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Macroscopic Distinguishability Between Quantum States Defining Different Phases of Matter

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The Aim of the Research

Characterizing regions of criticality that define (Quantum and Thermal) Phase Transitions

How?

Studying the fidelity between two ground/equilibrium states corresponding to two slightly different values of the parameters

Quantum Phase Transitions

Defined by the Regions of Criticality:

- Non-analyticity of the ground state energy density
- Existence of Gapless Excitations
- Diverging Correlation Lengths
- Extremal Behavior of Entanglement Measures
- Non-vanishing Geometric (Berry) Phases
- Existence of the Order Parameter

Quantum State Distinguishability

Fidelity Function: $F(\hat{\rho}_1, \hat{\rho}_2) = \mathrm{Tr}\sqrt{\sqrt{\hat{\rho}_1}\hat{\rho}_2\sqrt{\hat{\rho}_1}}$

Pure states: $F(|\psi_1\rangle, |\psi_2\rangle) = |\langle\psi_1|\psi_2\rangle|$

Ground States: $|g\rangle \equiv |g(q)\rangle$ $|\tilde{g}\rangle \equiv |g(\tilde{q})\rangle$ $\tilde{q} \equiv q + \delta q$

$$F = |\langle g(q)|g(\tilde{q})\rangle|$$

The XY Spin Chain

- Hamiltonian: $\hat{H}(\gamma,\lambda) = -\sum_{i=-M}^{M}\left(\frac{1+\gamma}{2}\hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + \frac{1-\gamma}{2}\hat{\sigma}_i^y\hat{\sigma}_{i+1}^y + \frac{\lambda}{2}\hat{\sigma}_i^z\right).$

- Diagonalized: $\hat{H}(\gamma,\lambda) = \sum_{k=-M}^{M}\Lambda_k(\hat{b}_k^\dagger\hat{b}_k - 1).$

- Excitations: $\Lambda_k = \sqrt{\varepsilon_k^2 + \gamma^2\sin^2\frac{2\pi k}{N}}, \qquad \varepsilon_k = \cos\frac{2\pi k}{N} - \lambda.$

- Regions of Criticality:

  $\gamma = 0$ and $\lambda \in (-1,1)$ XX - criticality

  $\lambda = \pm 1$ XY - criticality

Ground State

$$|g(\gamma,\lambda)\rangle = \bigotimes_{k=1}^{M} \left(\cos\tfrac{\theta_k}{2}|0\rangle_k|0\rangle_{-k} - i\sin\tfrac{\theta_k}{2}|1\rangle_k|1\rangle_{-k}\right).$$

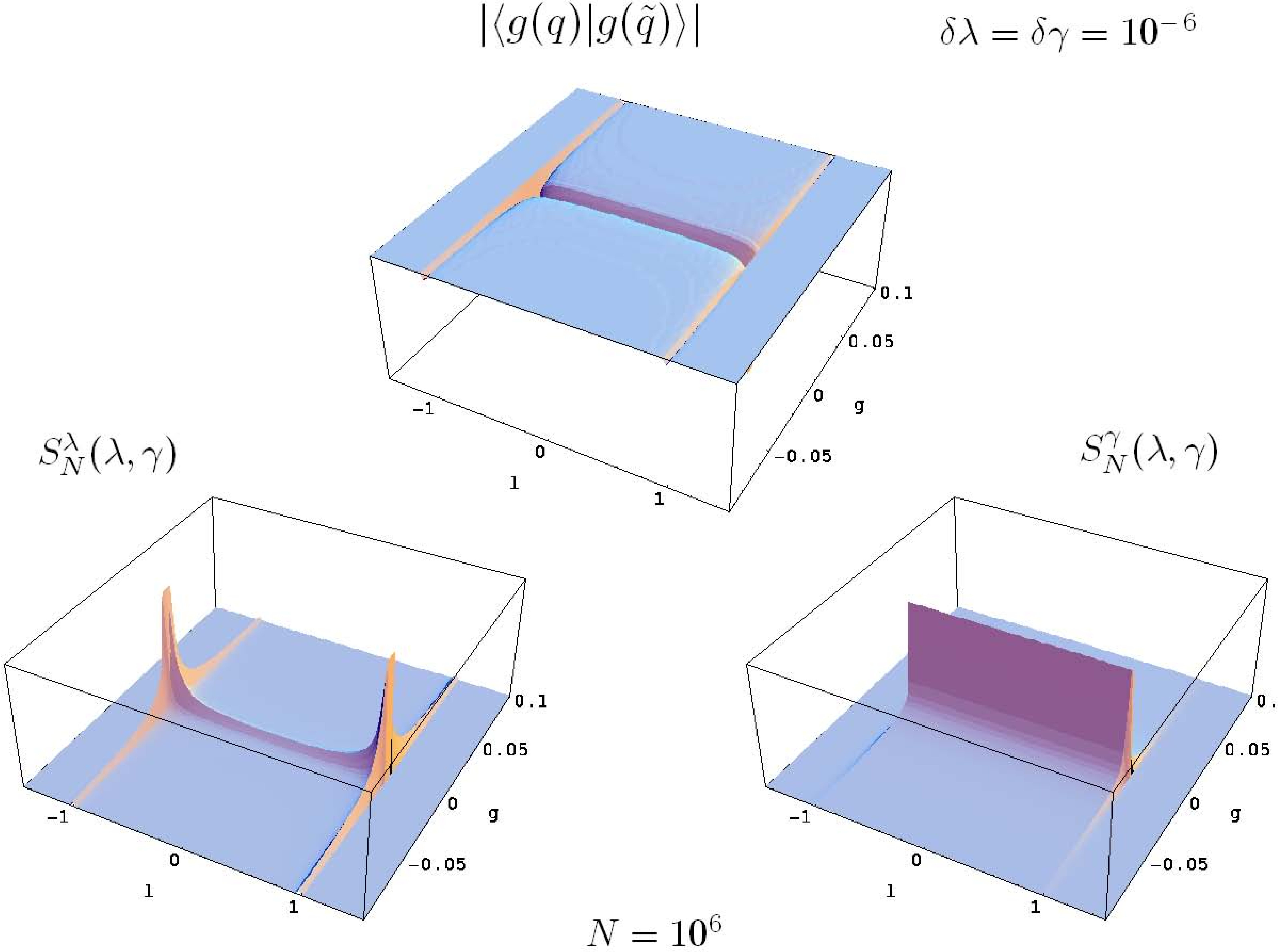
$$\cos\theta_k = \varepsilon_k/\Lambda_k.$$

Fidelity

$$|\langle g(q)|g(\tilde{q})\rangle| = \prod_{k=1}^{M} |\cos\tfrac{\theta_k-\tilde{\theta}_k}{2}|.$$

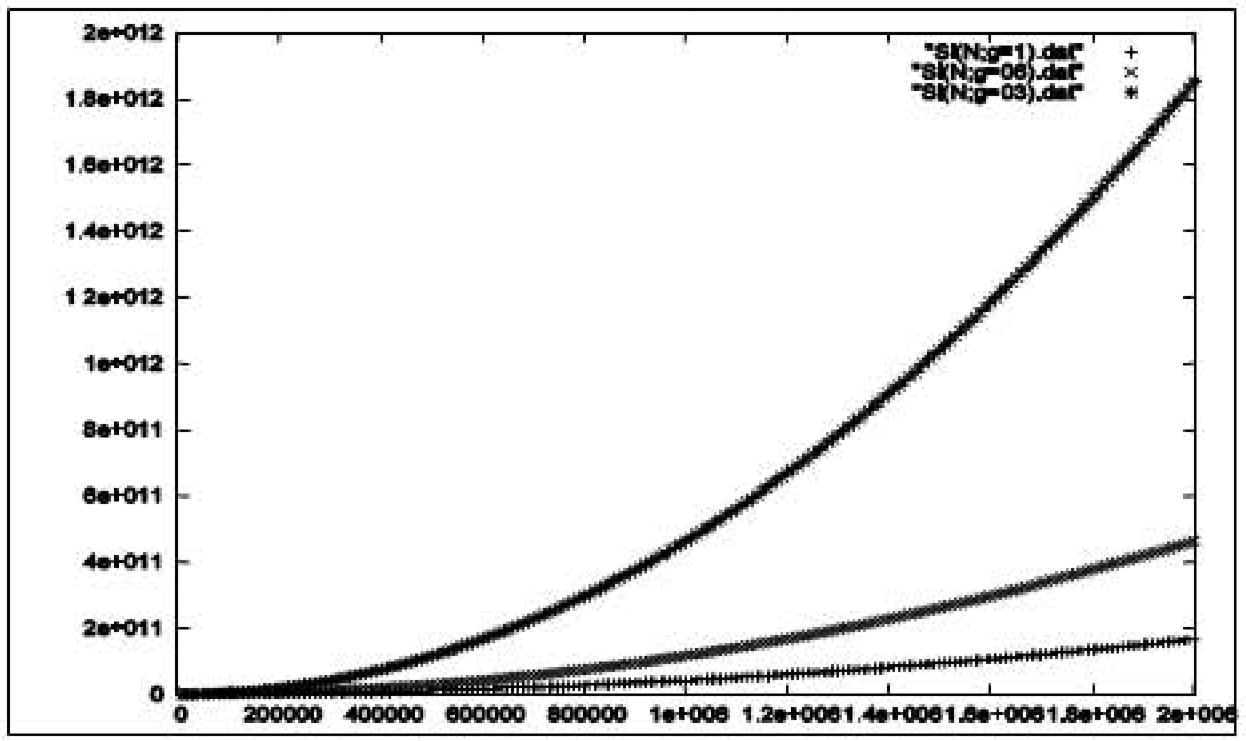
"Rates of Change"

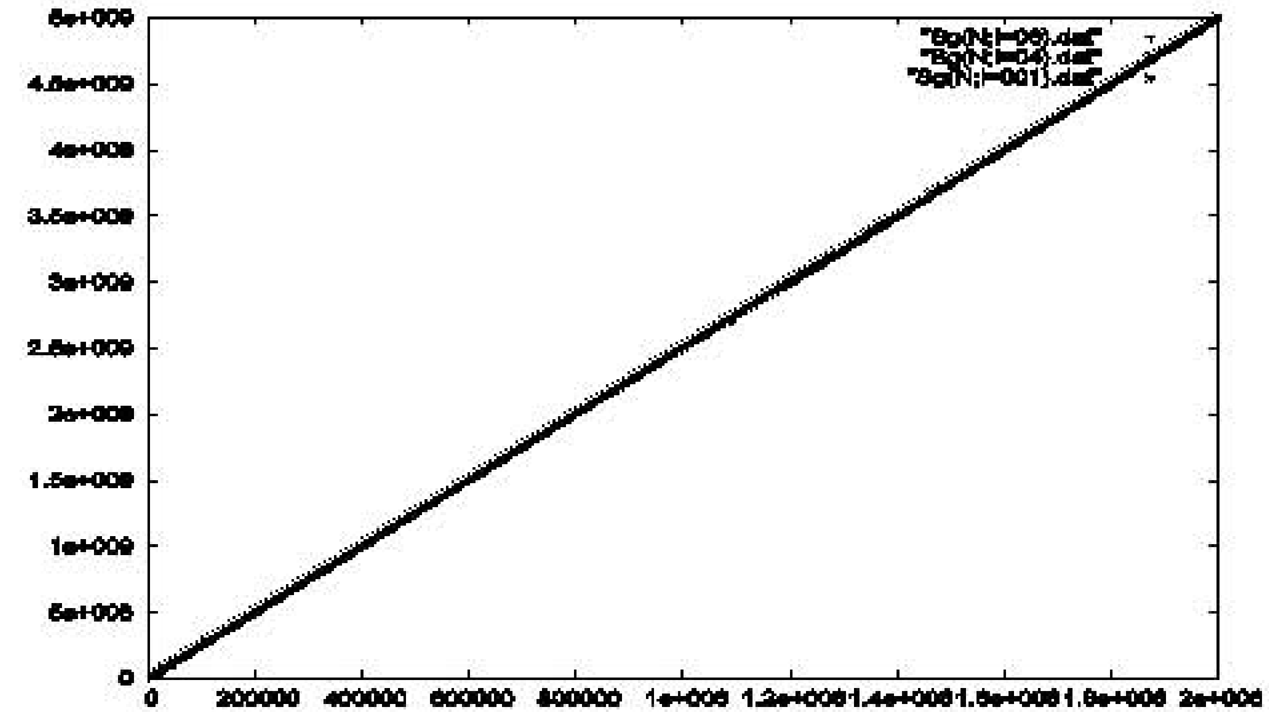
$$S_N^{\lambda}(\lambda,\gamma) \equiv \sum_{k=1}^{M}\left(\tfrac{\partial\theta_k}{\partial\lambda}\right)^2, \qquad S_N^{\gamma}(\lambda,\gamma) \equiv \sum_{k=1}^{M}\left(\frac{\partial\theta_k}{\partial\gamma}\right)^2.$$



$|\langle g(q)|g(\tilde{q})\rangle|$
$\delta\lambda = \delta\gamma = 10^{-6}$
0.1
0.05
0
g
−0.05
−1
0
1
1
$S_N^{\lambda}(\lambda, \gamma)$
$S_N^{\gamma}(\lambda, \gamma)$
0.1
0.05
0
g
−0.05
−1
0
1
1
0.1
0.05
0
g
−0.05
−1
0
1
1
$N = 10^6$

Scaling Behavior





$$S_N^{\lambda}(\lambda_c = 1, \gamma = \{1, 0.6, 0.3\}).$$

$$S_N^{\gamma}(\lambda = \{0.6, 0.4, 0.01\}, \gamma = 10^{-4}).$$

quadratic behavior

linear behavior

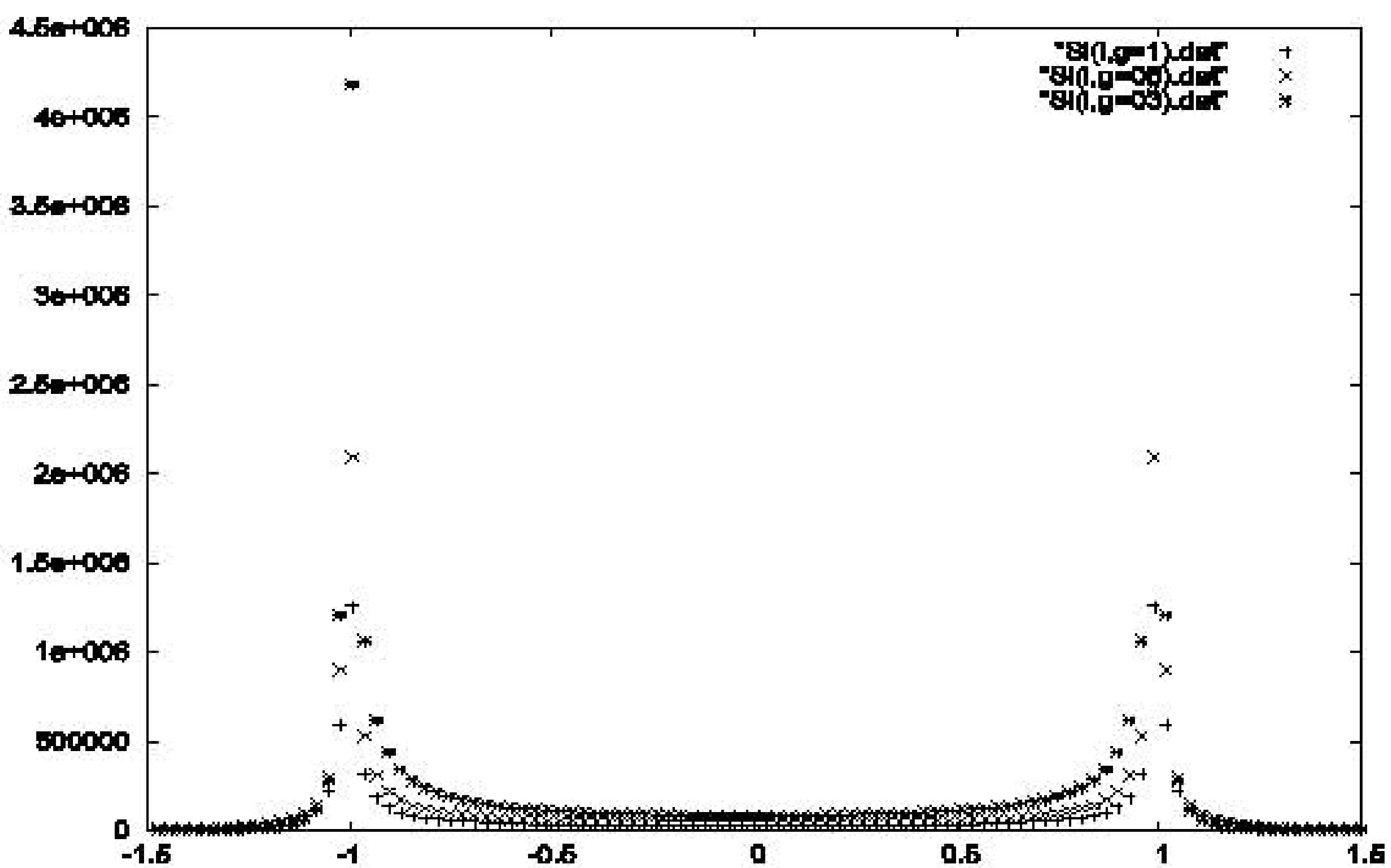
Asymptotic Behavior

$$S_N^{\lambda}(\lambda,\gamma) \propto \frac{a(\gamma,N)}{|1-\lambda|^{\alpha(\gamma,N)}}.$$

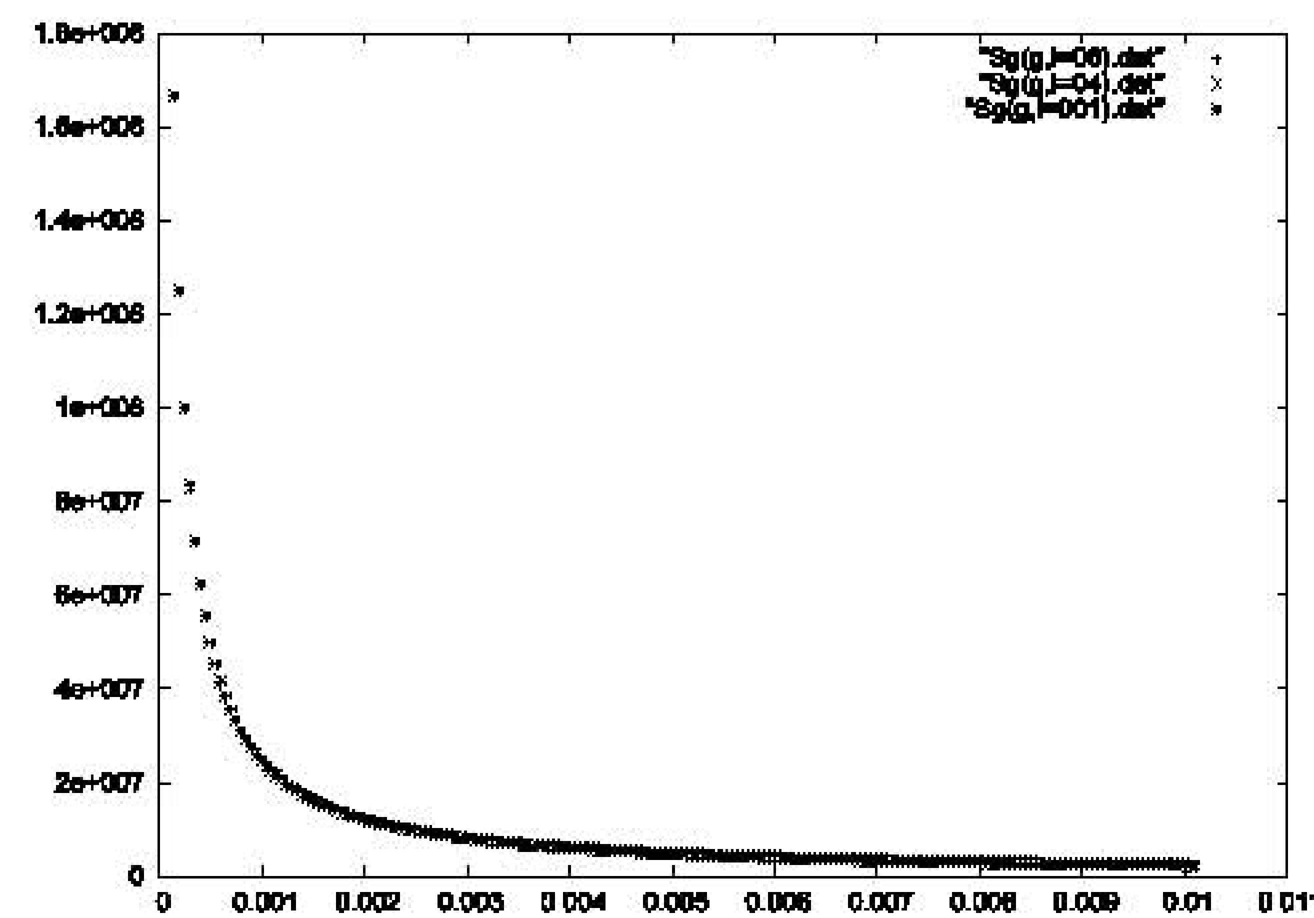
$$S_N^{\gamma}(\lambda,\gamma) \propto \frac{b(\lambda,N)}{\gamma^{\beta(\lambda,N)}}.$$

Vicinity of $\lambda = \pm 1$

Vicinity of $\gamma = 0$



$S_N^{\lambda}(\lambda, \gamma = \{1, 0.6, 0.3\})$



$S_N^{\gamma}(\lambda = \{0.6, 0.4, 0.01\}, \gamma)$

Orthogonality Catastrophe

Two mechanisms of "orthogonalization":

- infinite number of sub-systems (Anderson)
- different structure of ground states (in vicinity of QPT)

Loschmidt Echo

$$L(t) = |\langle \varphi_g(t) | \varphi_e(t) \rangle|^2$$

Density of States: $$D(\omega; q, \tilde{q}) \equiv \langle g(\tilde{q}) | \delta(\omega - \hat{H}(q)) | g(\tilde{q}) \rangle$$

$$—\langle g(q) | g(\tilde{q}) \rangle|^2 = 1 - \int_{E_1}^{\infty} D(\omega) d\omega$$

$$| \int_{-\infty}^{+\infty} D(\omega) e^{-i\omega t} d\omega |^2 = L(q, t).$$

Related Results

- Fermi Systems and Graphs
- Bose-Hubbard model
- Orders beyond Landau-Ginzburg-Wilson theory (topologically ordered QPT, MPS and Kosterlitz-Thouless)
- XXZ Heisenberg model
- QPTs and the renormalization group flaws

LGW Symmetry Breaking QPTs

- Hamiltonian: $\hat{H}(q) = \hat{H}_0 - h(q)\hat{S}$

- Fidelity:

$$\begin{aligned} F^2(q, q+dq) &= |\langle g(q)|g(q+dq)\rangle|^2 \approx |\langle g|(|g\rangle + |\partial g\rangle dq + \frac{1}{2}|\partial^2 g\rangle dq^2)|^2 \\ &= 1 + \langle \partial g|(|g\rangle\langle g| - \hat{I})|\partial g\rangle dq^2 = 1 - dq^2 \sum_{n>0} \frac{|\langle g|\hat{S}|n\rangle|^2}{(E_n - E_0)^2} \end{aligned}$$

- Susceptibility:

$$\begin{aligned} \chi_\infty &= \int_0^\infty d\tau \tau [\langle g|\hat{S}(\tau)\hat{S}|g\rangle - \langle g|\hat{S}|g\rangle^2] \\ &= \int_0^\infty d\tau \tau [\sum_{n>0} e^{-(E_n - E_0)\tau} |\langle g|\hat{S}|g\rangle|^2] = \sum_{n>0} \frac{|\langle g|\hat{S}|g\rangle|^2}{(E_n - E_0)^2} \end{aligned}$$

Differential Geometry and Berry Phases

Quantum Geometric Tensor:

$$\begin{aligned} Q_{\mu\nu} &= \langle \partial_\mu g(q) | \partial_\nu g(q) \rangle - \langle \partial_\mu g(q) | g(q) \rangle \langle g(q) | \partial_\nu g(q) \rangle \\ &= \sum_{n>0} \frac{\langle g(q) | \partial_\mu \hat{H}(q) | g(q) \rangle \langle g(q) | \partial_\nu \hat{H}(q) | g(q) \rangle}{[E_n(q) - E_0(q)]^2} \end{aligned}$$

Reimannian Metric Tensor:

$g_{\mu\nu} = \mathrm{Re}[Q_{\mu\nu}]$ where $ds^2 = \sum_{\mu\nu} g_{\mu\nu} dq^\mu dq^\nu = 2(1 - F(q, q+dq))$

Berry Curvature 2 - Form: $F_{\mu\nu} = \mathrm{Im}[Q_{\mu\nu}] = \partial_\mu A_\nu - \partial_\nu A_\mu$

Berry Adiabatic Connection: $A_\mu = \langle g | \partial_\mu g \rangle$

Thermal Phase Transitions

Thermal States ($T > 0$): $\hat{\rho}(q,T) = \frac{1}{Z} e^{-\beta \hat{H}(q)}$ (q,T) generalized parameter

$$F(\hat{\rho}_1,\hat{\rho}_2) = \mathrm{Tr}\sqrt{\sqrt{\hat{\rho}_1}\hat{\rho}_2\sqrt{\hat{\rho}_1}} \leq \sum_i \sqrt{p_1(i|\hat{A})p_2(i|\hat{A})} = F_c(\{p_1(i|\hat{A})\},\{p_2(i|\hat{A})\})$$

$$F(\hat{\rho}_1,\hat{\rho}_2) = \frac{Z(\hat{\hat{H}})}{\sqrt{Z(\hat{\hat{H}}-\Delta h\hat{S})Z(\hat{\hat{H}}+\Delta h\hat{S})}} \quad \text{for} \quad [\hat{H},\hat{S}] = 0$$

$$F|_{h=\Delta h} \simeq e^{-\frac{1}{2}\beta\chi(0)\Delta h^2}$$

where $\chi(0) = \beta\langle\hat{S}^2\rangle$ is the thermodynamic susceptibility.

The Uhlmann geometric phase given by $H - F$ where:

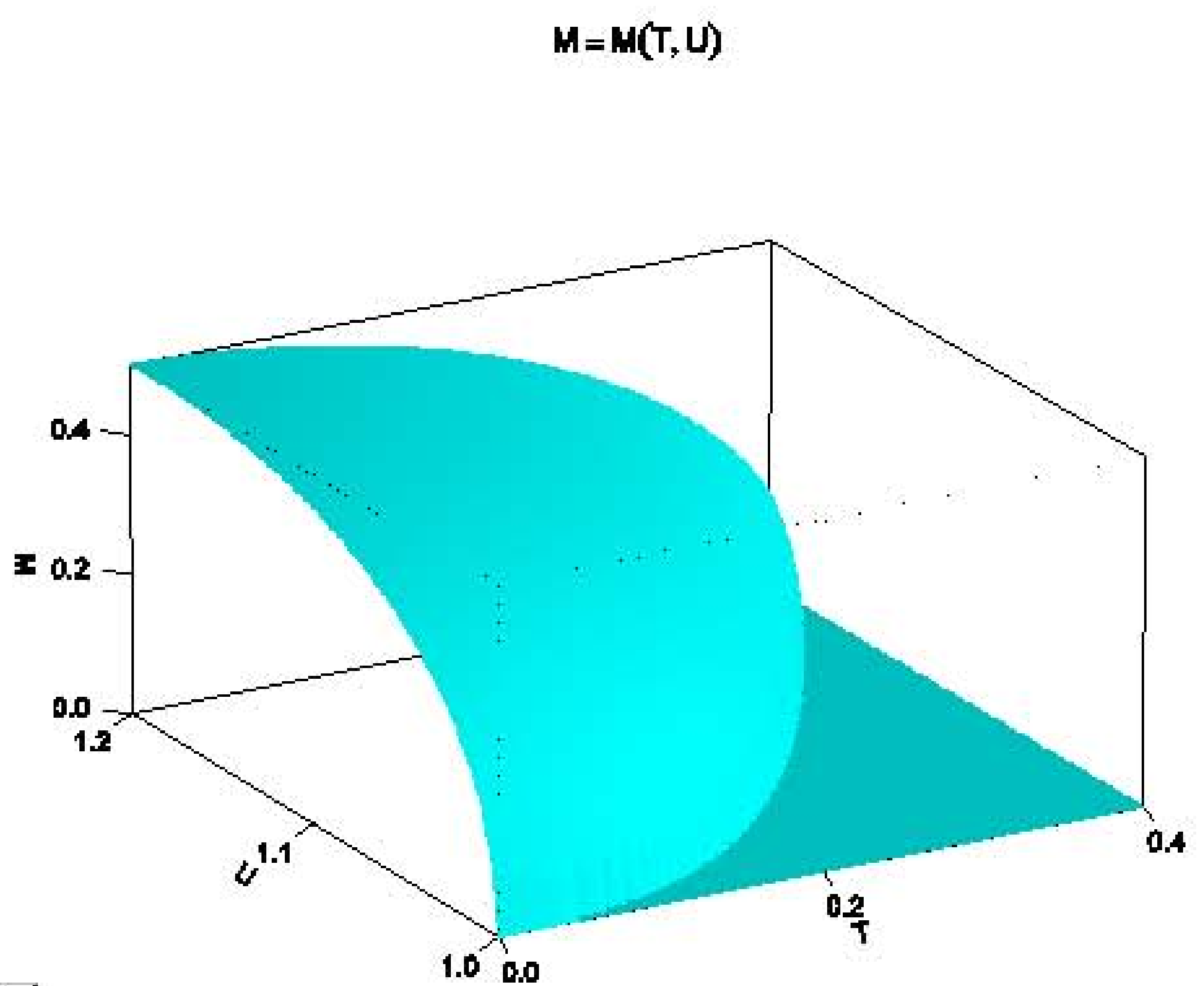
$$H(\hat{\rho}_1,\hat{\rho}_2) = \mathrm{Tr}\left[\sqrt{\hat{\rho}_1}\sqrt{\hat{\rho}_2}\right]$$

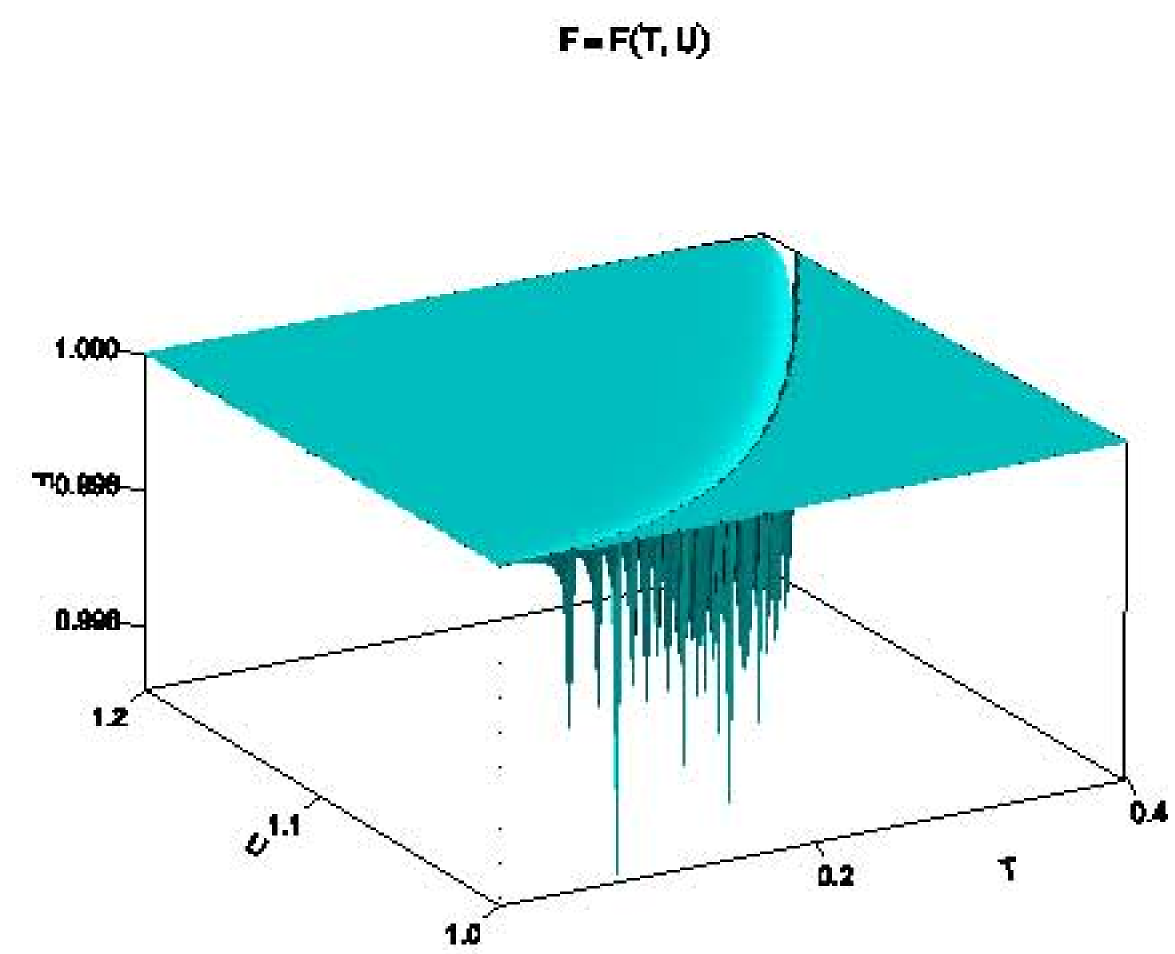
Stoner-Hubbard Model

$$\begin{aligned}\hat{H}_{SH} &= \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + U \sum_{l} \hat{n}_{l\uparrow}\hat{n}_{l\downarrow} \\ &\simeq \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + U \sum_{l} (\hat{n}_{l\uparrow} < \hat{n}_{l\downarrow} > + < \hat{n}_{l\uparrow} > \hat{n}_{l\downarrow} - < \hat{n}_{l\uparrow} >< \hat{n}_{l\downarrow} >)\end{aligned}$$

With the self-consistent symmetry breaking field $U(\langle \hat{n}_\uparrow \rangle - \langle \hat{n}_\downarrow \rangle)$

coupled to $\hat{S}_z = \frac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)$





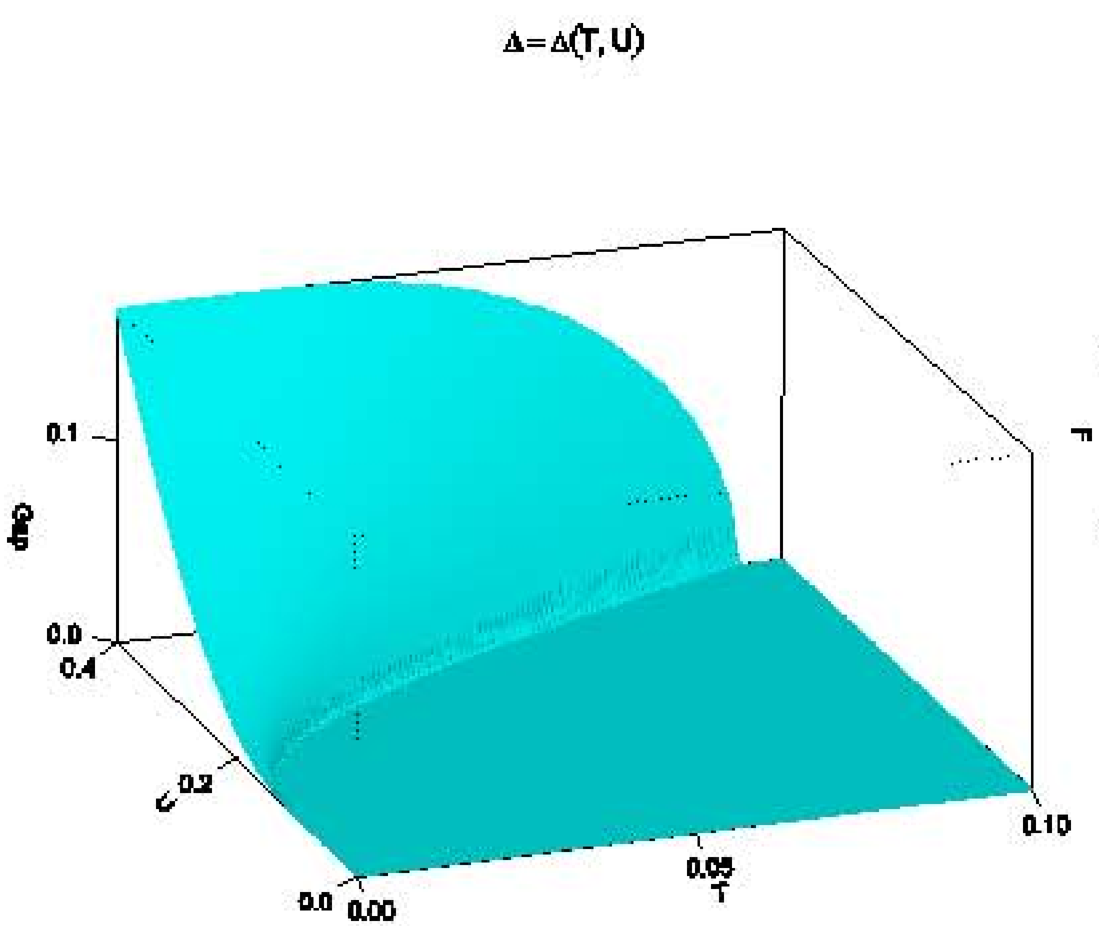
BCS Superconductivity

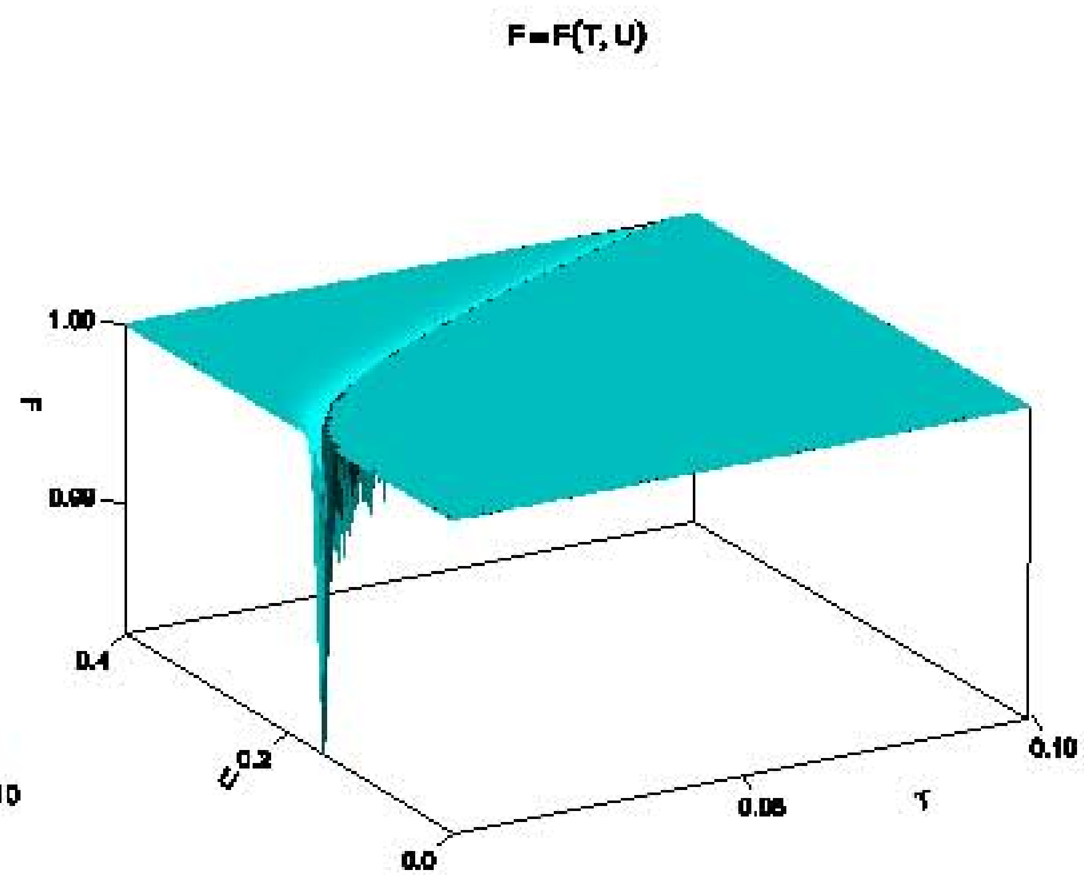
$$\hat{H}_{BCS} = \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + \sum_{kk'} V_{kk'} \hat{c}^\dagger_{k'\uparrow} \hat{c}^\dagger_{-k'\downarrow} \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow}$$

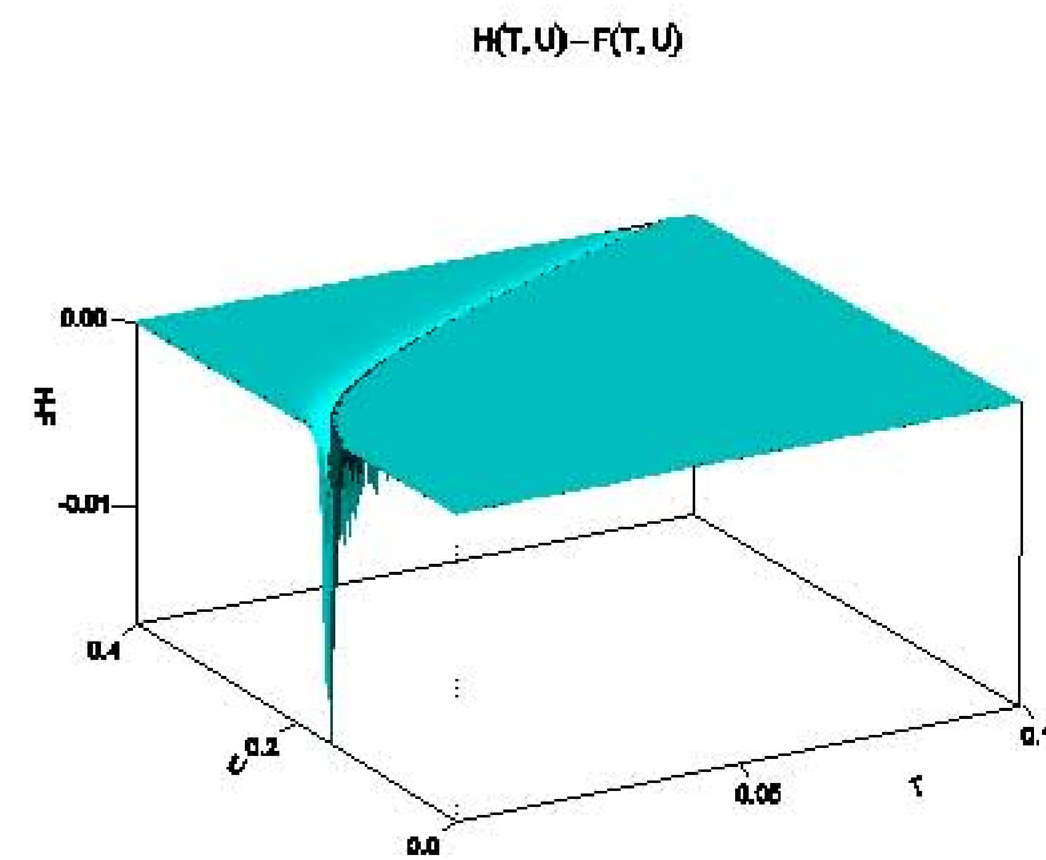
$$\simeq \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} - \sum_{k} \left(\Delta_k^* \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} + \hat{c}^\dagger_{k\uparrow} \hat{c}^\dagger_{-k\downarrow} \Delta_k - \Delta_k^* \hat{c}^\dagger_{-k\downarrow} \hat{c}^\dagger_{k\uparrow} \right)$$

With the self-consistent symmetry breaking fields Δ_k and Δ_k^* coupled to the Nambu operators

$\hat{T}^+ = \hat{c}^\dagger_{k\uparrow} \hat{c}^\dagger_{-k\downarrow}$ and $\hat{T}^- = \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow}$







$$H - F = \mathrm{Tr}[|\sqrt{\rho_1}\sqrt{\rho_2}|(\hat{V} - \hat{I})] < 0$$

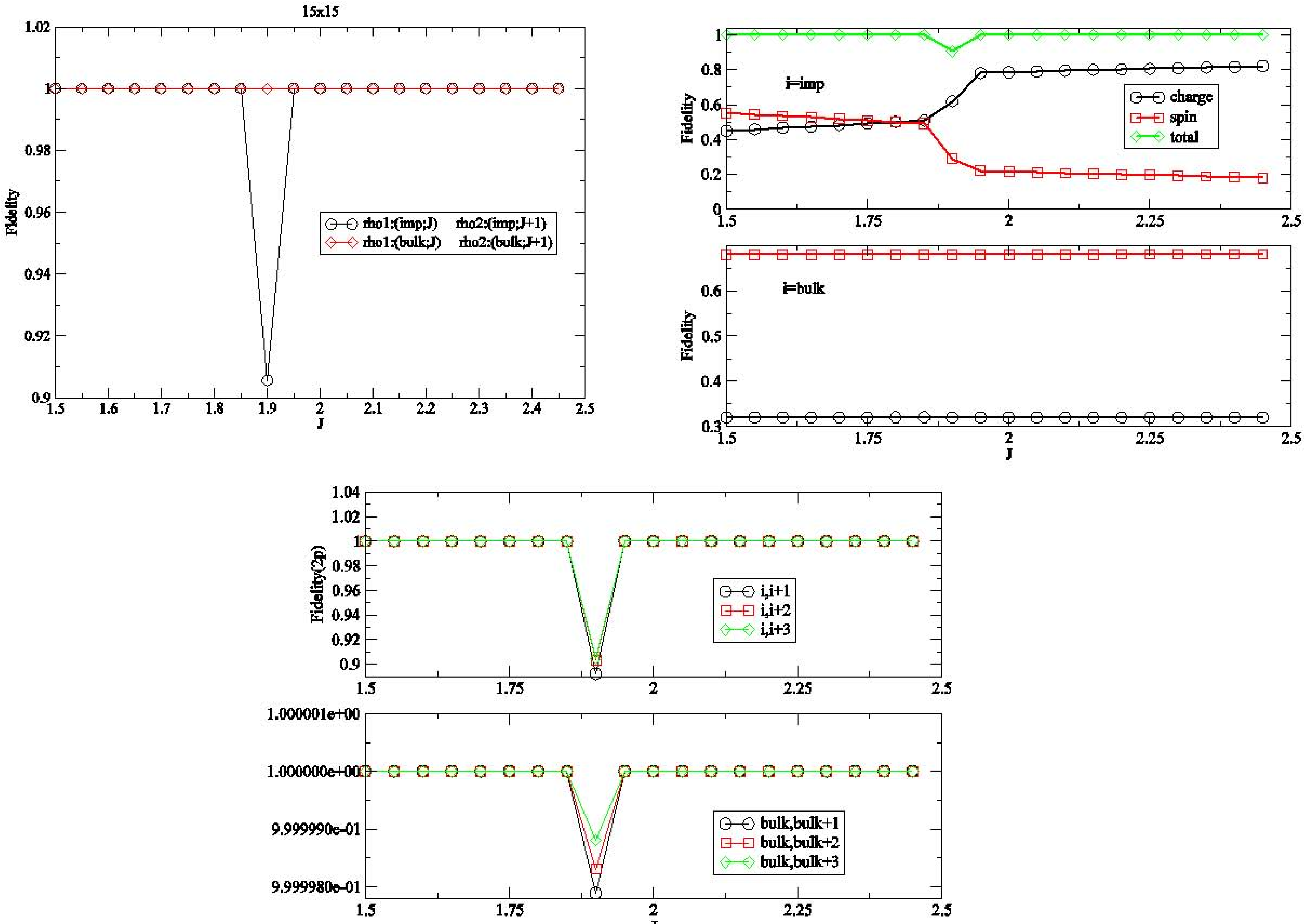
Uhlmann geometric phase

One Impurity in a Superconducting Lattice

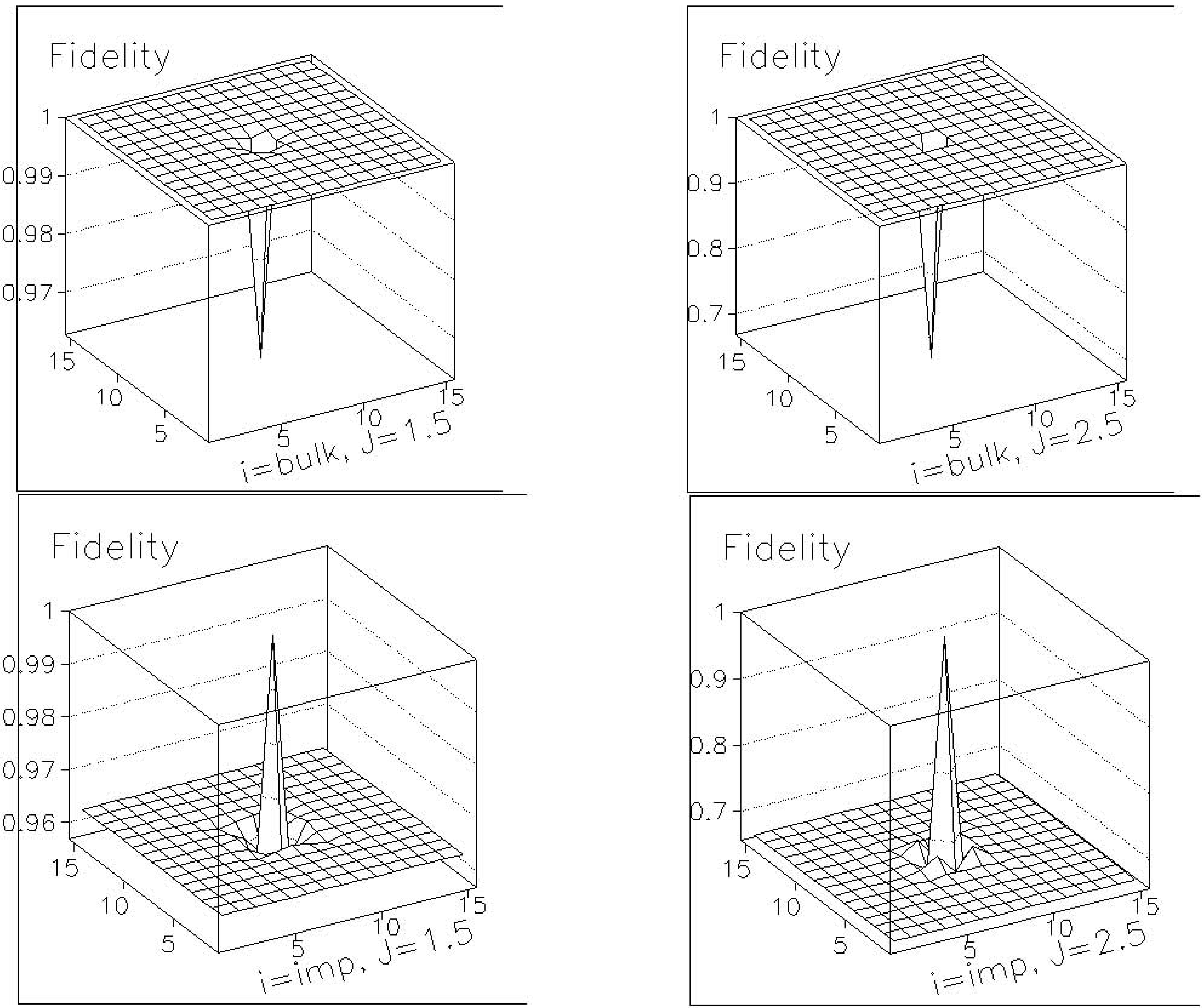
$$H = -\sum_{<i,j>,\sigma} t_{i,j} c^{\dagger}_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_i \left(\Delta_i c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} + \Delta^*_i c_{i\downarrow} c_{i\uparrow}\right)$$
$$- \sum_{i,\sigma,\sigma'} J\delta_{i,l}[\cos\varphi_l c^{\dagger}_{i\sigma} \sigma^x_{\sigma,\sigma'} c_{i\sigma'} + \sin\varphi_l c^{\dagger}_{i\sigma} \sigma^z_{\sigma,\sigma'} c_{i\sigma'}]$$

The one-site reduced density matrix is given by the correlation functions:

$$\rho_A = \begin{pmatrix} \langle(1-n_\uparrow)(1-n_\downarrow)\rangle & \langle c^{\dagger}_{\uparrow} c^{\dagger}_{\downarrow}\rangle & 0 & 0 \\ \langle c_\downarrow c_\uparrow\rangle & \langle n_\uparrow n_\downarrow\rangle & 0 & 0 \\ 0 & 0 & \langle n_\uparrow(1-n_\downarrow)\rangle & \langle c^{\dagger}_{\downarrow} c_\uparrow\rangle \\ 0 & 0 & \langle c^{\dagger}_{\uparrow} c_\downarrow\rangle & \langle(1-n_\uparrow)n_\downarrow\rangle \end{pmatrix}$$


15x15
Fidelity
J
rho1:(imp;J) rho2:(imp;J+1)
rho1:(bulk;J) rho2:(bulk;J+1)
i=imp
charge
spin
total
i=bulk
Fidelity(2p)
i,i+1
i,i+2
i,i+3
bulk,bulk+1
bulk,bulk+2
bulk,bulk+3
1.000001e+00
1.000000e+00
9.999990e-01
9.999980e-01

One-Site Fidelity and the Order Parameter – Local Magnetization



Conclusions

- The fidelity can be a good indicator of phase transitions;
- Proven for broad classes of systems (LGW, Free Fermions,…);
- Valid for other types of phase transitions (topological, matrix product states, Kosterlitz-Thouless, …);
- Induces metrics – connection with Berry and Uhlmann geometric phases;
- The partial state fidelity can also indicate QPTs;
- The fidelity as an order parameter.

• P. Zanardi and N. Paunković, *"Ground state overlap and quantum phase transitions"*, Phys. Rev. A **74**, 031123 (2006), arXiv:quant-ph/0512249;

• N. Paunković and V. R. Vieira, *"Macroscopic distinguishability between quantum states defining different phases of matter: Fidelity and the Uhlmann geometric phase"*, Phys. Rev. E **77**, 011129 (2008), arXiv:0707.4667v1 [quant-ph];

• N. Paunković, P. D. Sacramento, P. Nogueira, V. R. Vieira and V. K. Dugaev, *"Fidelity between partial states as signature of quantum phase transitions"*, Phys. Rev. A **77**, 052302 (2008), arXiv:0708.3494v1 [quant-ph];

Dicke Model

- Hamiltonian: $\hat{H}(\lambda) = \omega_0 \hat{J}_z + \omega \hat{a}^\dagger \hat{a} + \frac{\lambda}{\sqrt{2j}} \left(\hat{a}^\dagger + \hat{a}\right) \left(\hat{J}_+ + \hat{J}_-\right).$

- Critical Point: $\lambda_c = (\omega \omega_0)/2$

  $\lambda < \lambda_c$ normal phase

  $\lambda > \lambda_c$ super-radiant phase

- Normal Phase (TD limit):

$$\hat{H}^n(\lambda) = \omega_0 \hat{b}^\dagger \hat{b} + \omega \hat{a}^\dagger \hat{a} + \lambda \left(\hat{a}^\dagger + \hat{a}\right) \left(\hat{b}^\dagger + \hat{b}\right) - j\omega_0.$$

Ground State

$$g(x,y) = \left(\frac{\varepsilon_+\varepsilon_-}{\pi^2}\right)^{\frac{1}{4}} e^{-1/2\langle \mathbf{R}, A\mathbf{R}\rangle}$$

$[\mathbf{R} = (x,y)]$

$$A = \begin{bmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{bmatrix}^{-1} \begin{bmatrix} \varepsilon_- & 0 \\ 0 & \varepsilon_+ \end{bmatrix} \begin{bmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{bmatrix}$$

$$\gamma = (1/2)\arctan[4\lambda\sqrt{\omega\omega_0}/(\omega^2 + \omega_0^2)]$$

Fundamental Excitations

$$\varepsilon_\pm^2 = \frac{1}{2}\left(\omega^2 + \omega_0^2 \pm \sqrt{(\omega^2 - \omega_0^2)^2 + 16\lambda^2\omega^2\omega_0^2}\right).$$

Fidelity

$$|\langle g|\tilde{g}\rangle| = 2\frac{[\det A \det\tilde{A}]^{\frac{1}{4}}}{[\det(A+\tilde{A})]^{\frac{1}{2}}} = 2\frac{[\det A]^{\frac{1}{4}}}{[\det\tilde{A}]^{\frac{1}{4}}[\det(1+\tilde{A}^{-1}A)]^{\frac{1}{2}}}.$$

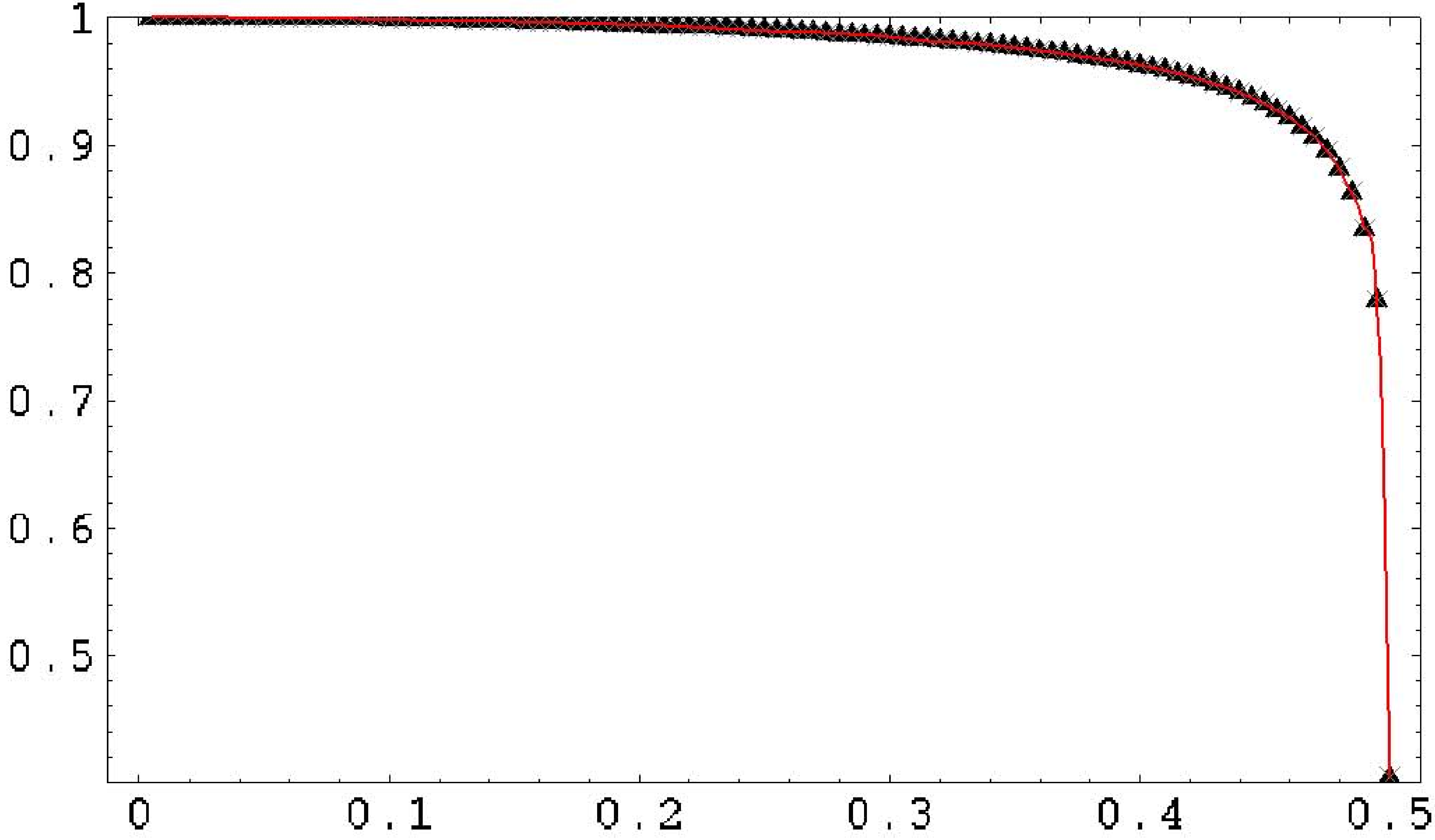
$(\lambda \to \lambda_c)$ $\delta\lambda > 0$

$$\det A = \varepsilon_+\varepsilon_- \to 0$$

$$\det\tilde{A} \geq \det\tilde{A}_c = \tilde{\varepsilon}^c_+\tilde{\varepsilon}^c_- > 0$$

$$\det(1+\tilde{A}^{-1}A) > 0$$

$|\langle g|\tilde{g}\rangle|$



$\omega_0 = \omega = 1 \qquad \delta\lambda = 10^{-6}$