Functional RG for impurities in 1d interacting fermion systems

work in collaboration with: V. Meden, W. Metzner, U. Schollwöck, S. Andergassen

Phys. Rev. B65, 045138 (2002)
J. Low Temp. Phys. 126, 1147 (2002)
⋮

1) Motivation
2) toy-model (single-particle scattering)
3) RG for model of spinless interacting fermions
4) Summary

1) Motivation

challenging issue:

Realistic calculation of transport through carbon nanotubes containing impurities

Do "both camps" have to contribute ?

A) LDA + Landauer-Büttiker ?

B) Luttinger liquid physics: Kane-Fisher scenario !

Kane + Fisher scenario :

Luttinger liquid + Delta potential of strength V_0

bosonization → local sine-Gordon model → weak coupling

RG in V_0 → " $V_0 \to \infty$ " (for repulsive two-body interaction)

An arbitrarily weak impurity "cuts a LL in half"

(complementary approach : weak link t' scales to zero)

⇒ i) $G \sim T^{2(\frac{1}{K_\rho}-1)}$ — boundary exponent α_B

ii) local spectral density suppression $|\varepsilon - \mu|^{\alpha_B}$

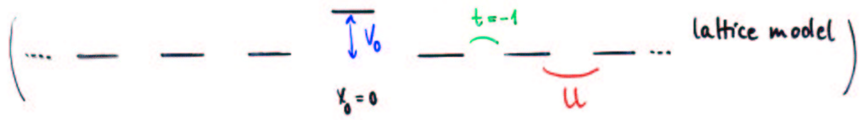
experimental verification (?) : Bockrath et. al. Nature **397**, 598 (1999)

simple fermionic picture ?

nonperturbative in V_0 !?

Interacting 1d-electrons : (spinless fermions)

Elementary attempt : Hartree-Fock ("half of the story")



To leading order in V_0 the change of the Hartree-potential is

$|x| \gg a$: $\delta V_H(x) \to U(2k_F)\, \delta\rho_{(1)}(x)$ — change of density

$\delta\rho_{(1)}(x) \sim V_0 \sin(2k_F|x| + \delta_F)/|x|$

Friedel oscillations for noninteracting electrons in d-dimensions decay $\sim 1/|x|^d$

for $d=1$ such an additional long-range potential leads to peculiar scattering behaviour and to drastic effects in the local density of states

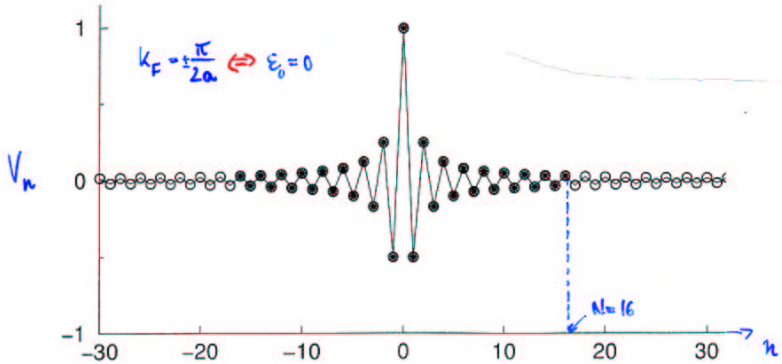
2) Toy – model

Noninteracting 1-d electrons in a potential (nearest neighbour hopping $t=-1$)

$$V = \sum_n |n\rangle V_n \langle n| \; + \; \sum_n \left(|n\rangle \delta t_n \langle n+1| + h.c.\right)$$

$$V_n = V_0 \, \delta_{n,0} + V' \frac{\sin(2k_F|n|a)}{|n|^\beta} \quad \text{for } n \le N$$

mostly $\beta = 1$:

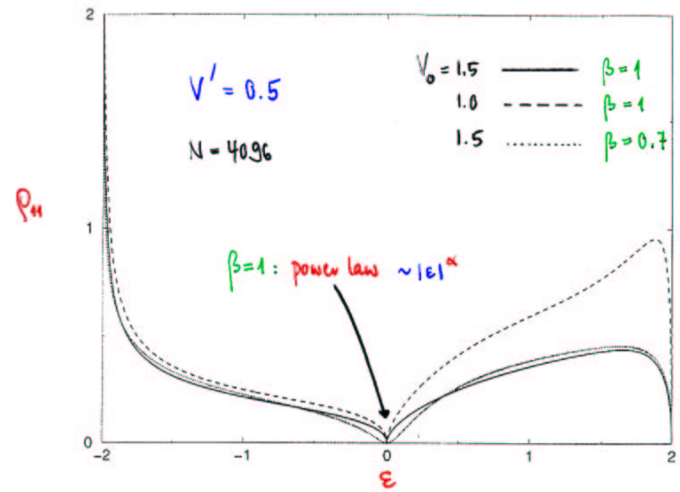


quantities of interest:

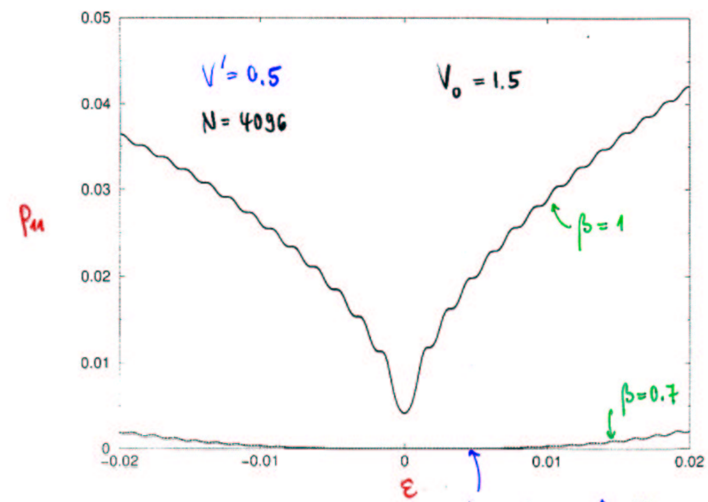
a) local density of states: $\rho_{nn}(\varepsilon) = \langle n|\delta(\varepsilon - H)|n\rangle$
(near the center of the potential)

b) transmission amplitude: $|t(\varepsilon)|$

local DOS next to the impurity site:

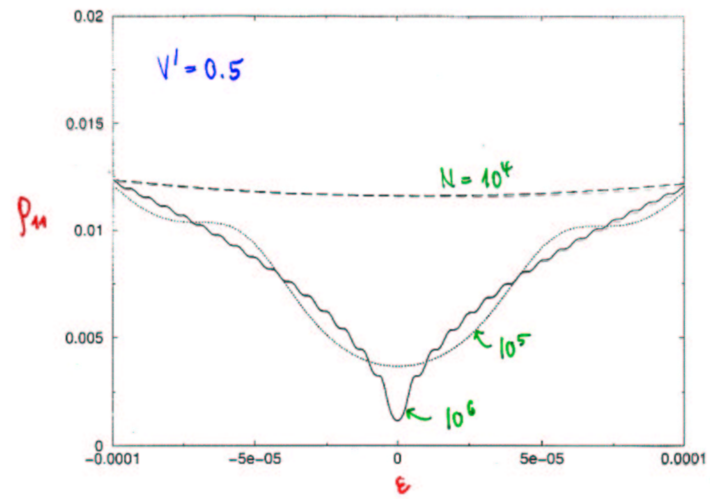


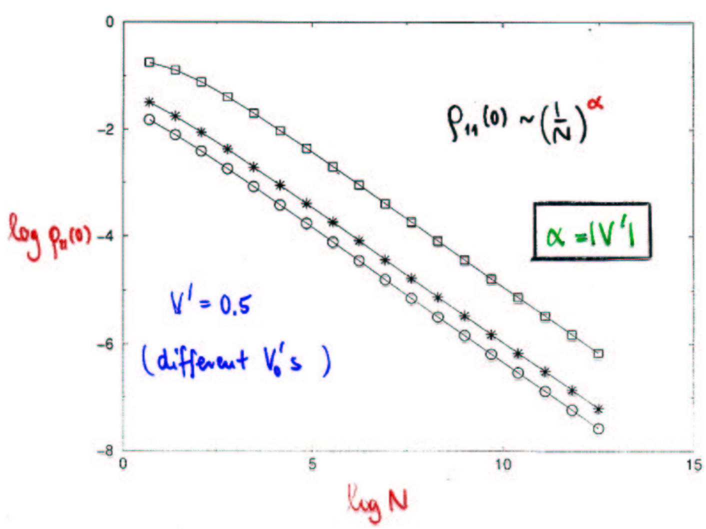
zooming in :



"pseudo-gap" ($\beta \to 0, N \to \infty$ real gap)
(A-B-chain)

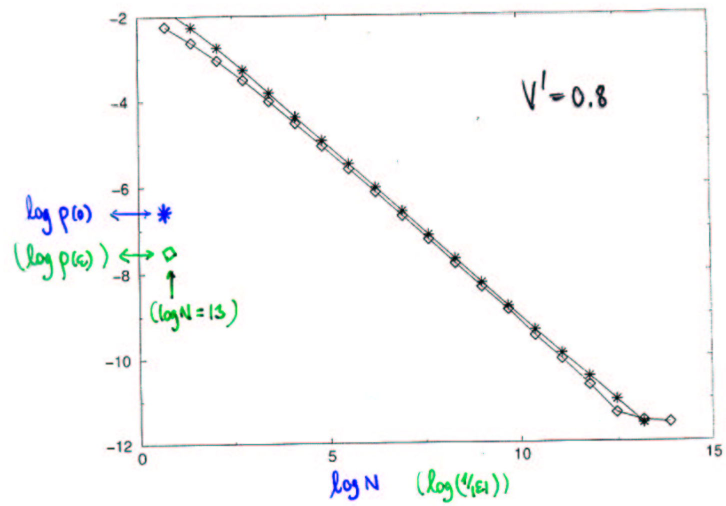
further zooming in :





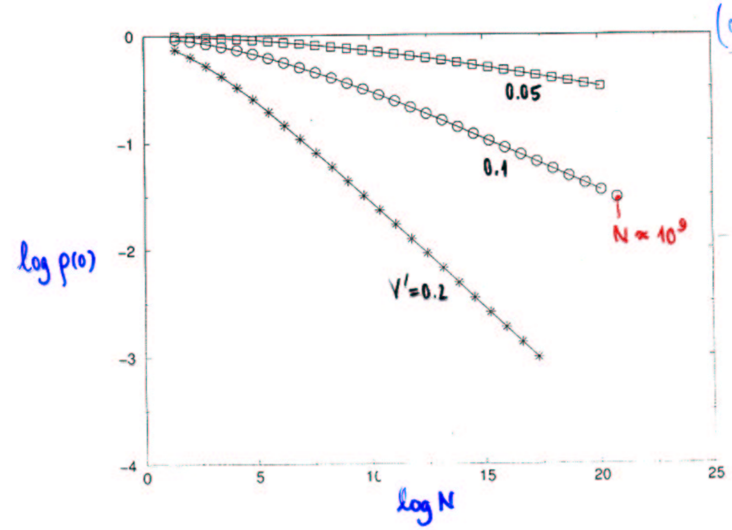
the power law $\rho(0) \sim (1/N)^{\alpha}$ is easier to detect than the

" " $\rho(\varepsilon) \sim |\varepsilon|^{\alpha}$

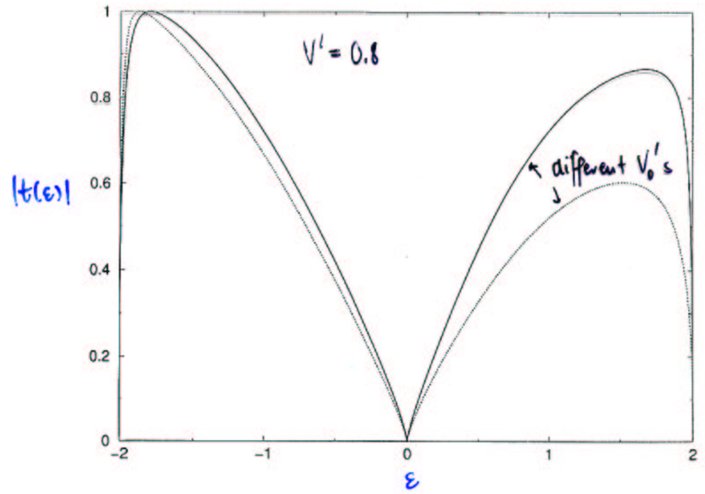


for smaller values of |V'| the approach to the power law is slow

$\left(\alpha + A\left(\frac{1}{N}\right)^{2\alpha}\right)$

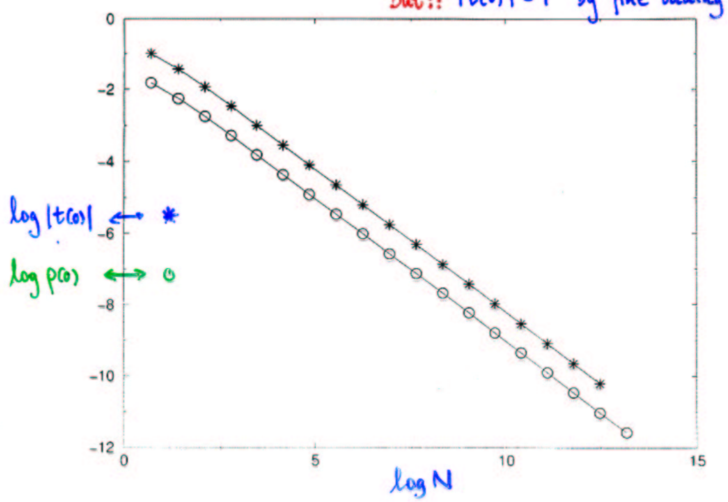


the transmission amplitude $|t(\varepsilon)|$ vanishes with a power law near $\varepsilon = 0$

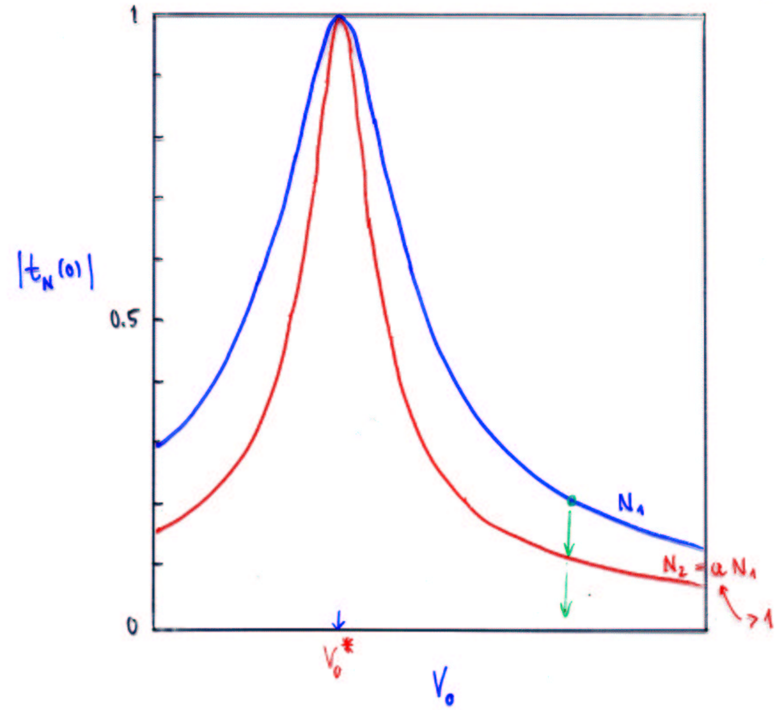


with the same exponent α as the LDOS ("generic")

but!: $|t(0)| = 1$ by fine tuning V_0



transmission resonance



1)

PHYSIKALISCHE ZEITSCHRIFT

vereinigt mit dem

JAHRBUCH DER RADIOAKTIVITÄT UND ELEKTRONIK

Nr. 15 — 1. August 1929 — 30. Jahrgang

Redaktionsschluß für Nr. 17 am 15. August 1929.

INHALT:

"About strange discrete eigenvalues"

"normal:" → E

"strange:" → E

ORIGINALMITTEILUNGEN.

Über merkwürdige diskrete Eigenwerte.

Von J. v. Neumann und E. Wigner.

1. Es sind in der quantentheoretischen Literatur mehrfach anschauliche Schlüsse von der Art gemacht worden, daß z. B. aus der Tatsache, daß ein Elektron genügend kinetische Energie hat, um sich aus einem atomaren System (klassisch gerechnet) ins Unendliche zu entfernen, geschlossen wurde, daß der betreffende Energiewert zum kontinuierlichen Spektrum des genannten Systems gehört. Im folgenden soll gezeigt werden, daß derartige Überlegungen mit äußerster Vorsicht zu handhaben sind, denn es kommt häufig ein entgegengesetztes Verhalten vor. Dieser Umstand, daß ein Elektron auf einer stationären Bahn verharrt (Punkteigenwert!), obwohl es Energie genug hätte, um sich aus dem Anziehungsbereich des ihn umgebenden Systems zu befreien, ist nur scheinbar paradox. Wir werden uns an zwei verschiedenen Beispielen klar machen, daß dieses Phänomen zwei ganz verschiedene Ursachen haben kann — aber in beiden Fällen bis zu einem gewissen Grade anschaulich deutbar ist.

Wir werden stets ein Elektron im Bereiche eines geeigneten kugelsymmetrischen Potentials betrachten, also die Wellengleichung

$$-\frac{h^2}{8\pi^2 m}\Delta\psi + (V(r) - E)\psi = 0$$

$\left(\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right.$, da wir uns auf kugelsymmetrische ψ beschränken und die Ableitungen nach den Winkeln θ und φ weglassen können). Damit $E = 0$ ein Punkteigenwert mit der kugelsymmetrischen Eigenfunktion $\psi = \psi(r)$ sei, muß also $V = \frac{h^2}{8\pi^2 m}\left(\frac{\psi''}{\psi} + \frac{2\psi'}{r\psi}\right)$ sein. Wir werden nun durch geeignete Wahl von ψ dem V die oben erwähnten, scheinbar paradoxen, Formen erteilen.

Sei zuerst $\psi = \frac{\sin(r^3)}{r^2}$, dann ergibt sich[1]) (unter Weglassung des unwesentlichen Faktors $\frac{h^2}{8\pi^2 m}$) $V = 2r^{-2} - 9r^4$. Ein ebener Schnitt durch den Potentialverlauf sieht also wie auf der Figur angedeutet aus. Nach allem Erwarten müßte das Elektron den Potentialabhang hinabstürzen und daher nur ein Streckenspektrum besitzen — dennoch ist eine stationäre Bahn und der Punkteigenwert $E = 0$ da!

Jedoch ist dieses Verhalten sogar auf Grund klassisch-mechanischer Analogien zu verstehen[2]).

1) Man setze versuchsweise $\psi(r) = r^a \sin(r^b)$. Damit das Quadratintegral von ψ, d.h. $\int_0^\infty 4\pi r^2 |\psi(r)|^2 dr = \int_0^\infty 4\pi r^{a+2} \sin^2(r^b) dr$ endlich sei, muß mit Rücksicht auf das Verhalten bei $r = 0$: $2a + b + 2 > -1$ und auf das Verhalten bei $r = \infty$: $2a + 2 < -1$ sein. Die Regularität von $V(r)$ für $r \neq 0$ erfordert $2a + b + 1 = 0$. Beides erfüllt $a = -2$, $b = 3$.

2) Diese Bemerkung rührt von Herrn L. Szilard her.

d = 3 : s-waves : $V(r) - E = -\frac{\hbar^2}{2m}\frac{\psi''(r)}{\psi(r)}$; $\psi(r) = f(r)\sin kr$

↑ clever choice

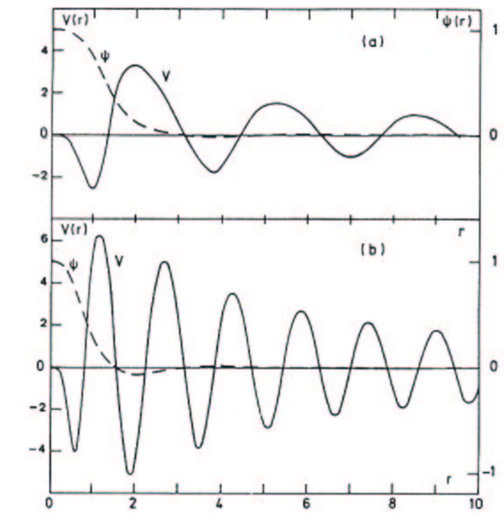


Fig. 1. Two examples of potential $V(r)$ that possess a bound state $\psi(r)$ with positive energy E; (a) $E = 1$; (b) $E = 4$.

$$V(r) = 16k^2\{-8A^2 \sin^4 kr\, f^2(r) + [6\sin^4 kr - (2kr - \sin 2kr)\sin 2kr]\, f(r)\}$$

$f(r) = [A^2 + s^2(r)]^{-1}$; $s(r) = 2kr - \sin(2kr)$.

$(A^2 = 4k^2)$

One verifies easily that $V(r) \sim -16k^2(\sin 2kr)/2kr$ for $r \to \infty$.

attempt to verify Kane + Fisher within HF (or LDA) successful ?

- power laws in LDOS and transmission
- exponent α depends on V_0

$$\alpha = \alpha_{HF}(U, k_F, V_0)$$

$$\neq \alpha_{boundary}(U, k_F) \quad \text{(Kane+Fisher)}$$

---

3) needed : better treatment of electron correlations to obtain the flow "$V_0 \to \infty$"

Method : "Exact" functional RG technique

- Polchinski
- Salmhofer
- → Wetterich (Morris) (1-PI)

The exact renormalization group and approximate solutions

(Wetterich 93, Morris 94) (fermions: $\underset{\sim}{x} \to$ Grassmann variables)

1) W : generator of connected Green's functions (real "fields")

$$e^{W(\underset{\sim}{h}, \alpha)} = \int e^{-V_{int}(\underset{\sim}{x})} e^{\underset{\sim}{x} \cdot \underset{\sim}{h}} \underbrace{e^{-\frac{1}{2} \underset{\sim}{x} C(\alpha)^{-1} \underset{\sim}{x}} \frac{d\underset{\sim}{x}}{(2\pi \det C(\alpha))^{1/2}}}_{d\mu(\underset{\sim}{x}, \alpha)}$$

$$\underset{\sim}{\varphi} := \left(\frac{\partial W}{\partial \underset{\sim}{h}}\right)_{\alpha} \quad \left(= \langle \underset{\sim}{x} \rangle_{\underset{\sim}{h}, \alpha} \right)$$

2) Legendre transformation : $\underset{\sim}{\varphi}$ as independent variables

$$\Gamma(\underset{\sim}{\varphi}, \alpha) := \underset{\sim}{\varphi} \cdot \underset{\sim}{h}(\underset{\sim}{\varphi}, \alpha) - W(\underset{\sim}{h}(\underset{\sim}{\varphi}, \alpha), \alpha) - \underbrace{\frac{1}{2} \underset{\sim}{\varphi}\, C(\alpha)^{-1} \underset{\sim}{\varphi}}_{\text{(convenient)}}$$

Straightforward differentiation yields

$$\left(\frac{\partial \Gamma(\underset{\sim}{\varphi}, \alpha)}{\partial \alpha}\right)_{\underset{\sim}{\varphi}} = \frac{1}{2} \mathrm{Tr} \left\{ \frac{\partial C(\alpha)}{\partial \alpha} \Gamma^{(2)} (1 + C\, \Gamma^{(2)})^{-1} \right\}$$

with $\underset{=}{\Gamma}^{(2)} = \left(\frac{\partial^2 \Gamma}{\partial \underset{\sim}{\varphi} \partial \underset{\sim}{\varphi}} \right)_{\alpha}$

3) initial condition :

$C(\alpha_0) = 0$ leads to $\Gamma(\underset{\sim}{\varphi}, \alpha_0) = V_{int}(\underset{\sim}{\varphi})$

If $C(\alpha_1)$ corresponds to the free propagator of the system to be studied, $\Gamma(\varphi, \alpha_1)$ is obtained by solving the differential equation approximately terminating the

4) hierarchy of coupled equations ("loop expansion")

The Taylor expansion (V_{int} even, e.g. $V_{int}(\varphi) = \frac{1}{4!} g_{ijkl}\varphi_i\varphi_j\varphi_k\varphi_l$)

$$\Gamma(\varphi, \alpha) = \Gamma_0(\alpha) + \frac{1}{2}\Gamma_{ij}(\alpha)\varphi_i\varphi_j + \frac{1}{4!}\Gamma_{ijkl}(\alpha)\varphi_i\varphi_j\varphi_k\varphi_l + \frac{1}{6!}\Gamma_{ijklmn}(\alpha)\varphi_i\varphi_j\varphi_k\varphi_l\varphi_m\varphi_n + \dots$$

yields an infinite hierarchy of coupled equations for the expansion coefficients ($\tilde{C} = (1 + C\Gamma_2)^{-1} C$)

$$\dot{\Gamma}_0 = \frac{1}{2}\mathrm{Tr}\{\dot{C}\Gamma_2(1 + C\Gamma_2)^{-1}\}$$

$$(\dot{\Gamma}_2)_{ij} = -\frac{1}{2}(\tilde{C}\dot{C}^{-1}\tilde{C})_{kl}\Gamma_{lkij}$$

$$\dot{\Gamma}_{ijkl} = -\frac{1}{2}(\tilde{C}\dot{C}^{-1}\tilde{C})_{mn}\Gamma_{nmijkl} + (\tilde{C}\dot{C}^{-1}\tilde{C})_{mn}\left[\Gamma_{mn'ij}\tilde{C}_{n'm'}\Gamma_{m'nkl} + (j \leftrightarrow k) + (j \leftrightarrow l)\right]$$

$$\dot{\Gamma}_{mnijkl} = \dots$$

$\vdots$

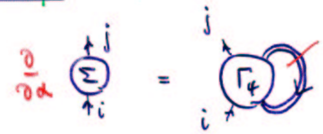
1-p-irreducible vertex functions

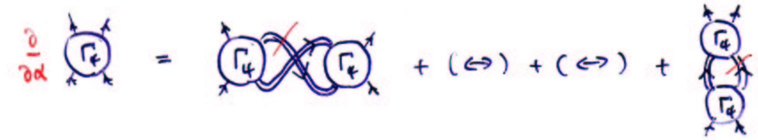
"1 loop" (error $\sim g^3 + \dots$)

"renormalization group enhanced perturbation theory"

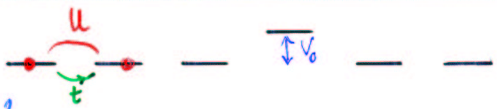
---

1 loop:





spinless fermions:



half filling: LL for $-2 < U \leq 2$

aim: anomalous dimension linear in U (V_0 arbitrary)

approximation: $\Gamma_4 \to U$ (antisymmetrized) ("no" flow)

(↯ with spin) (improvements "in the making")

cut-off in Matsubara frequencies ($\alpha \to \Lambda$): $(G^0_\Lambda(i\omega_n))_{kk} = \Theta(|\omega_n| - \Lambda)\frac{1}{i\omega_n - \varepsilon_k}$

⇒ (in site representation) — nonperturbative in the impurity strength, perturbative in U

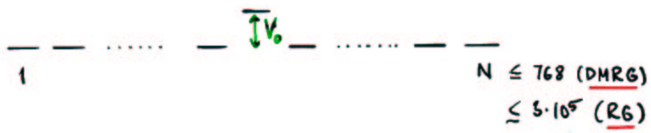
$$\dot{\Sigma}^{(\Lambda)}_{ii} = -\frac{1}{2\pi}U\left[G_{i+1,i+1}(i\Lambda) + G_{i-1,i-1}(i\Lambda) + (\Lambda \to -\Lambda)\right]$$

$$\dot{\Sigma}^{(\Lambda)}_{i,i\pm1} = \frac{1}{2\pi}U\left[G_{i,i\pm1}(i\Lambda) + G_{i,i\pm1}(-i\Lambda)\right]$$

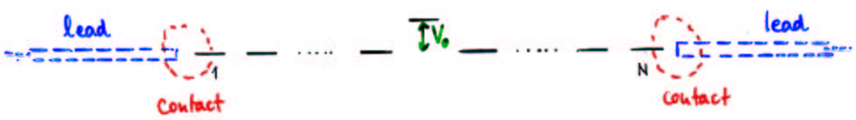
small V_0 allows analytical solution: $\Sigma^{(\Lambda)}_{k_F,-k_F} \sim \left(\frac{1}{\Lambda}\right)^{\frac{\tilde{v}(0) - \tilde{v}(2k_F)}{2\pi v_F}}$

(as long as $\Sigma_{k_F,-k_F}$ stays small) (Kane + Fisher) systems studied :

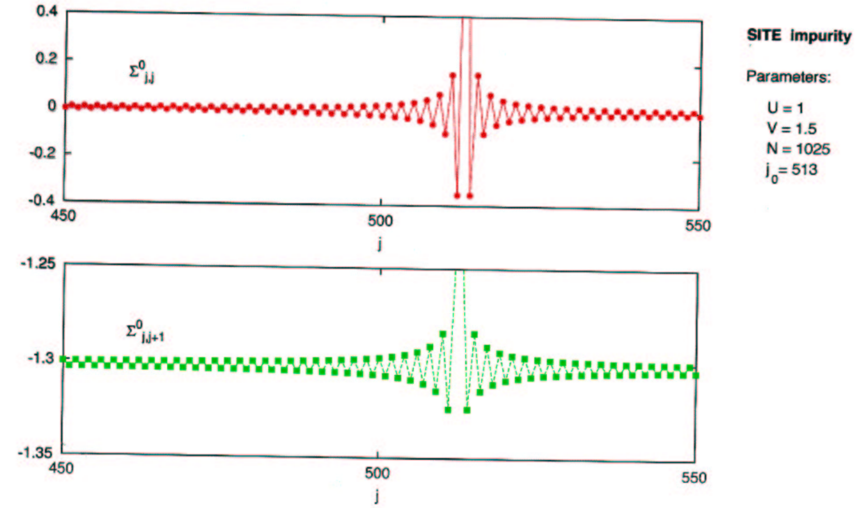
a) finite systems with open boundaries



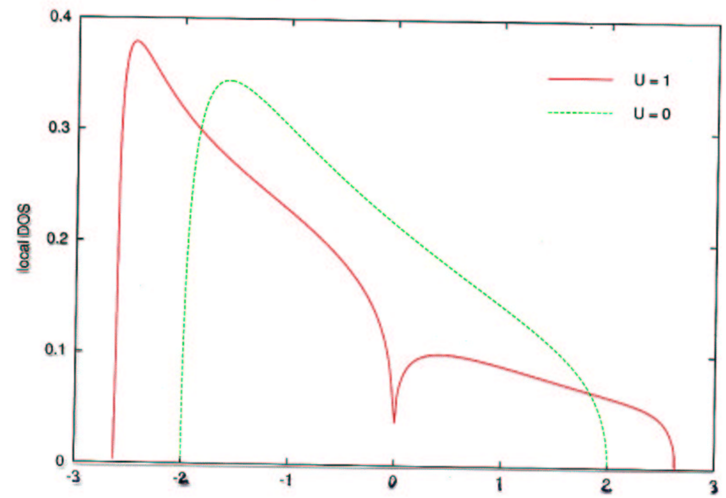
b) finite LL's with semiinfinite noninteracting leads



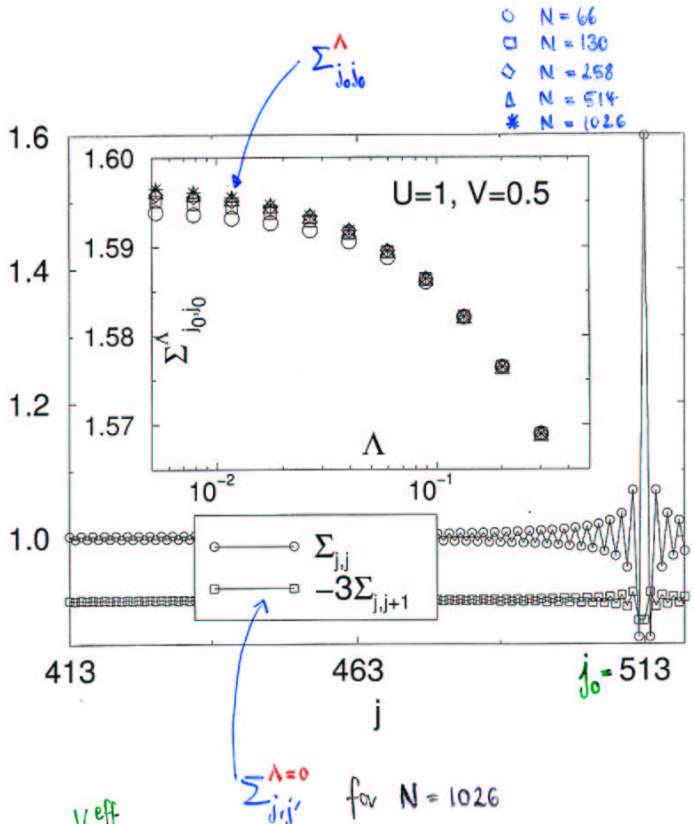
Results for **effective impurity potential**



Results for **DOS near impurity site**



site impurity:

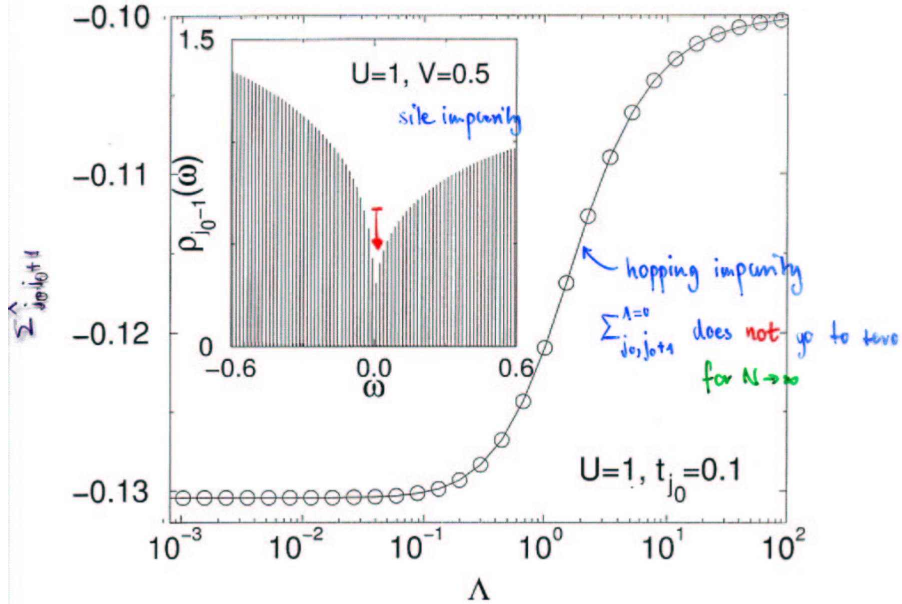


V_0^{eff}

$\Sigma^{\Lambda=0}_{j_0,j_0}$ goes to a finite constant for $N \to \infty$

$\Sigma^{\Lambda=0}_{k_F,-k_F}$ diverges for $N \to \infty$

finite chain : discrete spectrum

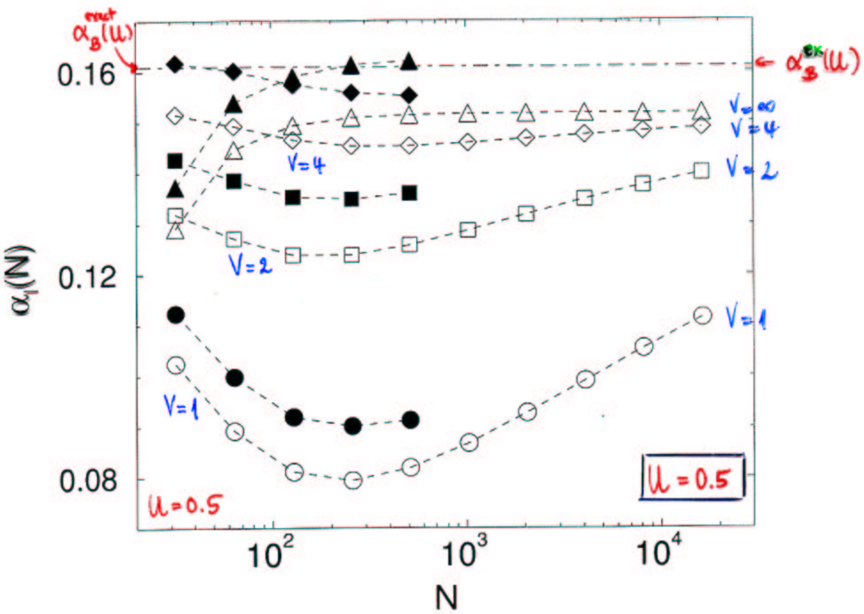


finite site scaling of peak at $\omega = 0$:

RG und DMRG

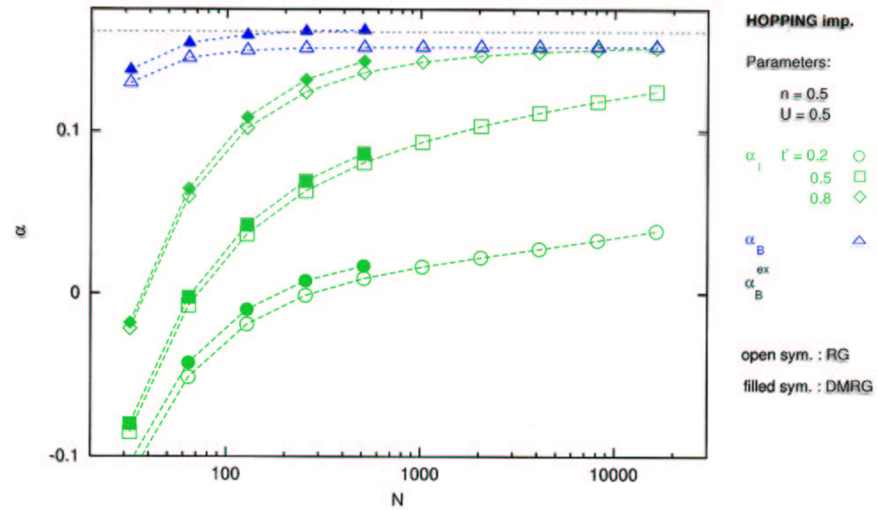
slow approach to the open boundary result

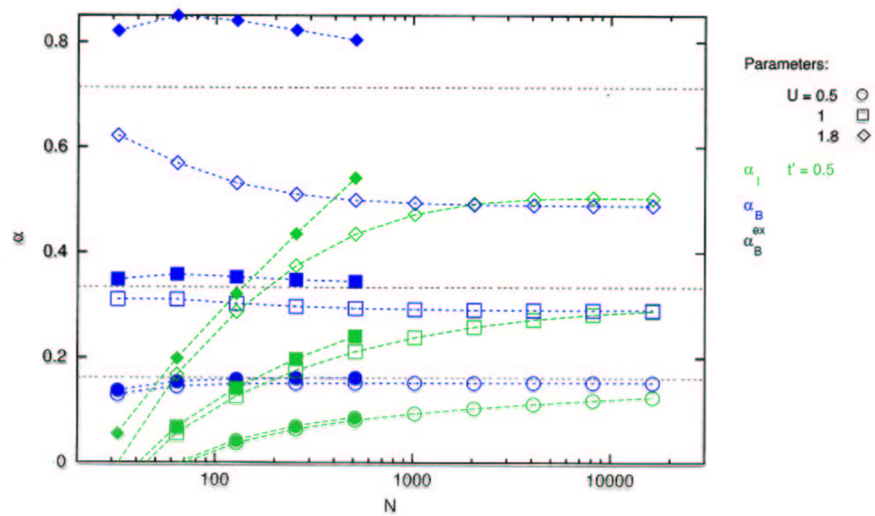
$\left(\alpha_I(N) \equiv - \frac{\Delta \log \rho_I(0)}{\Delta N} \right)$



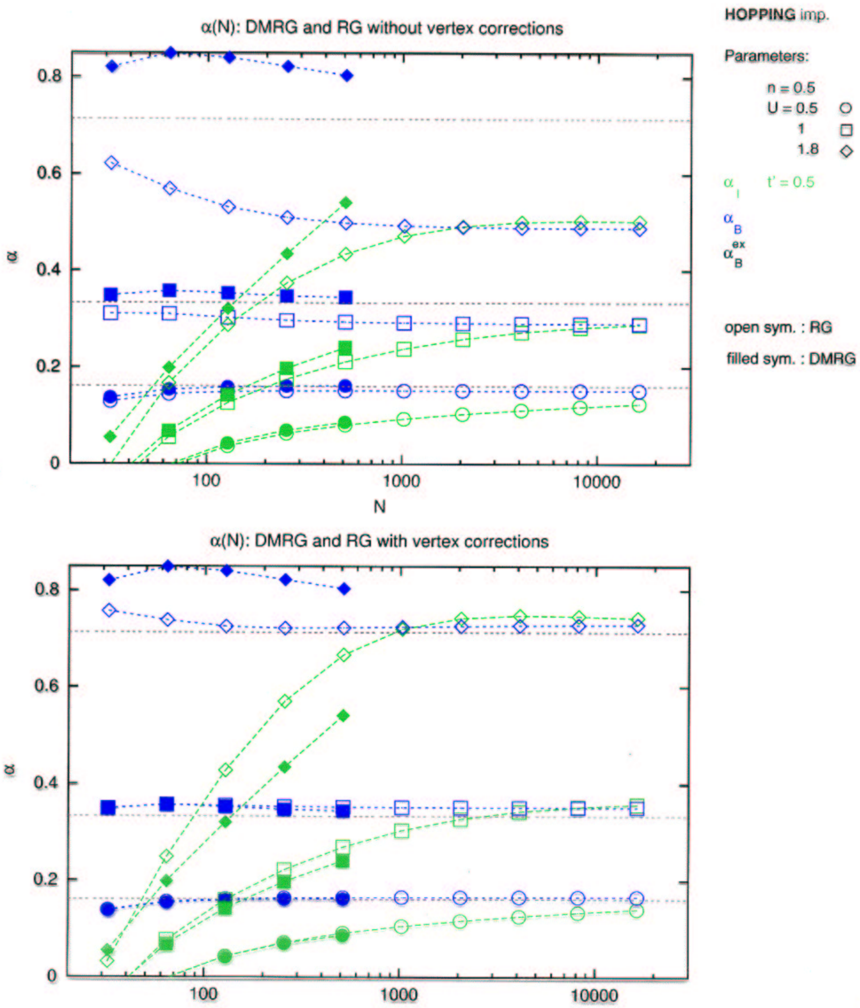
full symbols: DMRG

Results for exponent α(N)





Effect of the **VERTEX - Renormalization**



Conclusion

- The experimental verification of the asymptotic open boundary physics in transport in Luttinger liquids requires very long chains (e.g. nanotubes)

- The RG-method used (non-perturbative in the impurity strength, perturbative in the electron-electron interaction) shows the importance of oscillatory long range effective potentials for the understanding of the Kane-Fisher scenario directly in the fermionic language.