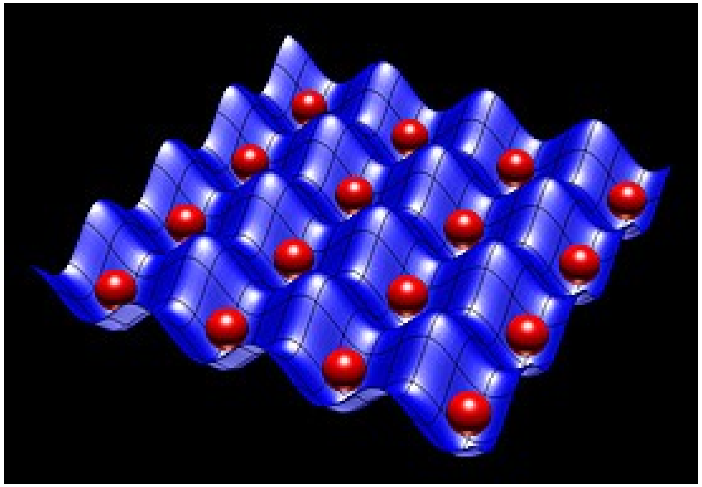
$$H = t \sum_{(i,j)\in n.n.} \sum_{\sigma=\uparrow,\downarrow} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i=1}^{N} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$n_{i\sigma} \equiv a^{\dagger}_{i\sigma} a_{i\sigma}$$

Kinetic energy and interactions with lattice

Interaction energy between electrons

Quantum simulations of Hubbard model

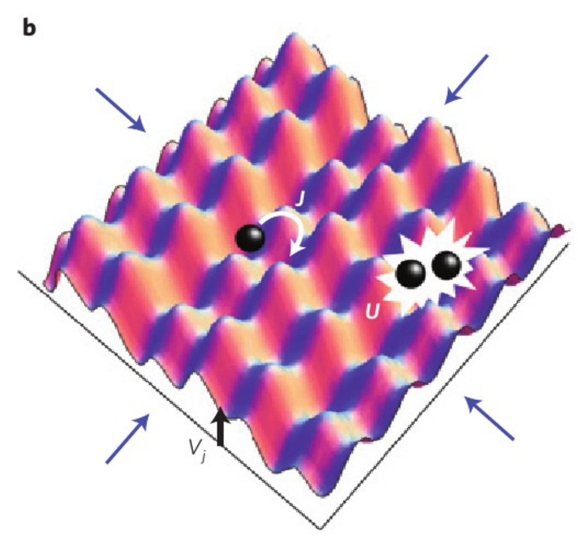


Hubbard model with disorder

$$H = t \sum_{(i,j)\in n.n.} \sum_{\sigma=\uparrow,\downarrow} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i} \sum_{\sigma=\uparrow,\downarrow} \epsilon_{i\sigma} n_{i\sigma} + \sum_{i=1}^{N} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Energy (external potential)
depends on lattice site

Quantum simulations of Hubbard model
with spin dependent disorder



How disorder influence magnetic phase?

L. Sanchez-Palencia, M. Lewenstein
Nature Physics, 2010

Type of disorder

In experiment $\epsilon_1, \ldots, \epsilon_n, \ldots$ fixed.

Statistical physics: averaging over probability distribution fof disorder:

We assume uncorrelated rectangular disorder:

$$\mathcal{P}(\epsilon_1, ..., \epsilon_n, ...) = \prod_i P(\epsilon_i)$$

$$P(\epsilon) = \begin{cases} \frac{1}{\Delta} & |\epsilon| < \frac{\Delta}{2} \\ 0 & |\epsilon| > \frac{\Delta}{2}. \end{cases}$$

What we investigate?

How interplay of spin disorder and interactions influence
-phase (paramagnetic, antiferromagnetic)
-susceptibility
-conductivity
-compressibility

Grand canonical potential (thermodynamics):

$$\Xi = \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} | \gamma_N \rangle$$

One-particle Green function:

$$G_{\alpha\beta}(\tau,\tau') = -\langle T_\tau \hat{a}_\alpha(\tau) \hat{a}^\dagger_\beta(\tau') \rangle$$

$$\langle \ldots \rangle = \frac{1}{\Xi} \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} \ldots | \gamma_N \rangle$$

"time" ordering

$$T_\tau \hat{a}_\alpha(\tau) \hat{a}^\dagger_\alpha(\tau') = \begin{cases} \hat{a}_\alpha(\tau)\hat{a}^\dagger_\alpha(\tau') & \text{dla} \quad \tau > \tau' \\ -\hat{a}^\dagger_\alpha(\tau')\hat{a}_\alpha(\tau) & \text{dla} \quad \tau < \tau' \end{cases}$$

Operator in Heisenberg picture

$$\hat{a}_\alpha(\tau) = e^{\tau(H-\mu N)} \hat{a}_\alpha e^{-\tau(H-\mu N)}$$

Green function for system with perturbation

$$H = H_0 + H_1$$

For H_0 :

$$G_{0,\alpha\beta}(\tau,\tau') = -\langle T_\tau \hat{a}_\alpha(\tau)\hat{a}^\dagger_\beta(\tau')\rangle$$

Hamiltonian in "average" and in „time" evolution

For H :

$$G_{\alpha\beta}(\tau,\tau') = -\langle T_\tau \hat{a}_\alpha(\tau)\hat{a}^\dagger_\beta(\tau')\rangle$$

Dyson equation:

$$G_0^{-1} = G^{-1} + \Sigma$$

Self-energy (diagrams)

Noninteracting system with disorder

$$H = t \sum_{(i,j)\in n.n.} \sum_{\sigma=\uparrow,\downarrow} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i} \sum_{\sigma=\uparrow,\downarrow} \epsilon_{i\sigma} n_{i\sigma}$$

Green function without disorder: $[G_0(\omega)]_{i\sigma j\sigma}$

Green function for system with disorder (Dyson equation):

$$[G_0^{-1}(\omega)]_{i\sigma j\sigma'} = [G^{-1}(\omega)]_{i\sigma j\sigma'} + \delta_{ij}\delta_{\sigma\sigma'}\epsilon_i$$

$$G_0^{-1} = G^{-1} + \epsilon$$

Green function averaged over disorder:

$$\langle G \rangle_{dis}$$

Coherent potential approximation

Dyson equation:

$$G_0^{-1} = G^{-1} + \epsilon$$

Definition of coherent potential Σ, which the same as ϵ is diagonal: $[\Sigma]_{ij} = \delta_{ij}\Sigma$

$$G_0^{-1} = \langle G \rangle^{-1} + \Sigma$$

yields:

$$G = \langle G \rangle + \langle G \rangle T \langle G \rangle$$

where $$T = (\epsilon - \Sigma)[1 - \langle G \rangle (\epsilon - \Sigma)]^{-1}$$

Average leads to: $$\langle T \rangle = 0$$

Coherent potential approximation: $$[\langle G \rangle]_{ij} \approx \delta_{ij} [\langle G \rangle]_{ii}$$
leads to closed system of equations.

Hubbard model with disorder

$$H = t \sum_{(i,j)\in n.n.} \sum_{\sigma=\uparrow,\downarrow} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i} \sum_{\sigma=\uparrow,\downarrow} \epsilon_{i\sigma} n_{i\sigma} + \sum_{i=1}^{N} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Dynamical mean field approach

Metzner i Vollhardt, 1987 – limit of high dimensional lattice (Georges et al. (1996))

Dynamical mean field equations for disorder

Dyson equation:

$$G = G_0 + G_0 \Sigma G$$

Consequences of high dimension limit (local problem):

$$G_{00}(\tau,\tau') = -\langle \langle T_\tau c_{0\sigma}(\tau) c^*_{0\sigma}(\tau') \rangle_{S_{\rm eff}[\mathcal{G}_0]} \rangle_{dis}$$

QMC

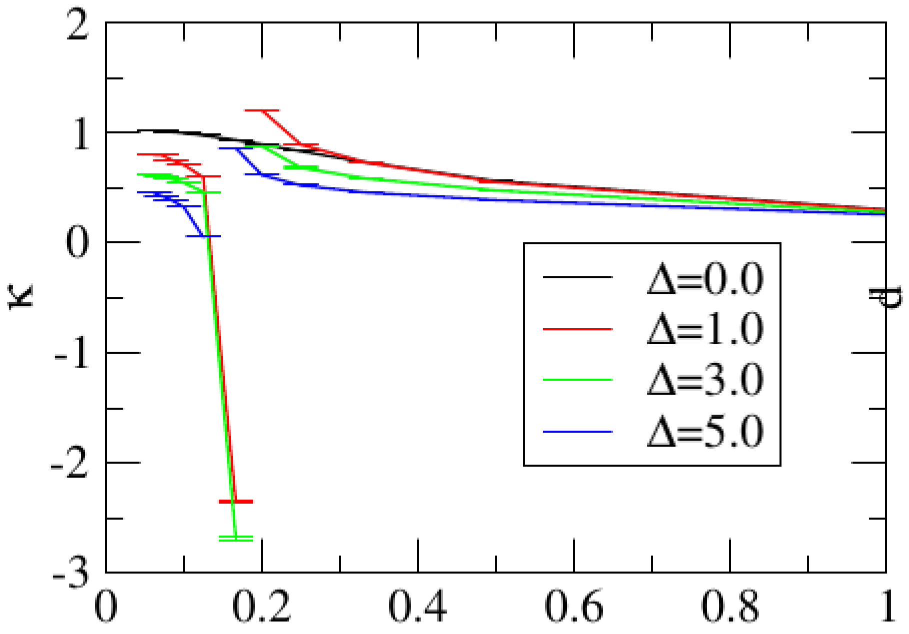
$$G_{00} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma G_{00}$$

$$S_{\rm eff} \approx \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau)(\mathcal{G}_0^{-1}(\tau,\tau') - \epsilon_0) c_{0\sigma}(\tau') + \int_0^\beta d\tau U n_{0\downarrow} n_{0\uparrow}$$

Actual results

Without disorder (Δ=0) – proper results.
Problem for disorder (Δ>0)

n=0.5   U=0.1



Thermodynamics: compressibility > 0

Where is the problem?

Fourier transform?

Asymptotic of Green function:

$$G(\omega) \sim 1/\omega \quad \text{for} \quad \omega \to \infty$$

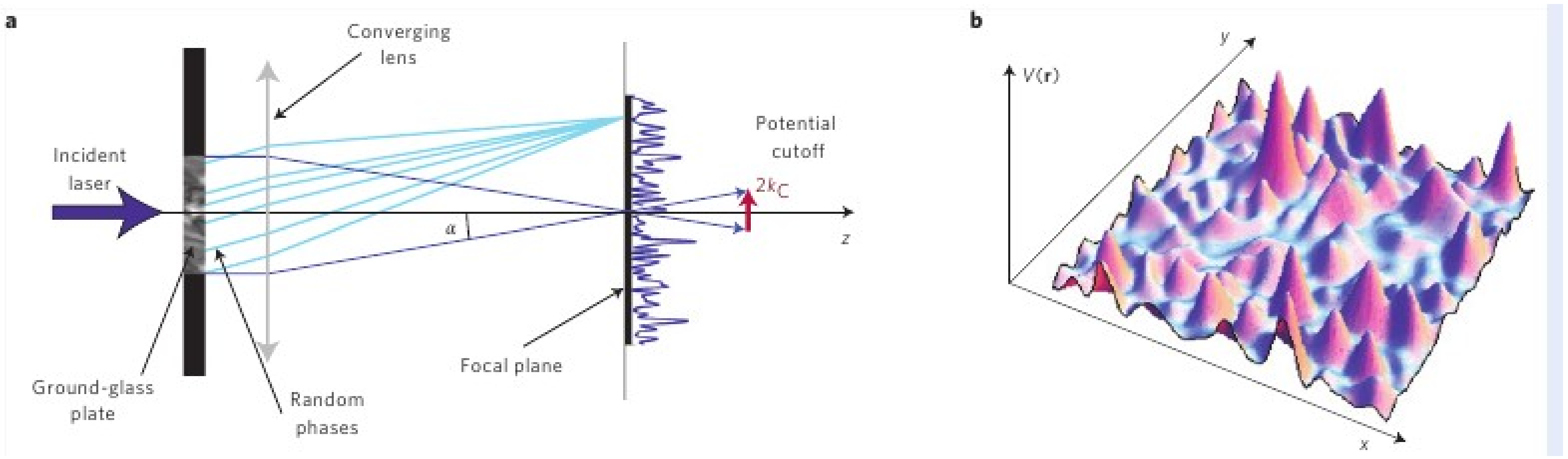
(Fourier transforms needs to be calculated properly)

No (program improved –
Ulmke trick avoided)

Transport coefficients?

To be checked...

Disorder in cold atoms



L. Sanchez-Palencia, M. Lewenstein
Nature Physics, 2010

Compressibility:

$$\kappa = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_T \qquad \kappa^{-1} \equiv -V\left(\frac{\partial p}{\partial V}\right)_T$$

Charge susceptibility:

$$\chi_c = \left(\frac{\partial n}{\partial \mu}\right)_T$$

Magnetic susceptibility:

$$\chi = \left(\frac{\partial m}{\partial h}\right)_T$$

Disorder and interaction competition

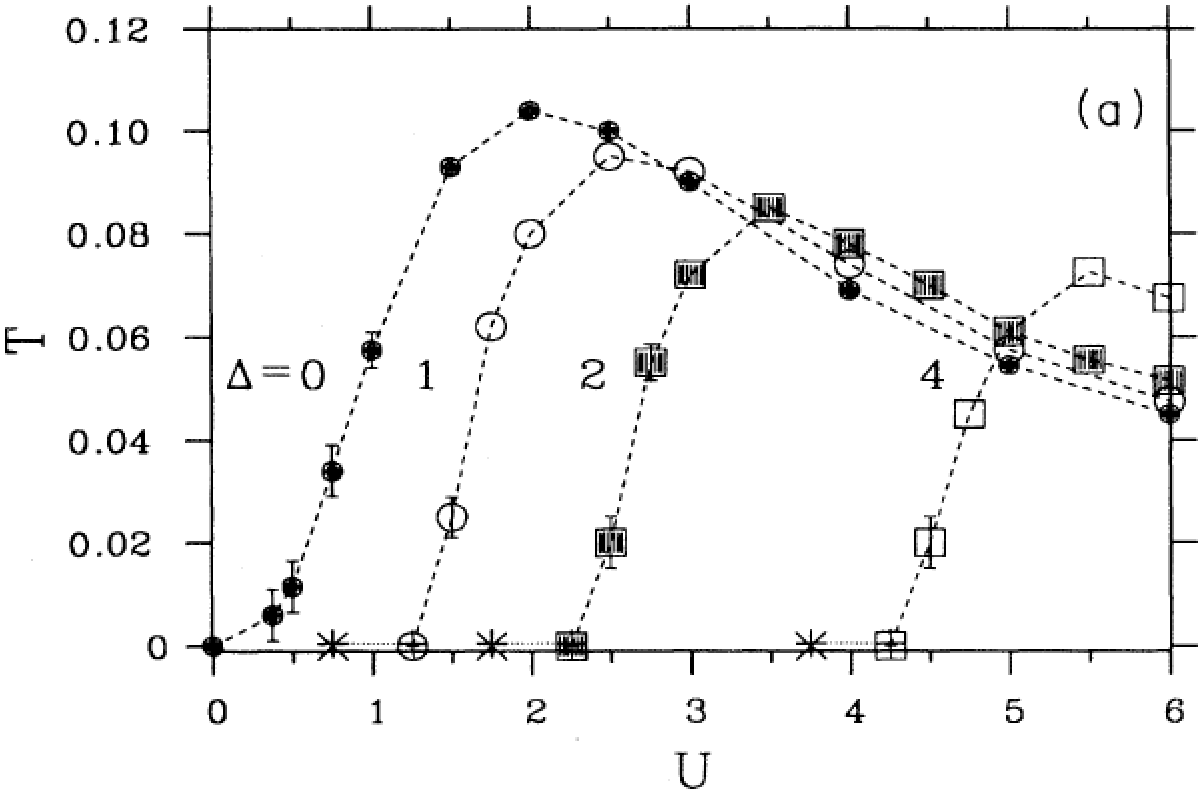


FIG. 4. (a) $T-U$-phase diagram for the binary alloy with $\Delta = 0, 1, 2, 4$ obtained from the zeroes of χ_{AF}^{-1} (see Fig. 3). The AF phase is stable below the curves. The dotted lines at $T = 0$ depict the regimes where the Curie law would give negative transition temperatures. Below the crosses χ_{AF}^{-1} has no zeroes but a minimum and an AF phase can no longer be expected. (b) $T-U$-phase diagram for the semielliptic distribution of the random energies with width $\Delta = 0, 2, 4, 6$.

M. Ulmke,V. Janis, D. Vollhardt (1995)

Hubbard model

Georges et al. (1996): cuprate (tlenki miedzi) superconductors (transition metals – niecałkowicie zapełniona powłoka d)

Ulmke trick

It smoothed Green function(?)

$$\overline{G}_n = \delta\tau/[1 - \exp(\delta\tau/G_n)],$$

$$\overline{G}(\tau) = \beta^{-1}\sum_n e^{i\omega_n\tau}\overline{G}_n,$$

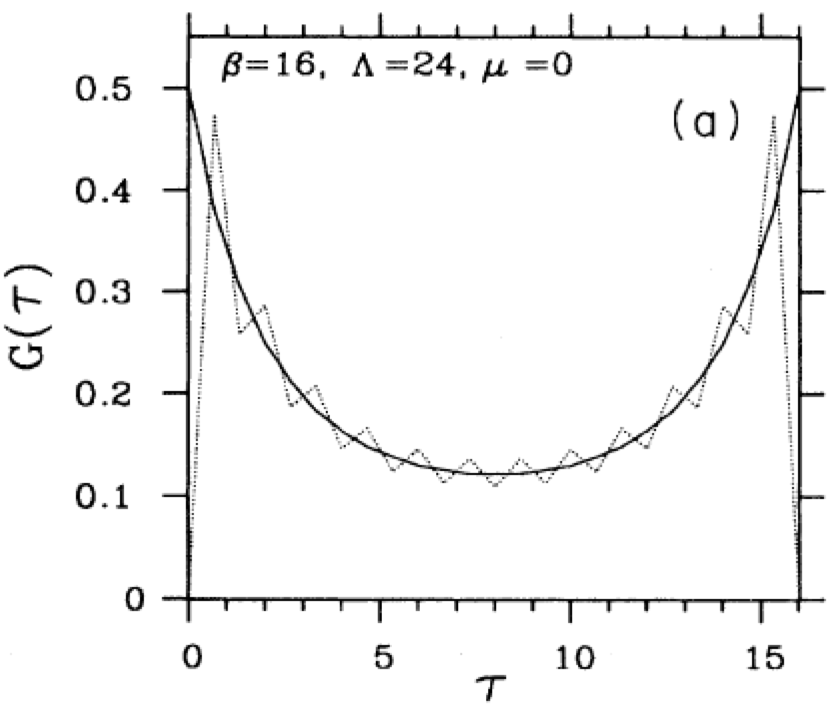


FIG. 1. Local Green function $G(\tau)$ for $U = 0$ and $\mu = 0$ (a), $\mu = 0.5$ (b) obtained by usual Fourier transformation (dotted line) and by redefinition according to Eq. (13) (solid line).

Picture from: M. Ulmke,V. Janis, D. Vollhardt (1995)