Part III: Impurities in Luttinger liquids

1. Luttinger liquids
2. Impurity effects
3. Microscopic model
4. Flow equations
5. Results

Phys. Rev. B 65, 045318 (2002); Europhys. Lett. 64, 769 (2003);
1. Luttinger liquids

One-dimensional interacting Fermi systems without correlation gaps are Luttinger liquids.
(1D counterpart of Fermi liquid in 2D or 3D)

One-dimensional electron systems:

- Complex chemical compounds containing chains
- Quantum wires (in heterostructures)
- Carbon nanotubes
- Edge states

(Dekker’s group)
Electronic structure of 1D systems:

Dispersion relations:
\[ \epsilon_k = \frac{k^2}{2m} \quad \text{(low carrier density)} \]
\[ \epsilon_k = -2t \cos k \quad \text{(tight binding)} \]

"Fermi surface": 2 points \( \pm k_F \)

Dispersion relation near Fermi points:
\[ \xi_k = \epsilon_k - \epsilon_F = v_F (|k| - k_F) \]
Electron-electron interaction:

has stronger effects than in 2D and 3D systems:

no fermionic quasi-particles, Fermi liquid theory not valid.

Fermi liquid replaced by Luttinger liquid:

• only bosonic low-energy excitations
  (collective charge/spin density oscillations)

• power-laws with non-universal exponents

⇒ Luttinger liquid theory

Bulk properties of Luttinger liquids:

- **Bosonic** low-energy excitations with linear dispersion relation
  \[
  \xi^c_q = u_c q, \quad \xi^s_q = u_s q \quad \text{(charge and spin channel)}
  \]
  \[\Rightarrow \quad \text{specific heat} \quad c_V \propto T\]

- **DOS** for single-electron excitations:
  \[
  D(\epsilon) \propto |\epsilon - \epsilon_F|^\alpha
  \]
  vanishes at Fermi level \((\alpha > 0)\)

DOS in principle observable by photoemission or tunneling.
• **Density-density** correlation function $N(q)$:

finite for $q \to 0$ (compressibility)

divergent as $|q - 2k_F|^{-\alpha_{2k_F}}$ for $q \to 2k_F$

($\alpha_{2k_F} > 0$ for repulsive interactions)

$\Rightarrow$ enhanced back-scattering ($2k_F$) from impurity.

For spin-rotation invariant (and spinless) systems all exponents can be expressed in terms of one parameter $K_\rho$. 
Asymptotic low energy behavior (power-laws) of Luttinger liquids described by Luttinger model:

\[ H_{LM} = \text{linear } \epsilon_k + \text{forward scattering interactions} \]

It is exactly solvable and scale-invariant (fixed point).

For spinless fermions only one coupling constant, parametrizing interaction between left- and right-movers:

\[ H_I = g \int dx \, n_+(x) \, n_-(x) \]
2. Impurity effects

How does a single non-magnetic impurity (potential scatterer) affect properties of a Luttinger liquid?

Non-interacting system:

Impurity induces Friedel oscillations (density oscillations with wave vector $2k_F$)

DOS near impurity finite at Fermi level

Conductance reduced by a finite factor (transmission probability)
Kane, Fisher ’92: impurity in interacting system (spinless Luttinger liquid)

• Weak impurity potential:

Backscattering amplitude $V_{2k_F}$ generated by impurity grows as $\Lambda^{K_\rho - 1}$ for decreasing energy scale $\Lambda$.
($K_\rho < 1$ for repulsive interactions; $V_{2k_F}$ is ”relevant” perturbation of pure LL)

⇒ Low energy probes see high barrier even if (bare) impurity potential is weak!

• Weak link:

\[ t_{wl} \]

DOS at boundary of LL vanishes as $|\epsilon - \epsilon_F|^{\alpha_B}$ ⇒

Tunneling amplitude $t_{wl}$ between two weakly coupled chains scales to zero as $\Lambda^{\alpha_B}$ with $\alpha_B = K_\rho^{1 - 1} - 1 > 0$ at low energy scales. ($t_{wl}$ is ”irrelevant” perturbation of split chain)
Hypothesis (Kane, Fisher):

Any impurity effectively "cuts the chain" at low energy scales and physical properties obey weak link or boundary scaling.  ⇒

DOS near impurity:

\[ D_i(\epsilon) \propto |\epsilon - \epsilon_F|^{\alpha_B} \quad \text{for } \epsilon \to \epsilon_F \text{ at } T = 0 \]

Conductance through impurity:

\[ G(T) \propto T^{2\alpha_B} \quad \text{for } T \to 0 \]

supported within effective bosonic field theory by:

refermionization (Kane, Fisher '92)
QMC (Moon et al. '93; Egger, Grabert '95)
Bethe ansatz (Fendley, Ludwig, Saleur '95)
3. Microscopic model

Spinless fermion model:

\[
H_{sf} = -t \sum_j \left( c_{j+1}^{\dagger} c_j + c_j^{\dagger} c_{j+1} \right) + U \sum_j n_j n_{j+1}
\]

Properties (without impurities):

• **exactly solvable** by Bethe ansatz

• **Luttinger liquid** except for \(|U| > 2t\) at half-filling

• **charge density wave** for \(U > 2t\) at half-filling
**Impurity potential** added to bulk hamiltonian $H_{sf}$:

**general form:**  
$$H_{\text{imp}} = \sum_{j,j'} V_{j'j} c_{j'}^\dagger c_j$$

"site impurity":  
$$H_{\text{imp}} = V n_{j_0} \quad (j_0 \text{ impurity site})$$

"hopping impurity":  
$$H_{\text{imp}} = (t - t') \left( c_{j_0+1}^\dagger c_{j_0} + c_{j_0}^\dagger c_{j_0+1} \right)$$

Later also **double barrier** (two site or hopping impurities)
4. Flow equations

Starting point (for approximations):

**Exact hierarchy of differential flow equations** for 1-particle irreducible vertex functions with infrared cutoff $\Lambda$:

\[
\frac{d}{d\Lambda} \Sigma^\Lambda = \frac{\mathcal{S}^\Lambda}{\Gamma^\Lambda}
\]

\[
\frac{d}{d\Lambda} \Gamma^\Lambda = \frac{\mathcal{S}^\Lambda}{G^\Lambda} + \frac{\Gamma_3^\Lambda}{\Gamma_3^\Lambda}
\]

where

\[
G^\Lambda = \left[ (G_0^\Lambda)^{-1} - \Sigma^\Lambda \right]^{-1}
\]

\[
S^\Lambda = \left[ 1 - G_0^\Lambda \Sigma^\Lambda \right]^{-1} \frac{dG_0^\Lambda}{d\Lambda} \left[ 1 - \Sigma^\Lambda G_0^\Lambda \right]^{-1}
\]

etc. for $\Gamma_3^\Lambda$, $\Gamma_4^\Lambda$, ...
Cutoff:

At $T = 0$ sharp frequency cutoff: $G_0^\Lambda = \Theta(|\omega| - \Lambda) G_0$

At finite $T$ (discrete Matsubara frequencies) soft cutoff with width $2\pi T$

$G_0$ bare propagator without impurities and interaction
Approximations:

Scheme 1 (first order):

Approximate $\Gamma^\Lambda \approx \Gamma^{\Lambda 0}$ (ignore flow of 2-particle vertex)

$\Rightarrow \Sigma^\Lambda$ tridiagonal matrix in real space

Flow equation very simple; at $T = 0$:

$$\frac{d}{d\Lambda} \Sigma^\Lambda_{j,j} = -\frac{U}{2\pi} \sum_{s=\pm1} \sum_{\omega=\pm\Lambda} \tilde{G}^\Lambda_{j+s,j+s}(i\omega)$$

$$\frac{d}{d\Lambda} \Sigma^\Lambda_{j,j\pm1} = \frac{U}{2\pi} \sum_{\omega=\pm\Lambda} \tilde{G}^\Lambda_{j,j\pm1}(i\omega)$$

where $\tilde{G}^\Lambda(i\omega) = [G_0^{-1}(i\omega) - \Sigma^\Lambda]^{-1}$.

Kane/Fisher physics already qualitatively captured!
Scheme 2 (second order):

Neglect $\Gamma^\Lambda_3$; approx. $\Gamma^\Lambda$ by flowing nearest neighbor interaction $U^\Lambda$

$\Rightarrow$ 1-loop flow for $U^\Lambda$; flow of $\Sigma^\Lambda$ as in scheme 1 with renormalized $U^\Lambda$

$$\frac{d}{d\Lambda} \Sigma^\Lambda_{j,j} = -\frac{U^\Lambda}{2\pi} \sum_{s=\pm 1} \sum_{\omega=\pm \Lambda} \tilde{G}^\Lambda_{j+s,j+s}(i\omega) \quad \frac{d}{d\Lambda} \Sigma^\Lambda_{j,j\pm 1} = \frac{U^\Lambda}{2\pi} \sum_{\omega=\pm \Lambda} \tilde{G}^\Lambda_{j,j\pm 1}(i\omega)$$

Works quantitatively even for rather big $U$
Derivation of flow equation (scheme 1):

Flow equation for self-energy:

$$\frac{d}{d\Lambda} \Sigma^\Lambda(1', 1) = -T \sum_{2, 2'} e^{i\omega_2^0} S^\Lambda(2, 2') \Gamma_0(1', 2'; 1, 2)$$

Single-scale propagator

$$S^\Lambda = G^\Lambda [\partial_\Lambda(G_0^\Lambda)^{-1}] G^\Lambda = -\frac{1}{1 - G_0^\Lambda \Sigma^\Lambda} \frac{\partial G_0^\Lambda}{\partial \Lambda} \frac{1}{1 - \Sigma^\Lambda G_0^\Lambda}$$

Self-energy and propagator diagonal in frequency: $\omega_1 = \omega_1'$ and $\omega_2 = \omega_2'$.

$\Gamma_0$ frequency-independent $\Rightarrow \Sigma$ frequency-independent.
Sharp frequency cutoff \((T = 0): \quad G_0^\Lambda(i\omega) = \Theta(|\omega| - \Lambda) \, G_0(i\omega) \quad \Rightarrow \quad S^\Lambda(i\omega) = \frac{1}{1 - \Theta(|\omega| - \Lambda)G_0(i\omega)\Sigma^\Lambda} \delta(|\omega| - \Lambda)G_0(i\omega) \frac{1}{1 - \Theta(|\omega| - \Lambda)\Sigma^\Lambda G_0(i\omega)}

\delta(.) \text{ meets } \Theta(.) \text{: ill defined!}

Consider regularized (smeared) step functions \(\Theta_\epsilon\) with \(\delta_\epsilon = \Theta_\epsilon'\), then take limit \(\epsilon \rightarrow 0\), using

\[ \int dx \, \delta_\epsilon(x - \Lambda) \, f[x, \Theta_\epsilon(x - \Lambda)] \xrightarrow{\epsilon \rightarrow 0} \int_0^1 dt \, f(\Lambda, t) \quad \text{proof: substitution } t = \Theta_\epsilon \]

Integration can be done analytically, yielding

\[ \frac{d}{d\Lambda} \Sigma^\Lambda_{j_1'j_1} = -\frac{1}{2\pi} \sum_{\omega = \pm \Lambda} \sum_{j_2, j_2'} e^{i\omega 0^+} \tilde{G}^\Lambda_{j_2, j_2'}(i\omega) \Gamma^0_{j_1', j_2'; j_1, j_2} \]

where \( \tilde{G}^\Lambda(i\omega) = [G_0^{-1}(i\omega) - \Sigma^\Lambda]^{-1} \)
Insert real space structure of **bare vertex** for spinless fermions with nearest neighbor interaction $U$:

\[
\Gamma^0_{j_1',j_2';j_1,j_2} = U_{j_1,j_2} (\delta_{j_1,j_1'} \delta_{j_2,j_2'} - \delta_{j_1,j_2'} \delta_{j_2,j_1'})
\]

\[
U_{j_1,j_2} = U (\delta_{j_1,j_2-1} + \delta_{j_1,j_2+1})
\]

⇒ Flow equations

\[
\frac{d}{d\Lambda} \Sigma^\Lambda_{j,j} = -\frac{U}{2\pi} \sum_{s=\pm 1} \sum_{\omega=\pm \Lambda} e^{i\omega_0^+} \tilde{G}^\Lambda_{j+s,j+s}(i\omega)
\]

\[
\frac{d}{d\Lambda} \Sigma^\Lambda_{j,j\pm 1} = \frac{U}{2\pi} \sum_{\omega=\pm \Lambda} e^{i\omega_0^+} \tilde{G}^\Lambda_{j,j\pm 1}(i\omega)
\]

Convergence factor $e^{i\omega_0^+}$ matters only for $\Lambda \rightarrow \infty$
Initial condition at $\Lambda = \Lambda_0 \to \infty$: 

$$
\Sigma_{j_1,j'_1}^{\Lambda_0} = V_{j_1,j'_1} + \frac{1}{2} \sum_{j_2} \Gamma_{j'_1,j_2;j_1,j_2}^0
$$

where $V_{j_1,j'_1}$ is the bare impurity potential and the second term is due to the flow from $\infty$ to $\Lambda_0$ (!)

Flow equations at finite temperatures $T > 0$:

Replace $\omega = \pm \Lambda$ by $\omega = \pm \omega_n^{\Lambda}$ in flow equations, where $\omega_n^{\Lambda}$ is the Matsubara frequency most close to $\Lambda$. 
Calculation of conductance:

Interacting chain connected to semi-infinite non-interacting leads via smooth or abrupt contacts

Conductance \[ G(T) = -\frac{e^2}{h} \int d\epsilon f'(\epsilon) |t(\epsilon)|^2 \] with \[ |t(\epsilon)|^2 \propto |G_{1,N}(\epsilon)|^2 \]

Propagator \( G_{1,N}(\epsilon) \) calculated in presence of leads, which affect the interacting region only via boundary contributions \( \Sigma_{1,1}(\epsilon) \) and \( \Sigma_{N,N}(\epsilon) \) to the self-energy

Vertex corrections vanish within our approximation (no inelastic scattering) (see Oguri '01)
fRG features:

- perturbative in $U$ (weak coupling)
- non-perturbative in impurity strength
- arbitrary bare impurity potential (any shape)
- full effective impurity potential
  (cf. Matveev, Yue, Glazman '93: only $V_{2k_F}$)
- cheap numerics up to $10^5$ sites for $T > 0$ and $10^7$ sites at $T = 0$.
- captures all scales, not just asymptotics.
5. Results

Renormalized impurity potential (from self-energy $\Sigma_{jj}$ at $\Lambda = 0$):

![Graph showing long-range $2k_F$-oscillations](image)

**long-range $2k_F$-oscillations**! (associated with **Friedel** oscillations of density)

$2k_F$-oscillations also in renormalized **hopping** amplitude around impurity
Results for local DOS near impurity site:
(half-filling, ground state, $U = 1$, $V = 1.5$, 1000 sites)

Strong suppression of DOS near Fermi level

Power law with boundary exponent $\alpha_B$ for $\omega \to 0$, $N \to \infty$

Spectral weight at $\omega = 0$ in good agreement with DMRG for $U < 2$. 
Log. derivative of spectral weight at Fermi level as fct. of system size:

- near boundary (solid lines)
- near hopping impurity (dashed lines)

circles: quarter-filling, $U = 0.5$
squares: quarter-filling, $U = 1.5$

open symbols: fRG
filled symbols: DMRG

top panel: without vertex renorm.
bottom panel: with vertex renorm.

horizontal lines: exact boundary exponents
Friedel oscillations from open boundaries:
(half-filling, ground state)

Excellent agreement between fRG and DMRG
One parameter scaling of conductance ($T = 0$):

Single impurity, smooth contacts: $G(N) = \frac{e^2}{h} \tilde{G}_K(x)$, $x = \left[\frac{N}{N_0(U, V)}\right]^{1-K}$

Crossover size as function of bare reflection amplitude
Conductance at $T > 0$ — smooth contacts

Asymptotic power law $G(T) \propto T^{2\alpha}$ reached on accessible scales only for sufficiently strong impurities
Resonant tunneling through double barrier:

Treated theoretically by many groups; controversial results!

Model setup:

(Dekker’s group ’01)
Resonance peaks in conductance as a function of gate voltage:

At $T = 0$, width $w \sim N^{K-1}$

$T$-dependence of $|t(\epsilon)|^2$ important
fRG results for $G_p(T)$ (symmetric double barrier):

Various distinctive power laws, in particular (Furusaki, Nagaosa '93,'98):

- exponent $2\alpha_B$ (looks like independent impurities in series)
- exponent $\alpha_B - 1$ ("uncorrelated sequential tunneling")

No indications of exponent $2\alpha_B - 1$ ("correlated sequential tunneling")
Summary

• fRG is reliable and flexible tool to study Luttinger liquids with impurities

• can be applied to microscopic models, restricted to "weak" coupling

• provides simple physical picture

• interplay of contacts, impurities, and correlations

• method covers all energy scales

• resonant tunneling: universal behavior and crossover captured
and outlook

• include spin
  (extended Hubbard model: Andergassen et al., PRB 73, 045125 (2006))

• more complex geometries
  (Y-junctions: Barnabé-Thériault et al., PRL 94, 136405 (2005))

• include bulk anomalous dimension

• include inelastic processes

• extend to non-linear transport