量子シミュレーションによる強相関電子系の研究

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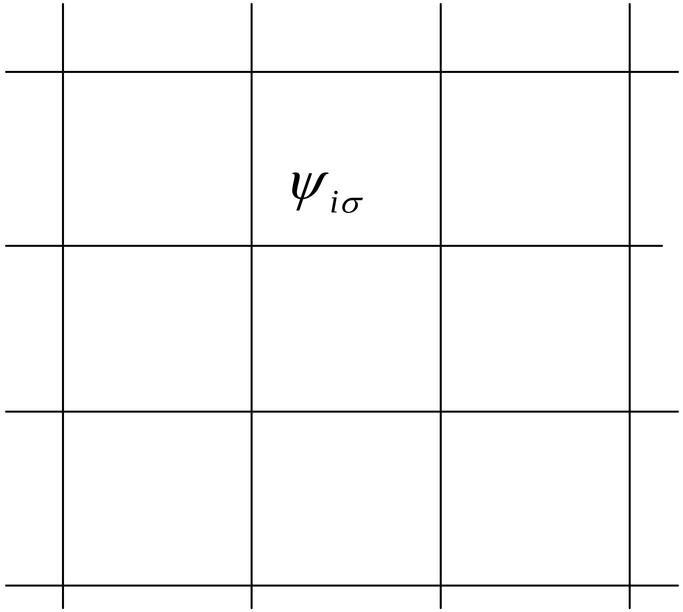
格子上のフェルミ粒子系

格子上のフェルミ粒子

ハミルトニアン

$$H = \sum_{ij\sigma} t_{ij} \psi^{+}_{i\sigma} \psi_{j\sigma} + V(\{\psi^{+}_{i\sigma}, \psi_{i\sigma}\})$$

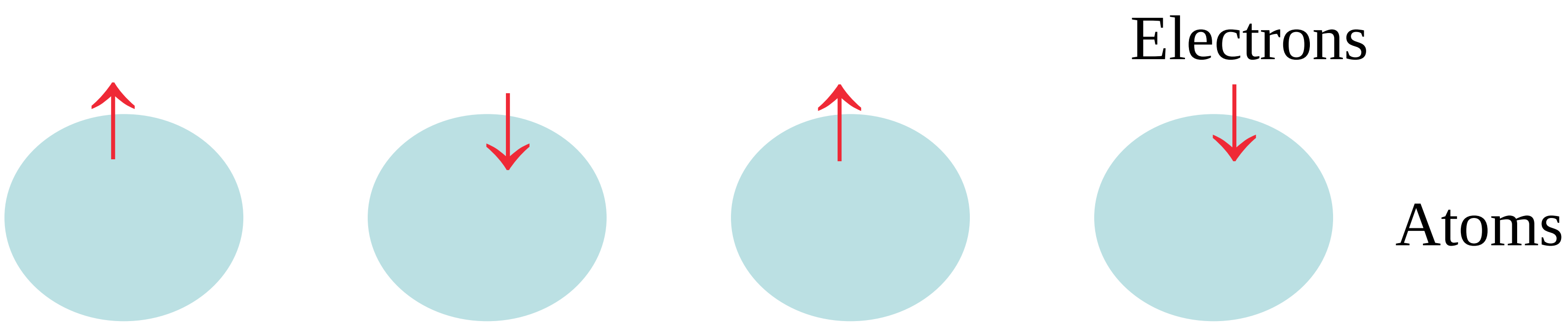
V: 相互作用項



ハバードモデル

Hubbard model

$$H = -t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{+}c_{j\sigma} + h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



Itinerant Electrons

モンテカルロ法

基底状態の波動関数

$$\psi = e^{-\tau H}\psi_0$$

ψ_0: initial function　　$\tau \to \infty$

$H = K + V$　ハバードモデル

$$K = -t\sum_{\langle ij\rangle\sigma}(c^{+}_{i\sigma}c_{j\sigma} + h.c.) \qquad V = U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

波動関数は

$$\psi = e^{-\tau H}\psi_0 = \left(e^{-\Delta\tau H}\right)^M \approx \left(e^{-\Delta\tau K}e^{-\Delta\tau V}\right)^M \psi_0$$

Hubbard-Stratonovich 変換

Wave function

$$\psi = e^{-\tau H}\psi_0 \approx \left(e^{-\Delta\tau K}e^{-\Delta\tau V}\right)^M \psi_0$$

H = K+V

Hubbard-Stratonovich transformation

2次形式に変換

$$\exp\left(-\alpha\sum_i n_{i\uparrow}n_{i\downarrow}\right) = \left(\frac{1}{2}\right)^N \sum_{s_i=\pm1} \exp\left[2a\sum_i s_i(n_{i\uparrow}-n_{i\downarrow}) - \frac{\alpha}{2}\sum_i (n_{i\uparrow}+n_{i\downarrow})\right]$$

$$\psi = \sum_j c_j \varphi_j$$

$$\langle Q\rangle = \frac{\sum_{ij} c_i^* c_j \langle \varphi_i Q \varphi_j\rangle}{\sum_{ij} c_i^* c_j \langle \varphi_i \varphi_j\rangle}$$

$c_i = const.$

$$\varphi_{\{s_i\}} = \prod_\ell \{\exp[2a\sum_i s(\ell)_i (n_{i\uparrow} - n_{i\downarrow}) - \frac{1}{2}\Delta\tau U \sum_i (n_{i\uparrow} + n_{i\downarrow})]\}\, \psi_0$$

$$= \prod_\sigma B_M^\sigma(s_i(M) B_{M-1}^\sigma(s_i(M-1)) \quad \cdot B_1^\sigma(s_i(1))\, \psi_0$$

$$B_\ell^\sigma(\{s_i(\ell)\}) = e^{-\Delta\tau K_\sigma} e^{-V_\sigma(\{s_i(\ell)\})}$$

負符号問題

期待値

$$\langle Q\rangle = \frac{\sum_{ij}\langle \varphi_i Q \varphi_j\rangle}{\sum_{ij}\langle \varphi_i \varphi_j\rangle} = \frac{1}{\sum_{ij}\langle \varphi_i \varphi_j\rangle}\sum_{mn}\langle \varphi_m \varphi_n\rangle \frac{\langle \varphi_m Q \varphi_n\rangle}{\langle \varphi_m \varphi_n\rangle} = \frac{1}{\sum_{ij} P_{ij}}\sum_{mn} P_{mn}\frac{\langle \varphi_m Q \varphi_n\rangle}{\langle \varphi_m \varphi_n\rangle}$$

$$P_{mn} = \langle \varphi_m \varphi_n\rangle = \det(\phi_m^{\uparrow}\phi_n^{\uparrow})\det(\phi_m^{\downarrow}\phi_n^{\downarrow})$$:weighting factor

Metropolis algorithm 出現確率 $\propto |P_{mn}|$

$$\langle Q\rangle = \frac{\sum_{mn} sign(P_{mn})\langle Q\rangle_{mn}}{\sum_{mn} sign(P_{mn})}$$

$$\sum_{mn} signP_{mn} \approx 0$$

Negative sign

Difficulty in calculations

Monte Carlo simulation without Negative sign

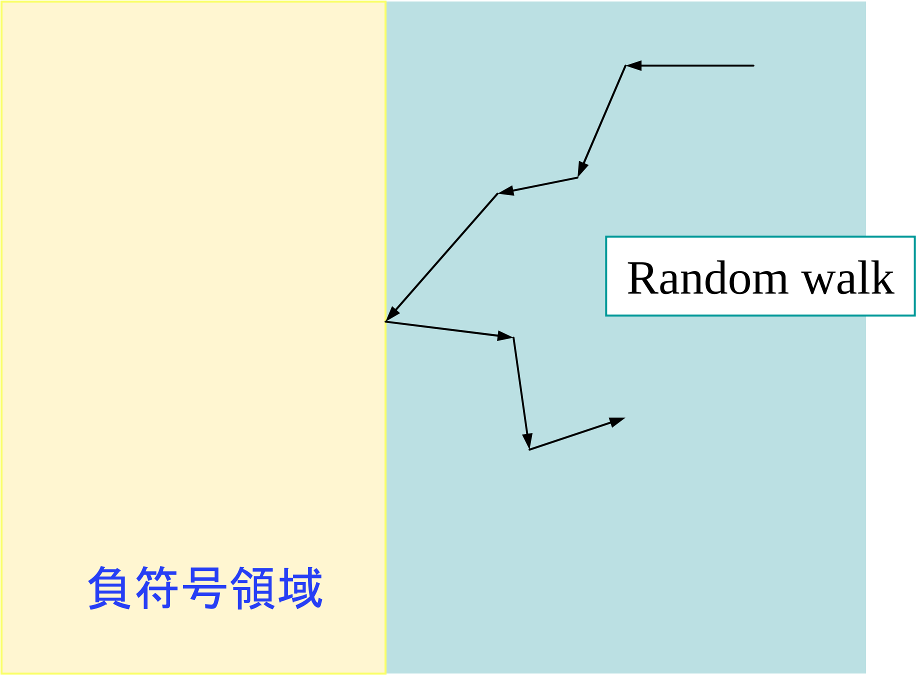
Constrained-path Quantum Monte Carlo method

基底の生成

$$\varphi_1, \varphi_2, \cdots, \varphi_n, \cdots$$

負符号領域 $\langle \varphi_m \varphi_n \rangle < 0$
を避ける

基底の空間



Diagonalization in Monte Carlo method

Diagonalization w.r.t. Basis functions

$$E = \langle H \rangle = \frac{\sum_{ij} c_i^* c_j \langle \varphi_i H \varphi_j \rangle}{\sum_{ij} c_i^* c_j \langle \varphi_i \varphi_j \rangle}$$

Generated basis functions

$$\{\varphi_1, \varphi_2, \cdots, \varphi_n, \cdots, \varphi_M\}$$

Eigenequation

$$\sum_m c_m \langle \varphi_n H \varphi_m \rangle - E \sum_m c_m \langle \varphi_n \varphi_m \rangle = 0 \qquad \partial E / \partial c_n = 0$$

$$\boxed{Hu = EAu}$$

$$H_{nm} = \langle \varphi_n H \varphi_m \rangle \qquad A = \langle \varphi_n \varphi_m \rangle$$

Optimization

1. Increase the number of basis functions

2. Improve each wave functions ϕ_m

Multiply ϕ_m by $B_\ell^\sigma(\{s_i(\ell)\})$

3. Genetic Algorithms

Search algorithms are methods to find optimized solution in complex spaces, based on the mechanics of natural selection and natural genetics.

T. Yanagisawa, Phys. Rev. B75, 224503 (2007)

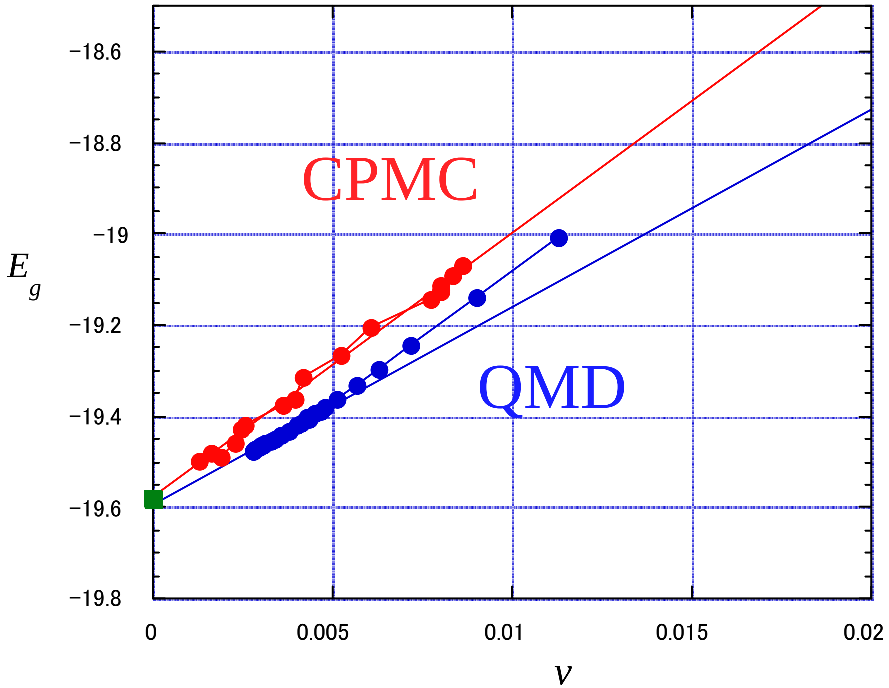
Approach to Exact wave function

The variance method:

期待値Q

$$Q - Q_{exact} \propto \frac{\left\langle \left(H - \langle H \rangle\right)^2 \right\rangle}{\langle H \rangle^2} = \frac{\langle H^2 \rangle - \langle H \rangle^2}{\langle H \rangle^2} \equiv v_E$$

エネルギー分散

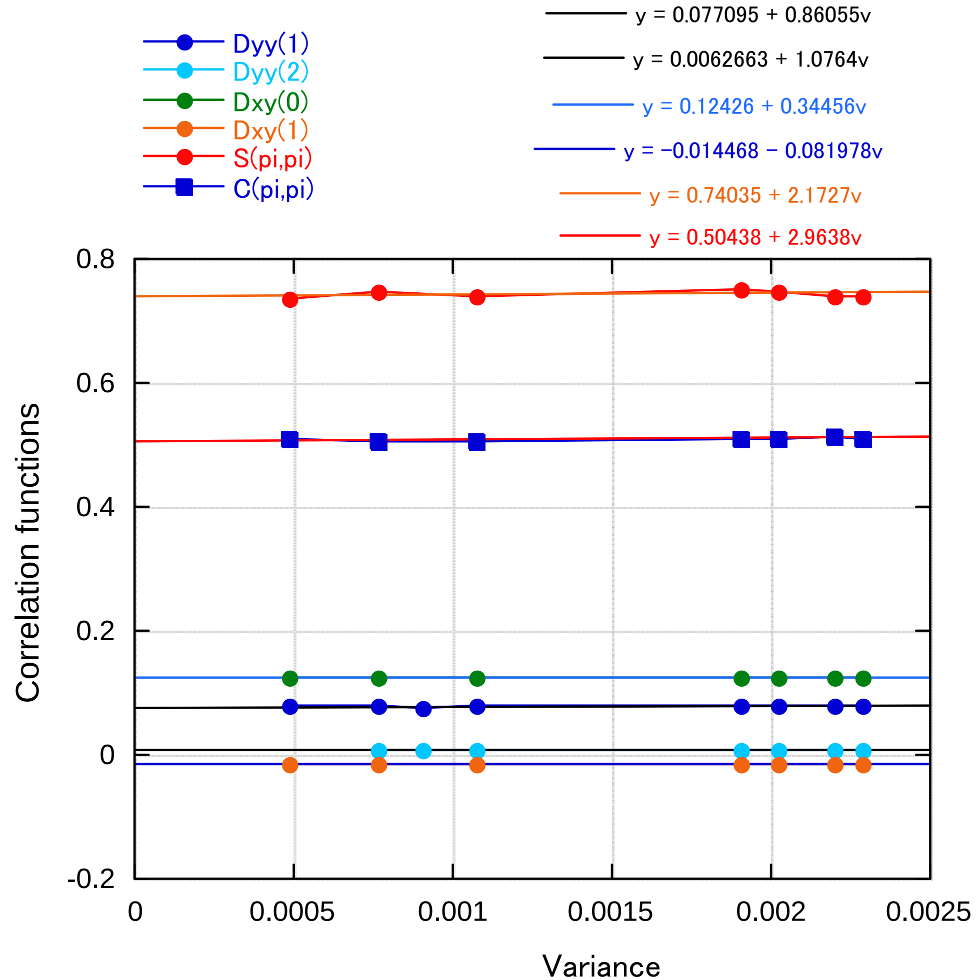


4x4 N_e= 10 U= 4

Examples of calculations I

4x4 N_e =10 U = 4 Correlation functions

CP-QMC



Examples of calculations II

Energy

Size	N_e	U	QMCD	VMC	CPMC	PIRG	QMC	Exact
4×4	10	4	-1.2237	-1.221(1)	-1.2238			-1.2238
4×4	14	4	-0.9836	-0.977(1)	-0.9831			-0.9840
4×4	14	8	-0.732(2)	-0.727(1)	-0.7281			-0.7418
4×4	14	10	-0.656(2)	-0.650(1)				-0.6754
4×4	14	12	-0.610(4)	-0.607(2)	-0.606			-0.6282
6×2	10	2	-1.058(1)	-1.040(1)				-1.05807
6×2	10	4	-0.873(1)	-0.846(1)				-0.8767
6×6	34	4	-0.921(1)	-0.910(2)		-0.920	-0.925	
6×6	36	4	-0.859(2)	-0.844(2)		-0.8589	-0.8608	

VMC: $\psi_\lambda^{(2)}$

4x4 Ne=10
U=10

Correlation function	QMCD	VMC	CPMC	Exact
$S(\pi,\pi)$	0.730(1)	0.729(2)	0.729	0.7327
$C(\pi,\pi)$	0.508(1)	0.519(2)	0.508	0.5064
$\Delta_{yy}(1)$	0.077(1)	0.076(1)		0.07685
$\Delta_{yy}(2)$	0.006(1)	0.006(1)		0.00624
$\Delta_{xy}(0)$	0.124(1)	0.120(2)		0.1221
$\Delta_{xy}(1)$	-0.015(1)	-0.015(1)		-0.0141
$s(0,0)$	0.529(1)			0.5331
$s(1,0)$	-0.091(1)			-0.0911
$c(0,0)$	0.329(1)			0.3263
$c(1,0)$	-0.0536(1)			-0.05394

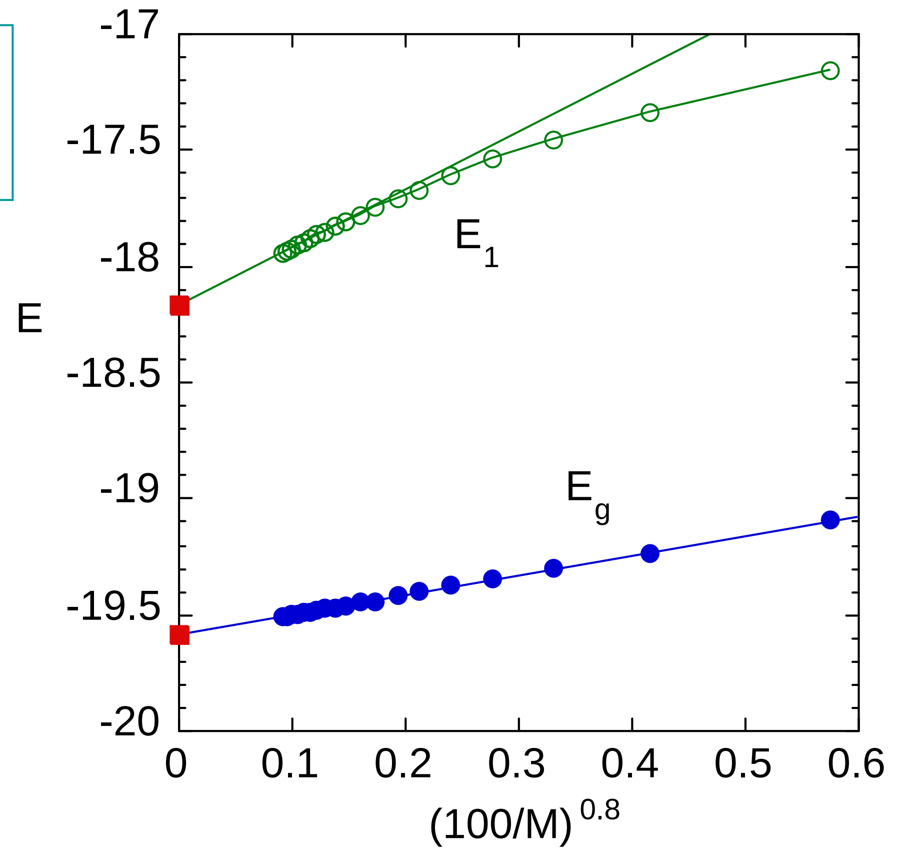
Excited states

The energies of excited states can be obtained by diagonalization.

Example

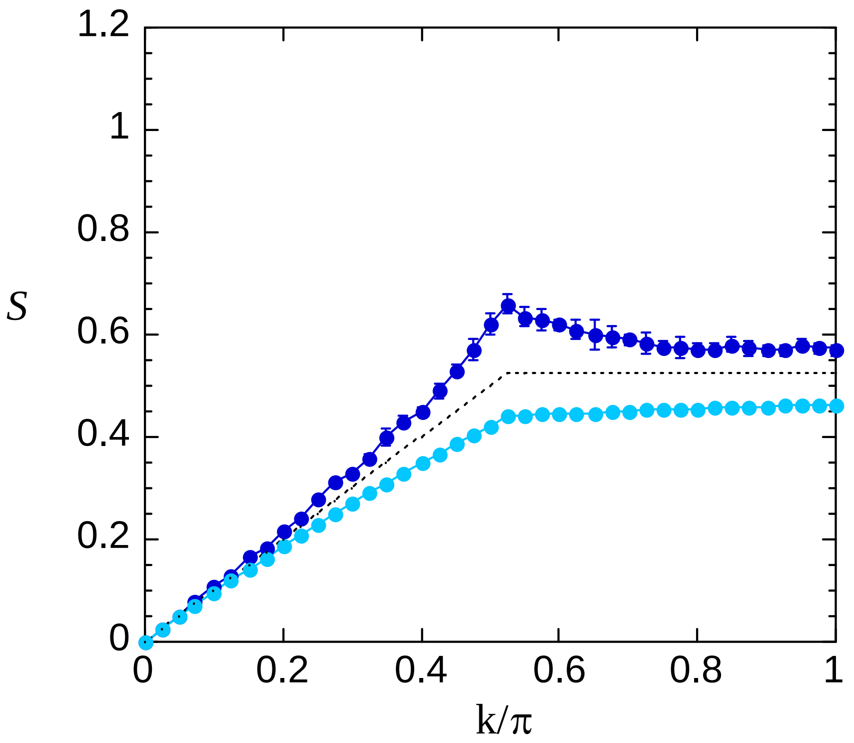
4x4 $N_e = 10$ $U = 4$
$E_g = -19.581$
$E_1 = -18.162$

(First excited state)

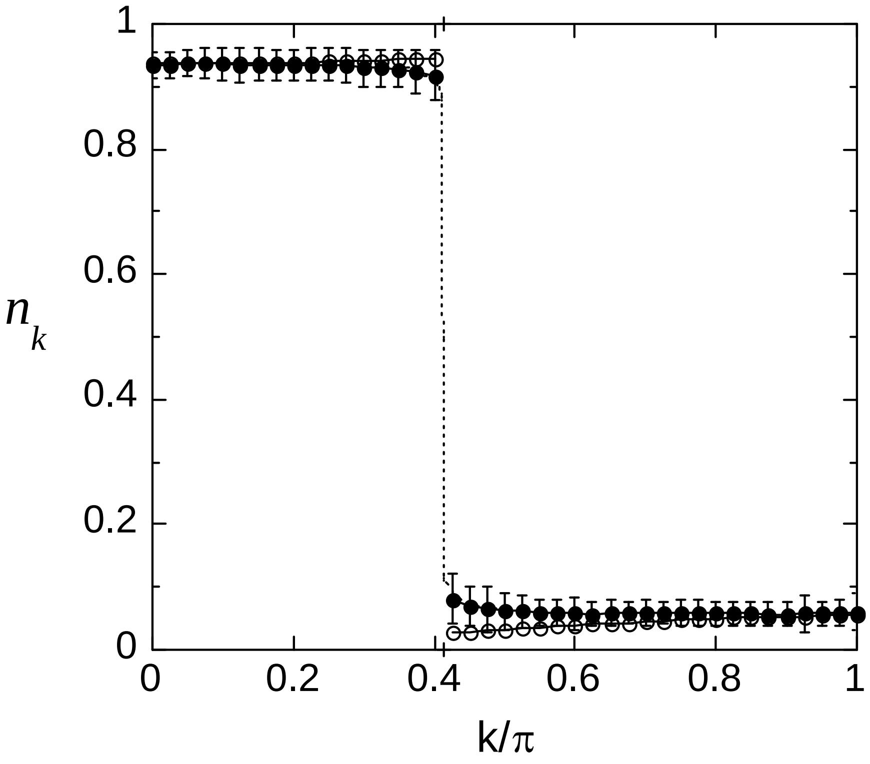


1D Hubbard Model

80 sites 66 electrons



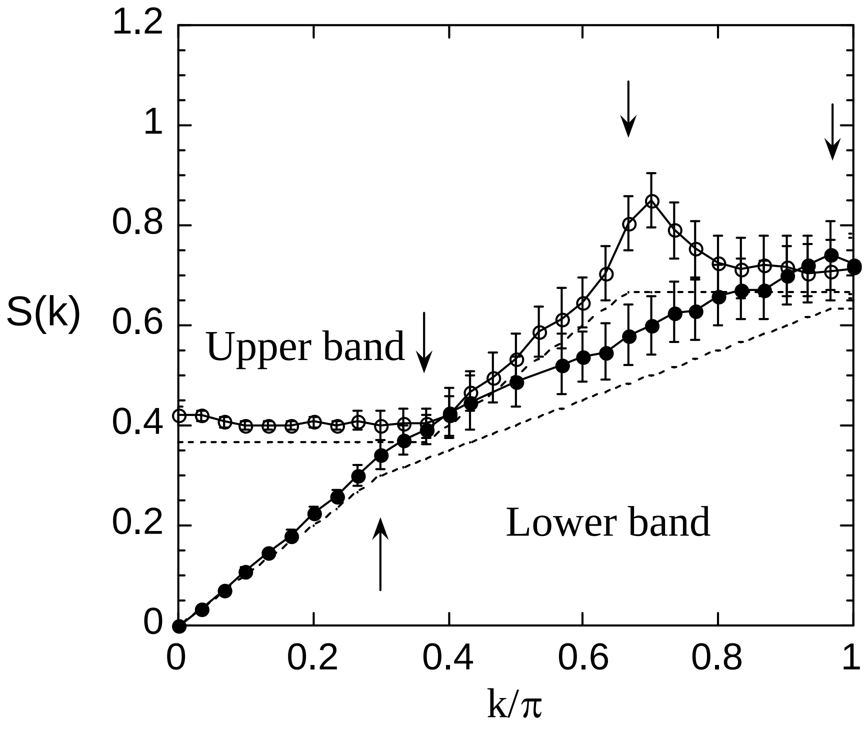
Spin correlation function S(k)

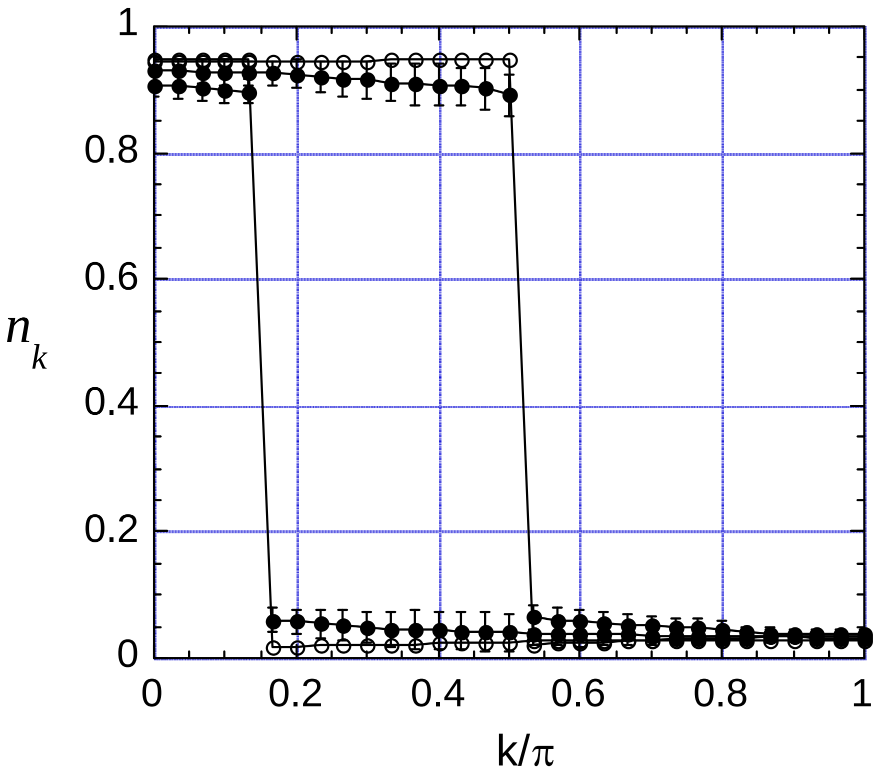


Momentum distribution

Ladder Hubbard Model

60x2 sites 80 electrons



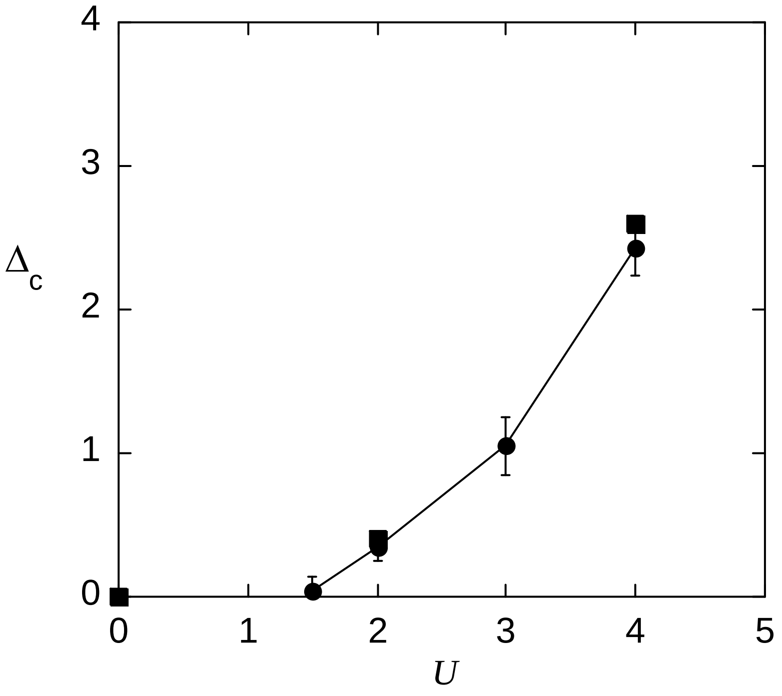


Ladder Hubbard: Charge gap

Charge gap at half-filling

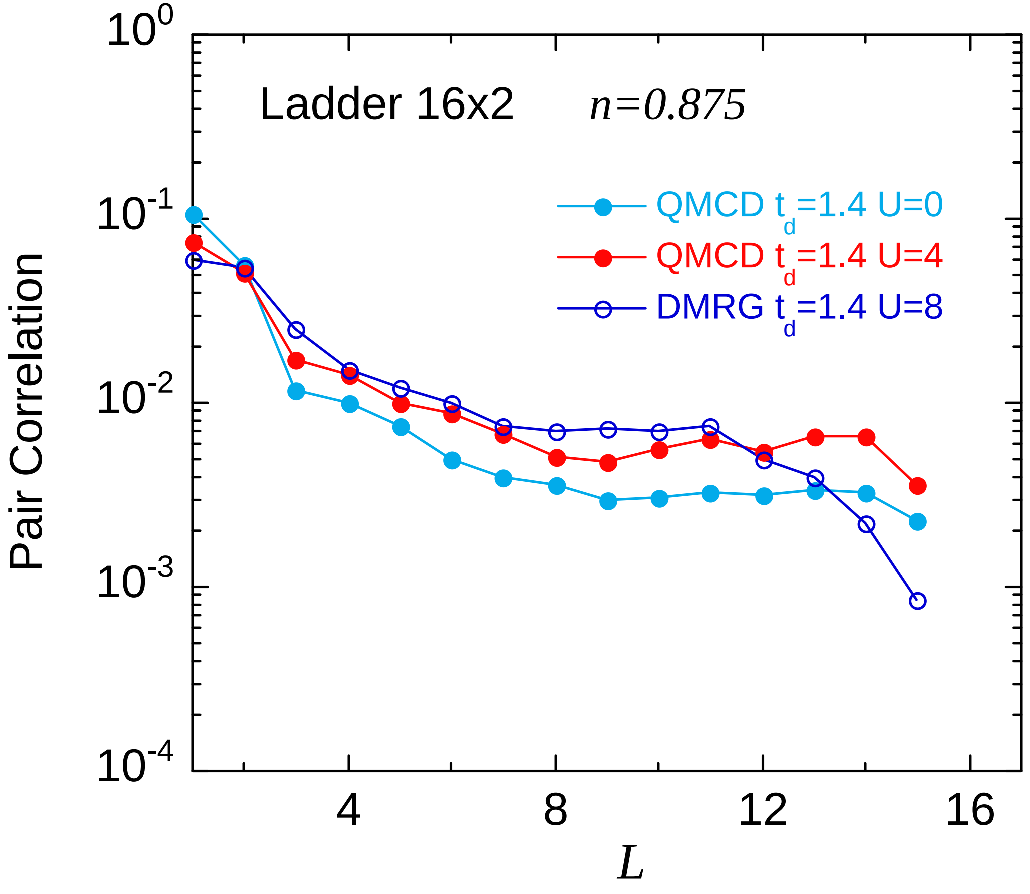
$$\Delta_c = E_g(N_e + 2) + E_g(N_e - 2) - 2E_g(N_e)$$

Comparison with DMRG



■ DMRG

Ladder Hubbard: Pair Correlation



ハバードモデルは超伝導を示すだろうか

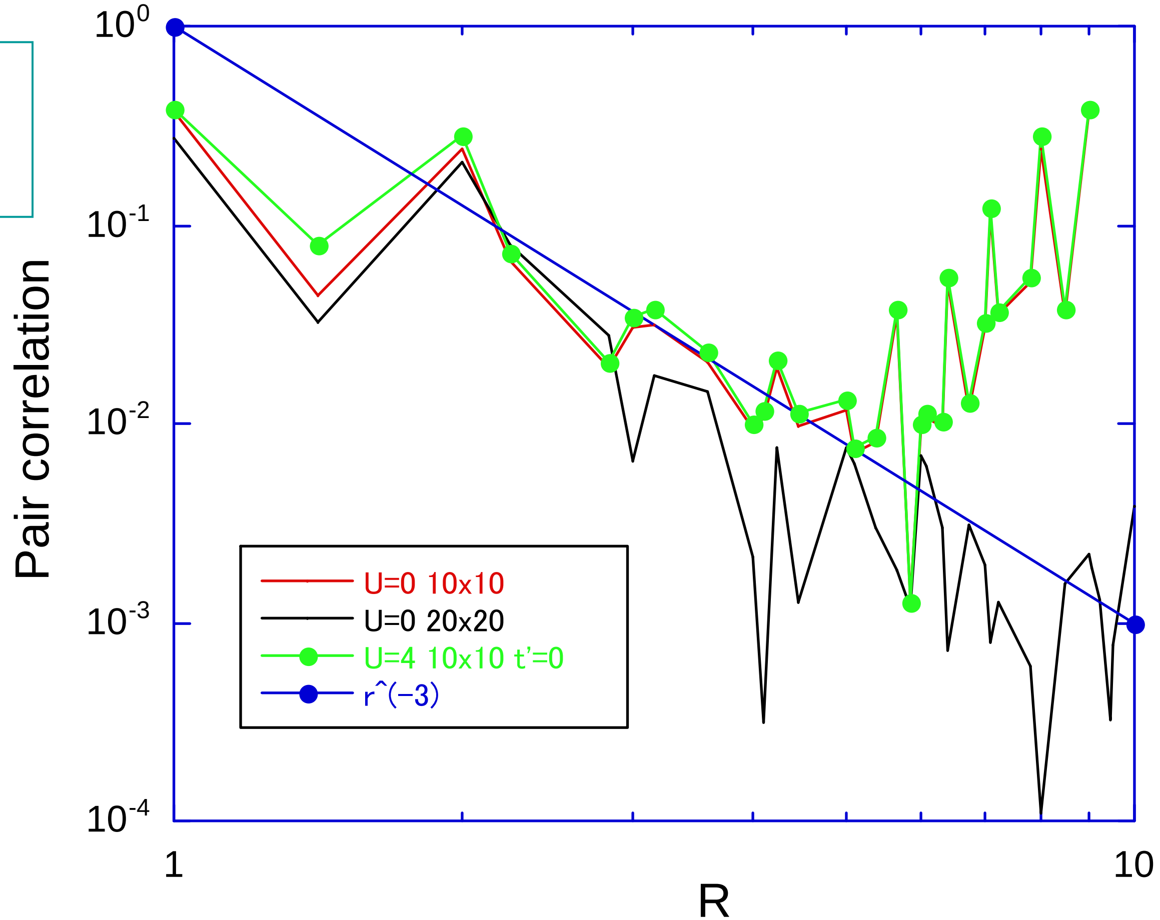
ハバードモデルによ高温超伝導を説明できるか

ペアー相関関数

10x10 Hubbard model Ne=82 U= 4 t’= 0 QMD

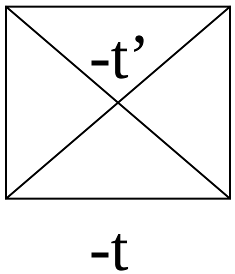
Pair相関は
早く減衰する

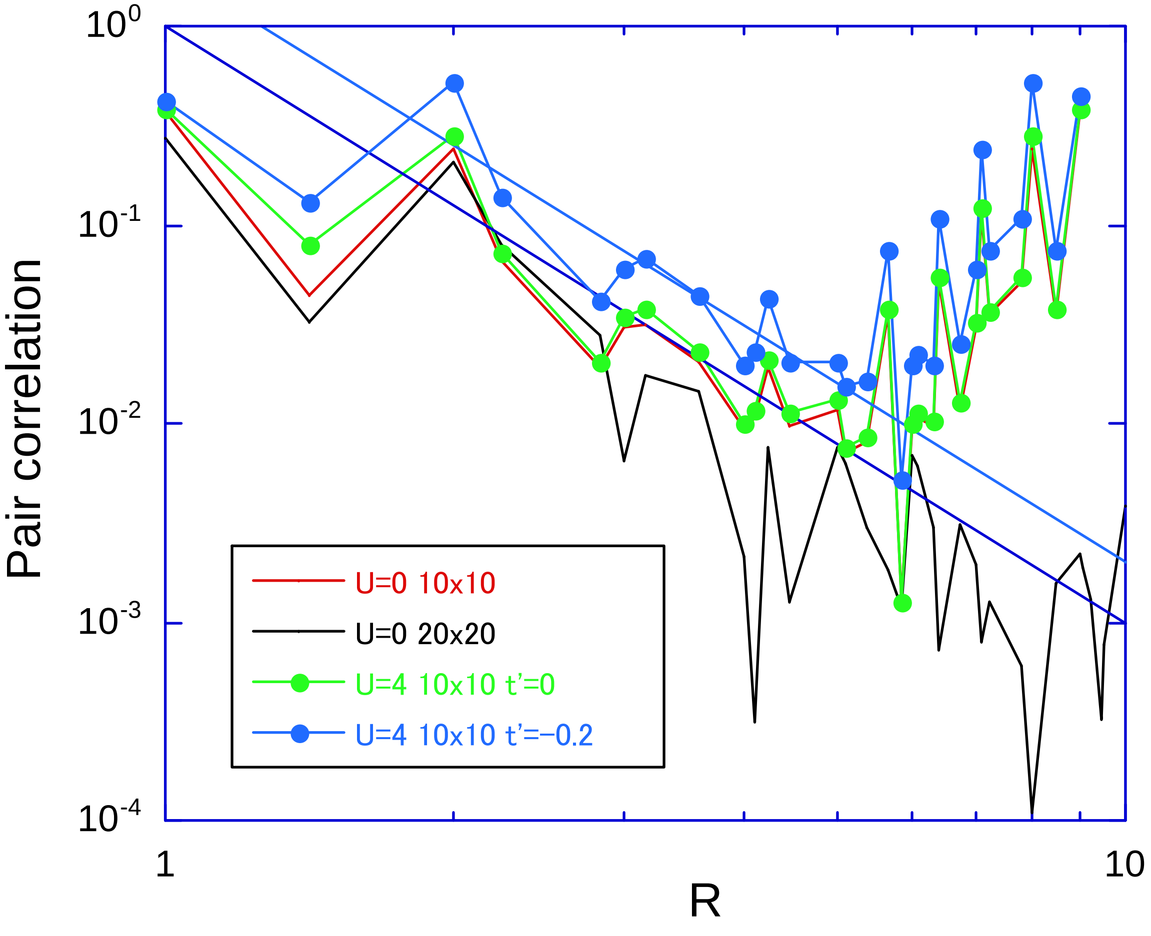
~1/r^3



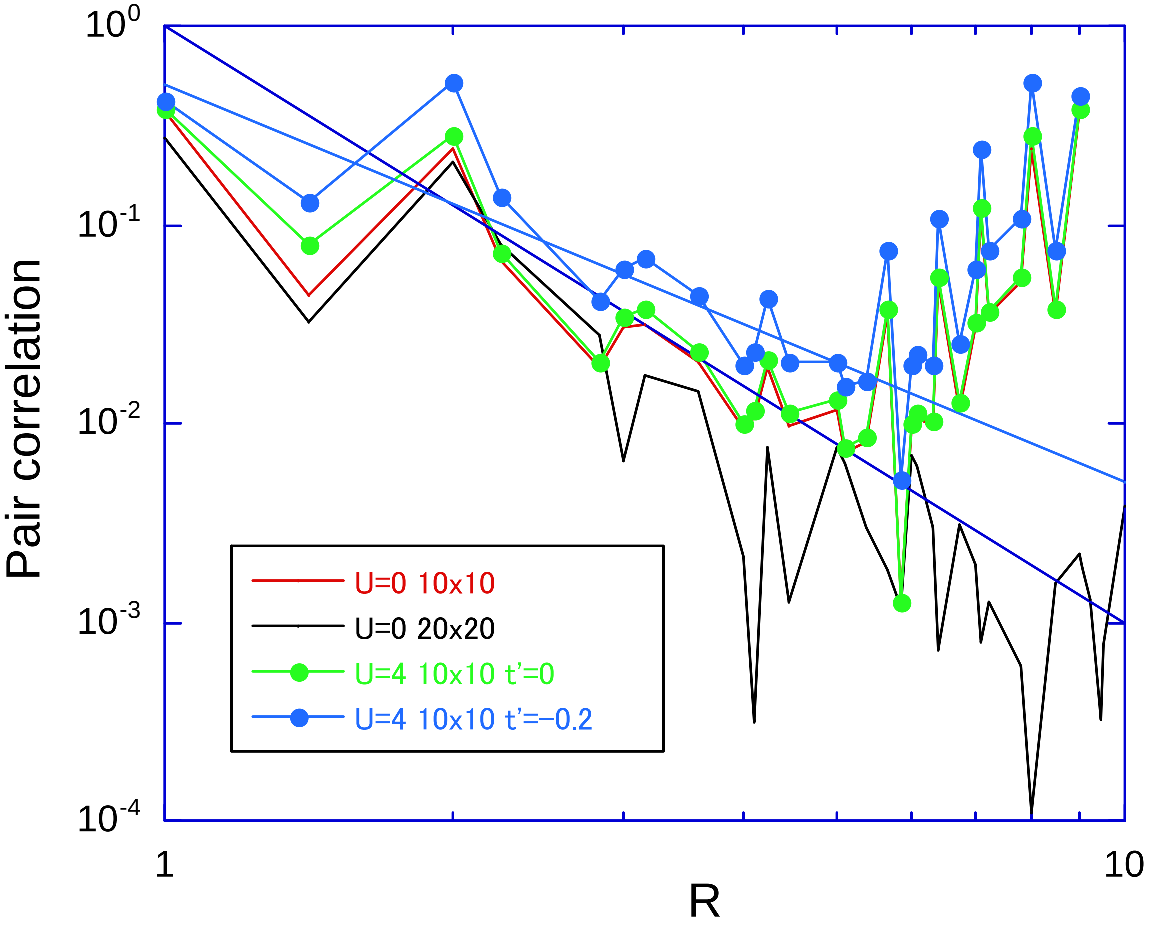
Aimi et al. JPSJ (2007) U=6

10x10 Hubbard model Ne=82 U= 4 t’= -0.2 QMD





10x10 Hubbard model Ne=82 U= 4 t’= -0.2 QMD



ハバードモデルにおけるペアー相関

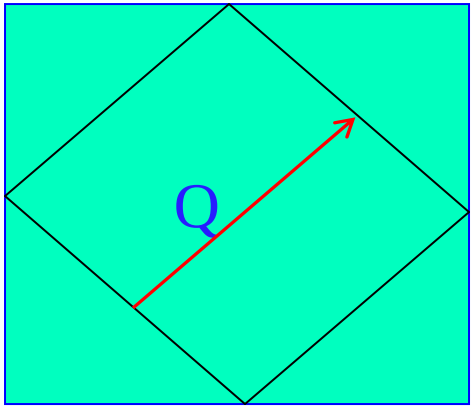
2次元ハバードモデルの超伝導相関

10x10 格子　超伝導相関はあまり増大しない。
次近接トランスファーt’< 0により増大
van Hove singularityによる
状態密度のよりピーク

大きい格子上での計算が必要

Long-range order in two dimensions

t'= 0

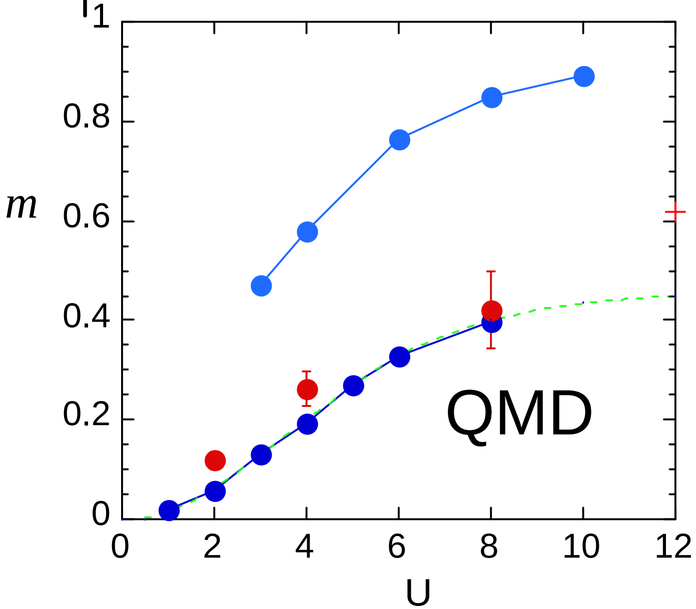


Half-filling at T= 0

Antiferromagnetic long-range order

Staggered Magnetization *m > 0*

$$m = \left| \frac{1}{N} \sum_j (-1)^j \langle n_{j\uparrow} - n_{j\downarrow} \rangle \right|$$



Hole-doped case

Is there any long-range order
in two space dimensions?

Kosterlitz-Thouless transition

2D $L \times L$ *System* Kosterlitz-Thouless transition

Susceptibility $\chi \sim \xi^{2-\eta}$ $\eta = 0$ $(T = 0)$ $\xi \approx L$

$= 1/4$ $(T = T_c)$ 相関長

Kosterlitz: J. Phys. C7, 1046 (1974)

$\chi \sim L^2$ *at T= 0*

Suceptibilities

2D LxL System $N = L \times L$

$Q=(\pi,\pi)$

$$\chi^{-+}(Q) = \int_0^{\beta} d\tau \langle T_\tau S_Q^-(\tau) S_{-Q}^+(0) \rangle$$

Spin susceptibility

$$\chi_{pair} = \frac{1}{N} \sum_{kk'} z_k z_{k'} \int_0^{\beta} d\tau \langle T_\tau b_{k'}(\tau) b_k^+(0) \rangle$$

Pair susceptibility

Size dependence in the non-interacting system

$$\chi^{-+}(Q) \sim (\ln L)^2$$

for t'= 0 half-filled band

$$\chi_{pair} \sim \ln L$$

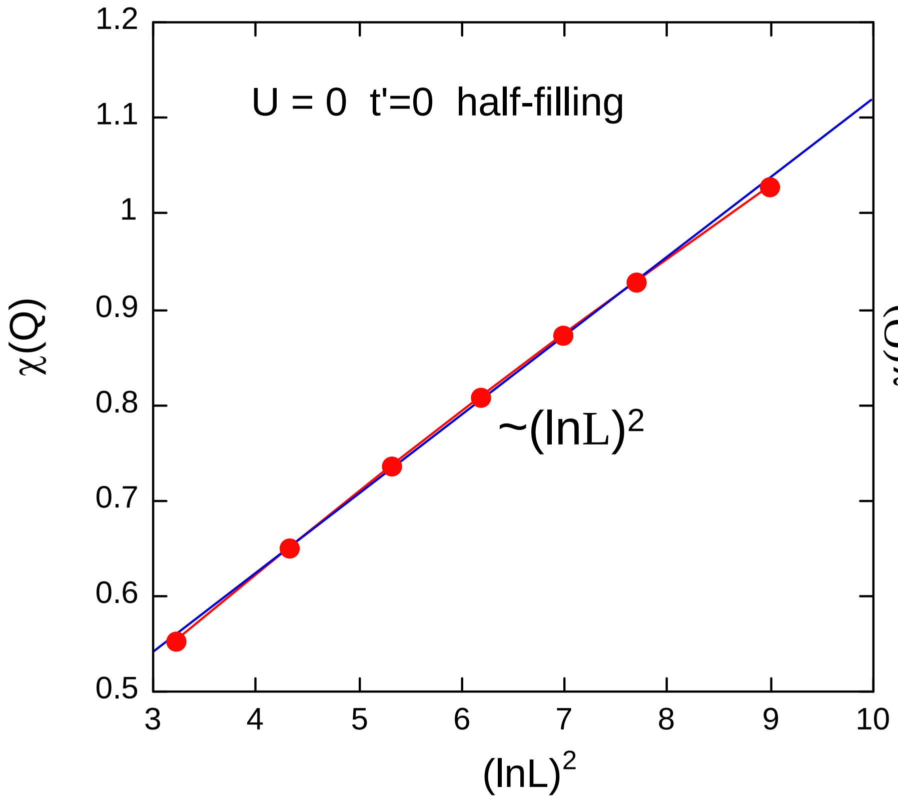
Size dependence of χ(Q)

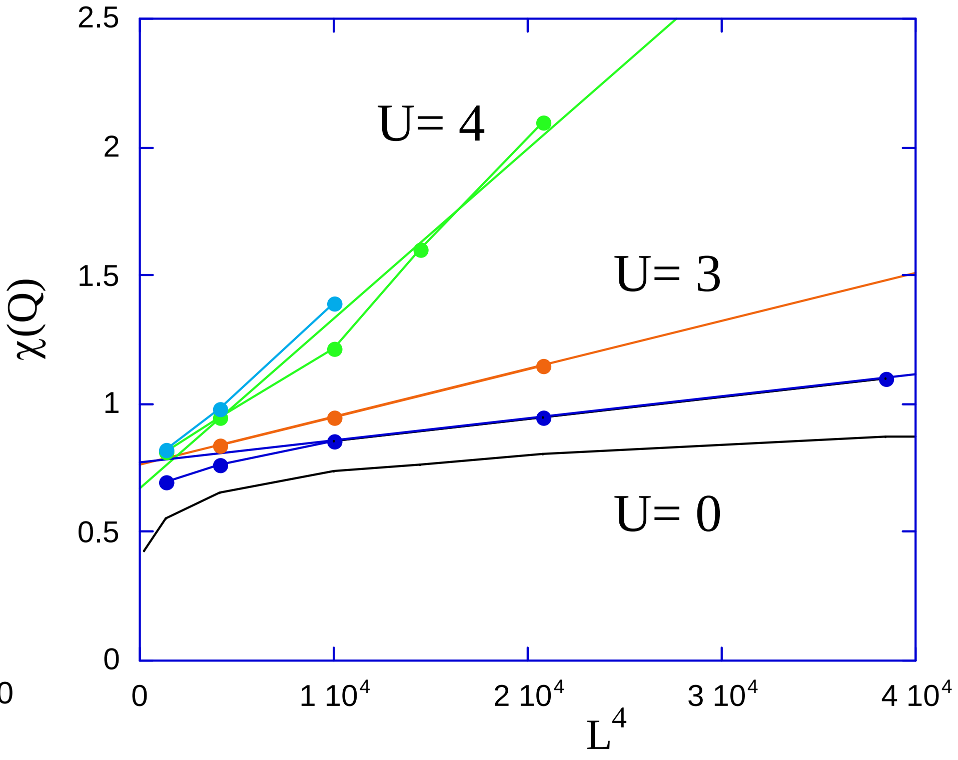
Non-interacting case

Half-filled t'=0

Quantum Monte Carlo Diagonalization

$$\chi^{-+}(Q) \sim L^4 \quad \text{if } U > 0$$





Pair susceptibility

$$\chi_{pair} = -\frac{1}{g}\frac{1}{N}\sum_{i,\mu(=x,y)} a_\mu \left\langle c^+_{i+\mu\uparrow} c^+_{i\downarrow} \right\rangle = -\frac{1}{g}\frac{1}{N}\sum_{i,\mu} a_\mu \left\langle c^+_{i+\mu} d_i \right\rangle$$

$$a_x = 1, a_y = -1$$
$$c_i = c_{i\uparrow}, d_i = c^+_{i\downarrow}$$

(nearest neighbor)

線形応答

レベル間隔とサイズ依存性

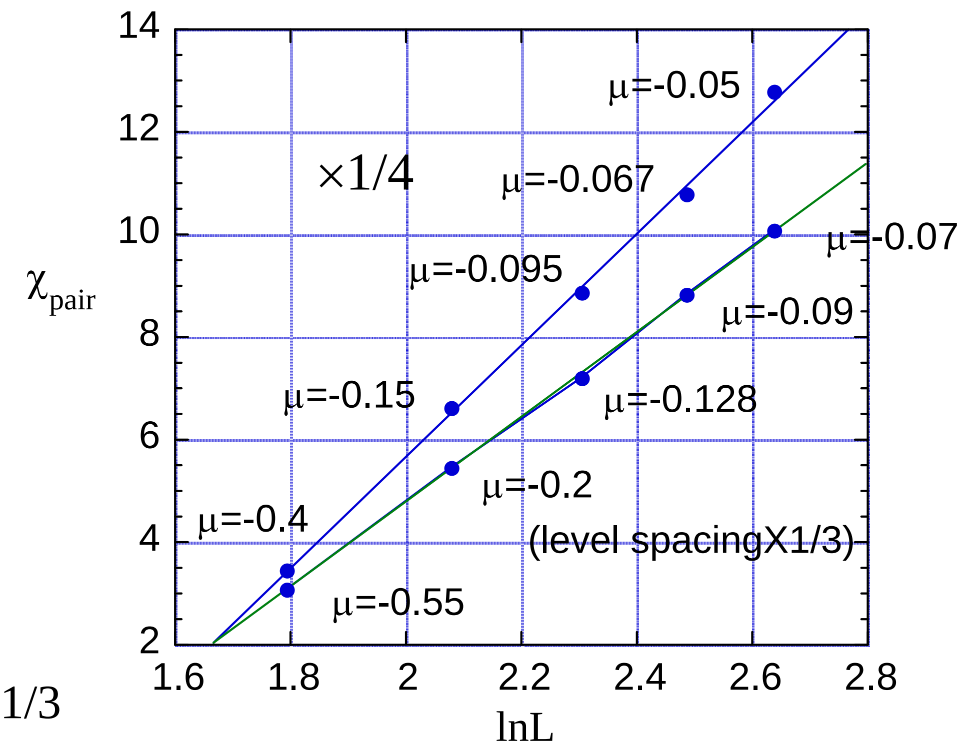
サイズLに依存

χ_{pair}はオーダー1の量だが、
サイズと共に増大する。

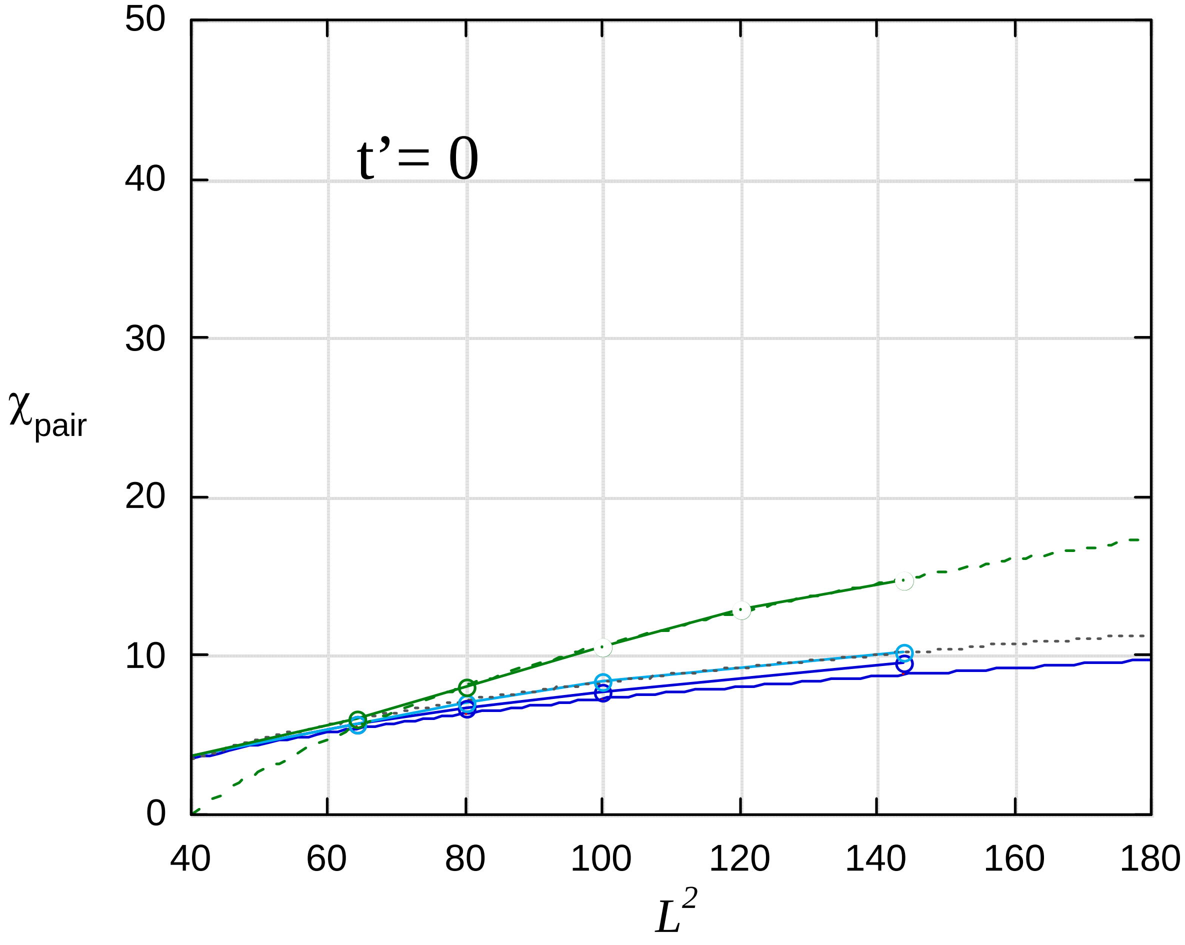
対数的に増大∼ln$L$

μ 1/3

2D Non-interacting case



Size dependence of χ_{pair}



ln依存性?

Long-range order and size dependence

Susceptibility

$$N = L^2$$

$\chi \sim N^2$ — Long-range order $\chi^{-+}(Q)$

Staggered susceptibility at half-filling

$\sim N$ — Quasi long-range order

Kosterlitz-Thouless transition

Pair susceptibility χ_{pair} ?

$\sim N^0(\log N)$ — No long-range order

No-interacting system

Summary

Quantum Monte Carlo methods without negative sign

$$\psi = e^{-\tau H} \approx \left(e^{-\Delta\tau K} e^{-\Delta\tau V}\right)^M \psi_0$$

- Quantum Monte Carlo diagonalization
- Constrained-path Monte Carlo method 並列化容易

Does the 2D Hubbard model exhibit superconductivity?

超伝導相関が大きく増大するかどうかは微妙

バンド構造の効果 t’

K-T転移として可能性がある