Out-of-equilibrium tunnel junction paradox and a new consistent Bosonization-deBosonization framework

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Bosonization: Why? How? What?

- Widely used theoretical method for tackling strongly correlated systems in low dimensions that are probed in a vast array of experimental setups and measurements
- Analytical method of choice for a large class of problems
- One of the few non-perturbative approaches that can be extended to study systems and devices out of equilibrium

- First used in the spin-boson problem (Schotte&Schotte 1969). Ideas developed in the context of the Tomonaga-Luttinger model through the 1960's and 70's in parallel in HET and CMT
- Modern algebraic formulation or "constructive bosonization" by Haldane (1981), who also coined the term "Luttinger liquid".

Bosonization: Why? How? What?

[continued…]

- Bosonization refers to the practical possibility of describing the excitations of fermionic systems via a description based on bosonic degrees of freedom.
- Constructive Bosonization: For a fermionic one-dimensional system with strictly linear dispersion and no cutoff, the excitations at constant fermion number are particle-hole pairs that can be used to construct bosonic operators which completely capture the full excitation spectrum.

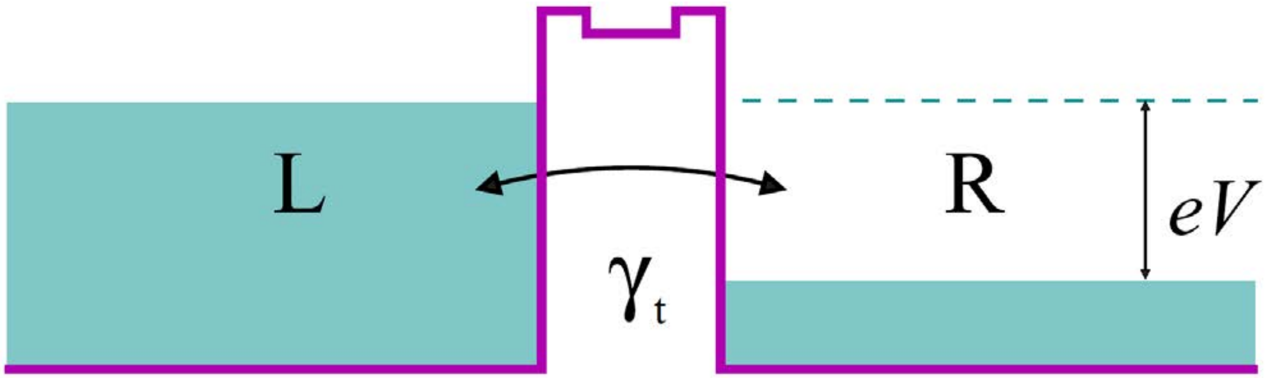
  [Review article: J. von Delft and H. Schoeller, Ann. Phys. **7**, 225 (1998)]
- The conceptual advantage of the constructive point of view is that it highlights the fact that bosonization is an exact correspondence between the two systems.
- There are also various complementary presentations based on the matching of correlators and known as the field-theoretic or the hydrodynamic approaches.

Question:

How to correctly and consistently carry out the bosonization program for an out-of-equilibrium (open) quantum system?

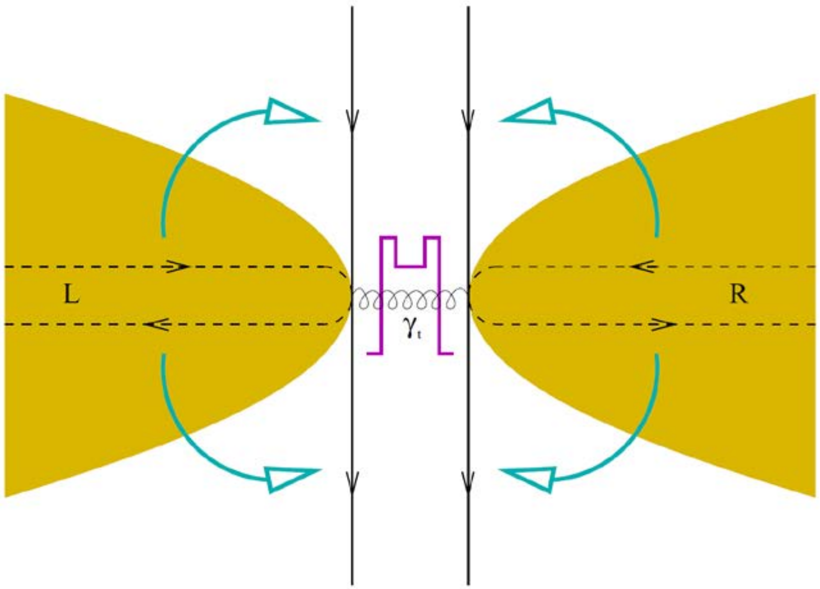
Let’s start at the very beginning, a very good place to start….

A Simple Tunneling Junction Problem



- Electrons tunnel across a barrier separating two electrodes in equilibrium at different chemical potentials
- The finite voltage drop makes the process irreversible
- Naturally modeled with a tunneling Hamiltonian

Mapping to One Dimension



Hamiltonian after "unfolding"

$$H = \sum_{\sigma,\ell} \left(\int \mathcal{H}_\ell^0 \, dx + H_{\text{tun}} \right)$$

$$\mathcal{H}_\ell^0 = v_{\text{F}} \, \psi_{\sigma\ell}^\dagger(x,t)(-i\partial_x)\psi_{\sigma\ell}(x,t)$$

$$H_{\text{tun}} = -\gamma_{\text{t}} \, \psi_{\sigma\ell}^\dagger(0,t)\psi_{\sigma\bar{\ell}}(0,t).$$

Here $\psi_{\sigma\ell}(x,t)$ are spin-1/2 ($\sigma = \uparrow, \downarrow$) chiral fermions in the two leads labeled by $\ell = \text{L}, \text{R} = \mp 1$

- Standard mapping in quantum impurity or "boundary" problems.
- Similar final Hamiltonian arise naturally in some setups of interest e.g. involving quantum-Hall edge states or certain topological states

Mapping to 1D (with choice of linear dispersion) means, the full technology of bosonization is now available!

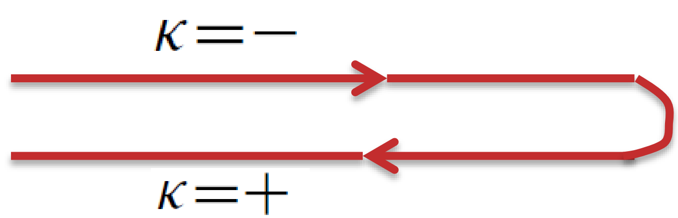
[Problem also amenable to Bethe Ansatz, CFT, etc.]

Direct Solution using Keldysh Local Action

Keldysh-augmented basis at the junction location ($x = 0$)

$$\Psi = \left(\psi_{\mathrm{L}}^{\kappa=-} \quad \psi_{\mathrm{L}}^{\kappa=+} \quad \psi_{\mathrm{R}}^{\kappa=-} \quad \psi_{\mathrm{R}}^{\kappa=+}\right)^T$$

Keldysh contour



$$G^{-1}(\omega) = -2i\,v_{\mathrm{F}} \begin{pmatrix} -s_{\mathrm{L}} & s_{\mathrm{L}}-1 & it & 0 \\ s_{\mathrm{L}}+1 & -s_{\mathrm{L}} & 0 & -it \\ it^* & 0 & -s_{\mathrm{R}} & s_{\mathrm{R}}-1 \\ 0 & -it^* & s_{\mathrm{R}}+1 & -s_{\mathrm{R}} \end{pmatrix}$$

where $\quad s_\ell(\omega) \equiv 1 - 2f\left(\frac{\omega-\mu_\ell}{T_\ell}\right)$

I-V Transport Characteristics

Steady-state current across the junction for a voltage drop $\mu_{\mathrm{L}} - \mu_{\mathrm{R}} = eV$

$$\hat{I} = \partial_t \frac{\Delta N}{2} = \frac{i}{2}[H, \Delta N] = \frac{i}{2}[H_{\mathrm{tun}}, N_{\mathrm{R}} - N_{\mathrm{L}}]$$

$$I = \langle \hat{I} \rangle = -\int \frac{d\omega}{2\pi}[\gamma_{\mathrm{t}} G_{\mathrm{RL}}^{-+} - \gamma_{\mathrm{t}}^{*} G_{\mathrm{LR}}^{-+}]$$

$$= \frac{4|t|^2}{\pi(1+|t|^2)^2} \int_{-\infty}^{+\infty} [f_{\mathrm{R}}(\omega) - f_{\mathrm{L}}(\omega)] d\omega$$

This includes finite temperatures that can be different in each lead (for thermal transport). At zero temperature it simplifies to:

$$\boxed{I \xrightarrow[T\to 0]{} \frac{4|t|^2 eV}{\pi(1+|t|^2)^2}}$$

where $\gamma_{\mathrm{t}} = 2v_{\mathrm{F}} t$

Now repeat the calculation using bosonization-debosonization…

But wait.

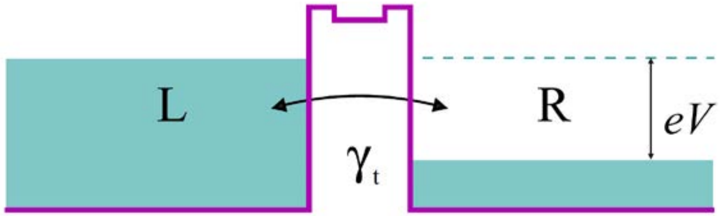
We need to first address the subtle question of how to bosonize when there is a finite voltage bias *i.e.* when there are two Fermi reference states or chemical potentials.

Will present a systematic way of doing this by going to the Lagrangian language and judiciously carrying out two gauge transformations of the fermionic field operators to ensure the validity of bosonization in the presence of voltage.

How to set up the out-of-equilibrium steady state problem to use bosonization?

The Lagrangian is not the full description, one needs to specify the chemical potentials

$$\mathcal{L}_\ell^0 = \psi_{\sigma\ell}^\dagger(x,t)(i\partial_t)\psi_{\sigma\ell}(x,t) - \mathcal{H}_\ell^0$$
$$= \psi_{\sigma\ell}^\dagger(x,t)(i\partial_t + i v_F\partial_x)\psi_{\sigma\ell}(x,t),$$
$$L_{tun} = -H_{tun} = \gamma_t \psi_{\sigma\ell}^\dagger(0,t)\psi_{\sigma\bar{\ell}}(0,t).$$



Time-dependent gauge transformation moves the chemical potentials from the distribution functions into the Lagrangian

$$\boxed{\psi_{\sigma\ell}(x,t) = e^{-i\mu_\ell t}\tilde{\psi}_{\sigma\ell}(x,t)}$$

Another gauge transformation factors out the fast oscillations or amounts to subtracting the vev's for each lead

$$\boxed{\tilde{\psi}_{\sigma\ell}(x,t) = e^{ik_F^\ell x}\breve{\psi}_{\sigma\ell}(x,t)}$$

$$k_F^\ell = \mu_\ell / v_F$$

$$\boxed{\begin{aligned} \mathcal{L}_\ell^0 &= :\breve{\psi}_{\sigma\ell}^\dagger(x,t)(i\partial_t + i v_F\partial_x)\breve{\psi}_{\sigma\ell}(x,t):, \\ L_{tun} &= e^{ieVt}\gamma_t\breve{\psi}_{\sigma L}^\dagger(0,t)\breve{\psi}_{\sigma R}(0,t) + e^{-ieVt}\gamma_t^*\breve{\psi}_{\sigma R}^\dagger(0,t)\breve{\psi}_{\sigma L}(0,t) \end{aligned}}$$

We have a normal-ordered problem with a global reference chemical potential. The tunneling term is now time dependent, but that is not a problem. One can now bosonize it in the standard way <u>and</u> the voltage appears explicitly!

Bosonization-deBosonization Program

1. Bosonization

$$\breve{\psi}_{\sigma\ell}(x,t) = \frac{1}{\sqrt{2\pi a}} F_{\sigma\ell}(t) e^{-i\phi_{\sigma\ell}(x,t)}$$ Mattis-Mandelstam formula

Here $F_{\sigma\ell}(t)$ are the so-called Klein factors

2. Change to a "physical" basis

$$\phi_{\sigma\ell} = \frac{1}{2}(\phi_c + \sigma\phi_s + \ell\phi_l + \sigma\ell\phi_{sl})$$ charge, spin, lead, spin-lead

Need to transform the Klein factors as well.

3. BdB-based Refermionization

$$\breve{\psi}_{\nu}(x,t) = \frac{1}{\sqrt{2\pi a}} F_{\nu}(t) e^{-i\phi_{\nu}(x,t)}$$ charge, spin, lead, spin-lead basis

Bosonization + change of basis + deBosonization results in a much simpler Hamiltonian in terms of new fermion fields

$$\mathcal{H}_{\nu}^{0} = :\breve{\psi}_{\nu}^{\dagger}(x,t)(-i v_{\mathrm{F}} \partial_x)\breve{\psi}_{\nu}(x,t):,$$

$$H_{\mathrm{tun}} = -[e^{ieVt}\gamma_{\mathrm{t}}\breve{\psi}_{l}(0,t) + e^{-ieVt}\gamma_{\mathrm{t}}^{*}\breve{\psi}_{l}^{\dagger}(0,t)] \times[\breve{\psi}_{sl}(0,t) - \breve{\psi}_{sl}^{\dagger}(0,t)].$$

Charge and spin degrees have disappeared from the problem!

The new problem can be regarded as arising from an original problem with the voltage acting as chemical potential shift of the lead fermions only.

The I-V characteristics are obtained in the same way as for the direct problem but starting with the Hamiltonian above.

[The local inverse Green's function is now 8 X 8 since the anomalous terms in the tunneling term need to be handled using a Nambu structure.]

$$I = \frac{|t'|^2}{(1+|t'|^2)} \int_0^{+\infty} [s_l(\omega) - \bar{s}_l(\omega)] \frac{d\omega}{2\pi}$$

Comparing two different ways of calculating the current…

Direct

(exact)

$$I \xrightarrow[T \to 0]{} \frac{4|t|^2 eV}{\pi(1+|t|^2)^2}$$

This is the "standard" <u>exact</u> result for the problem.

Conventional BdB

(expected to be exact)

$$I \xrightarrow[T_\nu \to 0]{} \frac{|t'|^2 eV}{\pi(1+|t'|^2)}$$

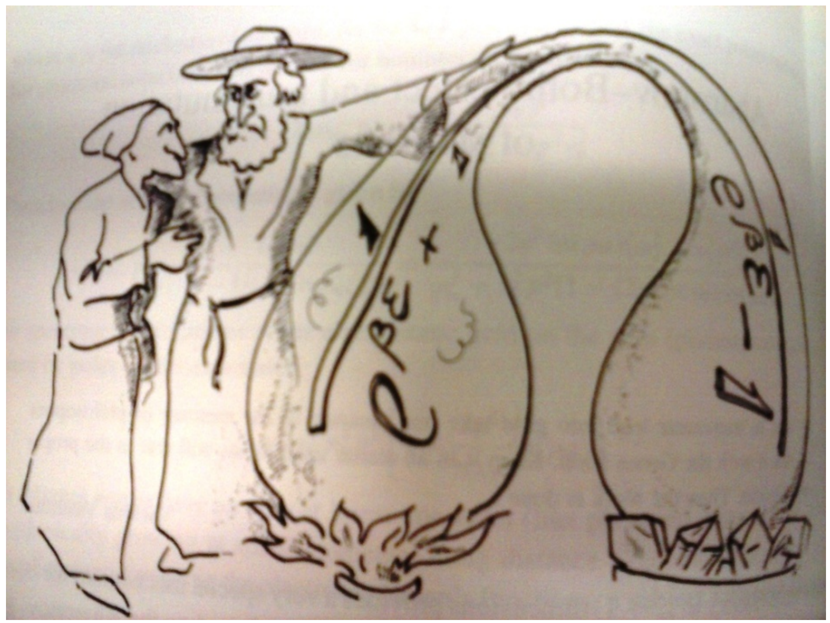
$$= \frac{(1+|t'|^2)}{4} \frac{4|t'|^2 eV}{\pi(1+|t'|^2)^2}$$

(i) Changed from t ………………to $t'=2t$

(ii) Overall factor of 1/4

(iii) Additional $(1+|t'|^2)$

This mismatch contradicts our *conventional* wisdom coming from decades of using the Bosonization-deBosonization Program



A. Tsvelik

Nonequilibrium Transport Paradox!

What is the resolution of this Paradox?

To get to the heart of the paradox
we need to first identify the correct diagnostic tool …

Observation: the two results coincide to $O(t^2)$

BdB-established Correspondence

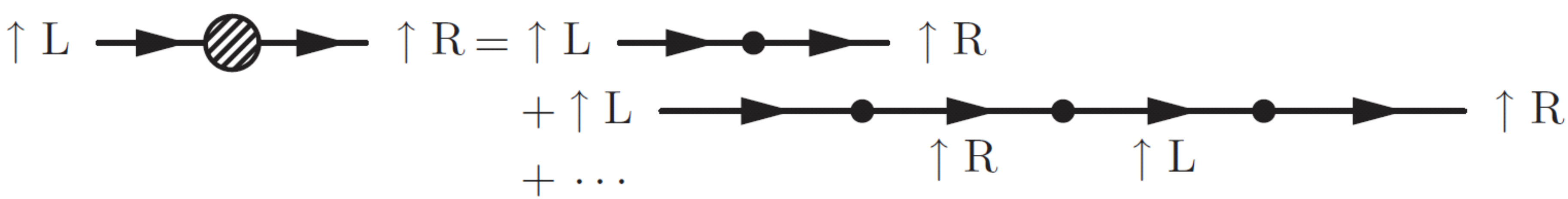
The BdB procedure effectively establishes a one-to-one correspondence between internal-labels in vertexes of *old* and *new* fermion bilinears.

Simple-junction Graph-vertex Dictionary			
Original Fermions		New Fermions	
$\psi^\dagger_{\uparrow\mathrm{R}}\psi_{\uparrow\mathrm{L}}$	$\uparrow\mathrm{L} \longrightarrow\bullet\longrightarrow \uparrow\mathrm{R}$	$\psi^\dagger_{sl}\psi^\dagger_{l}$	$l \longleftarrow\bullet\longrightarrow sl$
$\psi^\dagger_{\downarrow\mathrm{R}}\psi_{\downarrow\mathrm{L}}$	$\downarrow\mathrm{L} \longrightarrow\bullet\longrightarrow \downarrow\mathrm{R}$	$\psi^\dagger_{l}\psi_{sl}$	$sl \longrightarrow\bullet\longrightarrow l$
$\psi^\dagger_{\uparrow\mathrm{L}}\psi_{\uparrow\mathrm{R}}$	$\uparrow\mathrm{R} \longrightarrow\bullet\longrightarrow \uparrow\mathrm{L}$	$\psi_{l}\psi_{sl}$	$sl \longrightarrow\bullet\longleftarrow l$
$\psi^\dagger_{\downarrow\mathrm{L}}\psi_{\downarrow\mathrm{R}}$	$\downarrow\mathrm{R} \longrightarrow\bullet\longrightarrow \downarrow\mathrm{L}$	$\psi^\dagger_{sl}\psi_{l}$	$l \longrightarrow\bullet\longrightarrow sl$

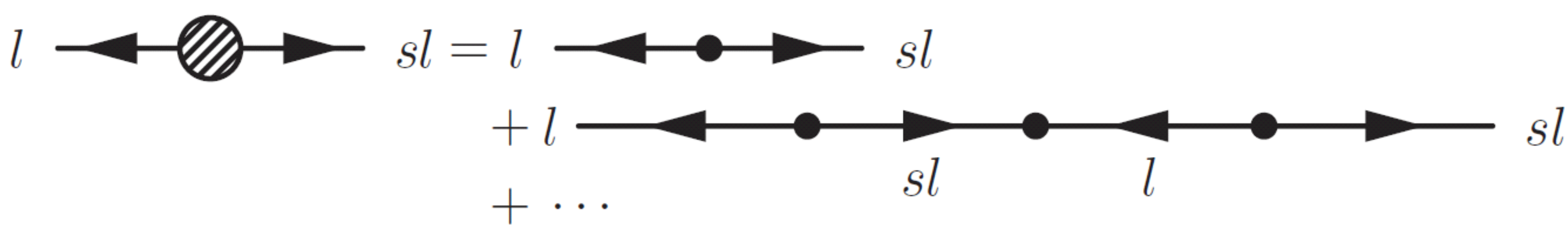
Going to new fermions, the smaller set in internal-label values is compensated by the appearance of anomalous fermion bilinears . . .

Diagrammatic Diagnosis Part 1:
An Exercise in Translation…

Consider how to dress a vertex using
the standard Feynman-Dyson perturbation theory:

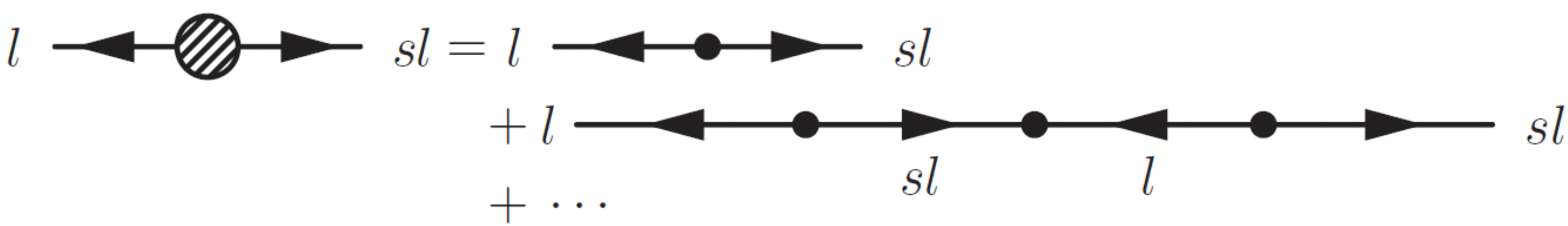


Then translate it using the BdB-generated dictionary:

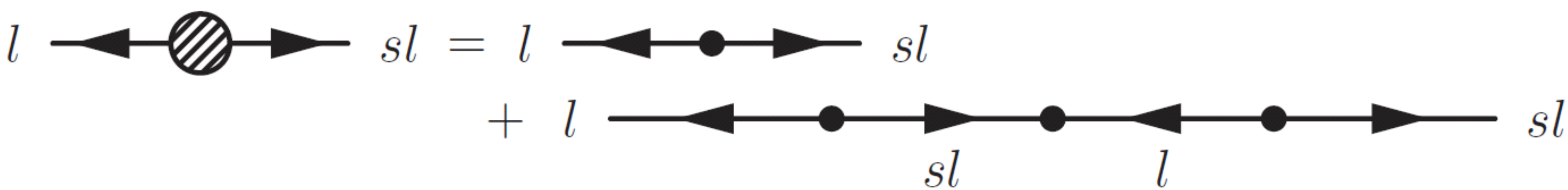


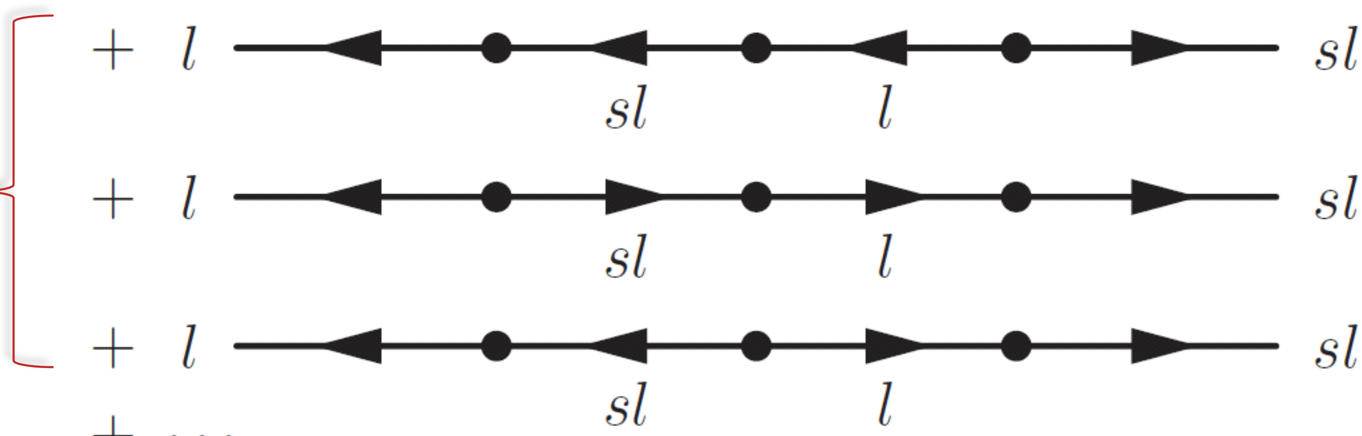
Diagrammatic Diagnosis Part 2:
Speaking in the New Languange…

Let us compare what we got after translating the Feynman-Dyson expansion…



… with a direct Feynman-Dyson dressing of the same vertex:

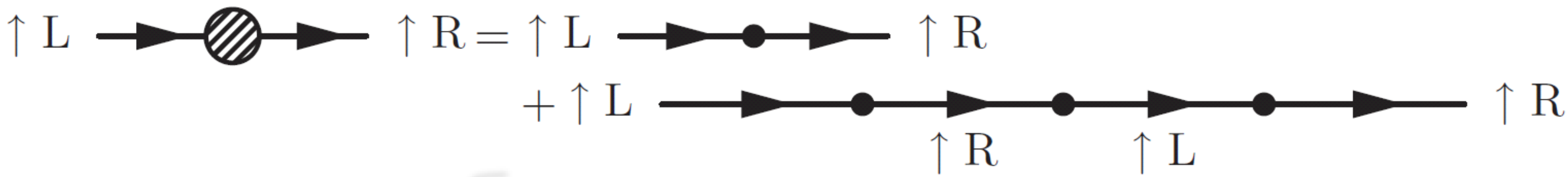


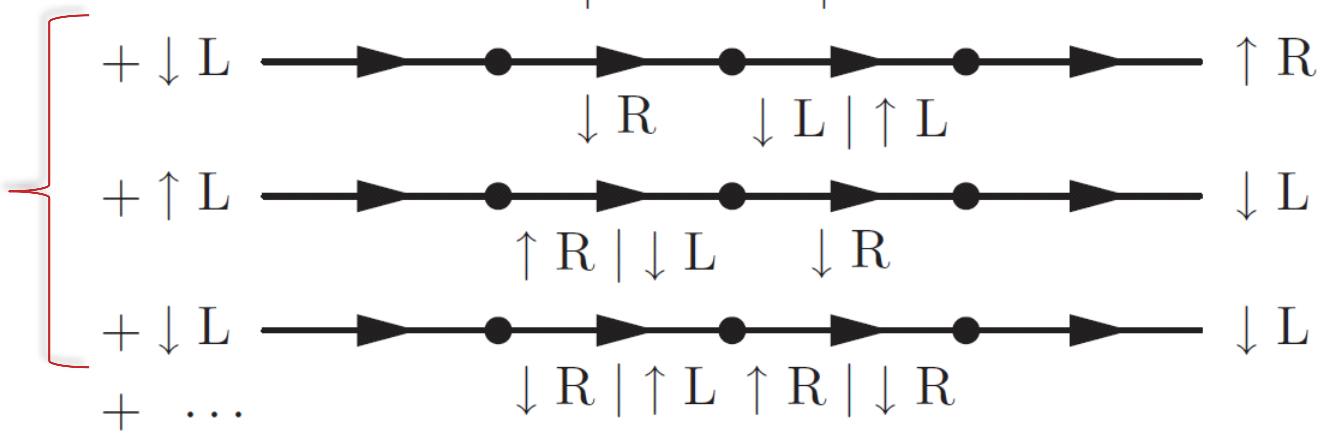


Saying *New* Things:
These three *new* processes are extra…

Diagrammatic Diagnosis Part 3:
Difficulties with Back-translation…

Higher-order Feynman-Dyson terms don't translate-back well:





<u>Spinning *Old* Words</u>:
The three *new* terms are not spin conserving…

- When translating back, the last three processes cannot be translated in terms of spin-conserving propagators.
- The last two processes cannot be translated back in terms of propagators conserving lead or flavor index (L or R) either.

Final Diagnosis: Violation of certain conservation laws in the Bosoization-deBosonization procedure

What is the resolution of the Paradox?

A new consistent formalism in which non-conserving terms are *not* generated while doing Feynman-Dyson perturbation theory in terms of *new* fermions.

Bringing back Consistency

Let us introduce the following definition:

Key idea $$\boxed{e^{\pm i\phi_{c,s}/2} e^{\mp i\phi_{c,s}/2} \mapsto \tilde{n}^{\pm}_{c,s}}$$

After bosonizing and changing basis, it is standard *(conventional)* to simplify products of boson exponentials (vertex operators) with opposite signs. This amounts to replacing $\tilde{n}^{\pm}_{\nu} \rightarrow 1$ everywhere

Let us not do that, but instead simply keep those products around. Then the tunneling Hamiltonian in terms of *new* fermions reads:

$$\begin{aligned} H_{\mathrm{tun}} = & -e^{ieVt}\gamma_{\mathrm{t}}\tilde{n}_c^{+}\tilde{n}_s^{+}\breve{\psi}_l\breve{\psi}_{sl} - e^{ieVt}\gamma_{\mathrm{t}}\tilde{n}_c^{+}\tilde{n}_s^{-}\breve{\psi}_{sl}^{\dagger}\breve{\psi}_l \\ & - e^{-ieVt}\gamma_{\mathrm{t}}^{*}\tilde{n}_c^{+}\tilde{n}_s^{+}\breve{\psi}_{sl}^{\dagger}\breve{\psi}_l^{\dagger} - e^{-ieVt}\gamma_{\mathrm{t}}^{*}\tilde{n}_c^{+}\tilde{n}_s^{-}\breve{\psi}_l^{\dagger}\breve{\psi}_{sl} \end{aligned}$$

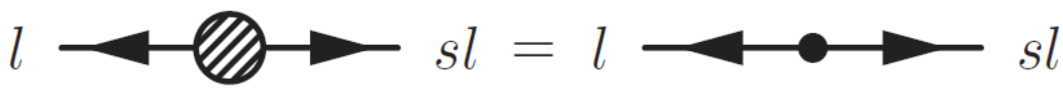
Keys to Consistency

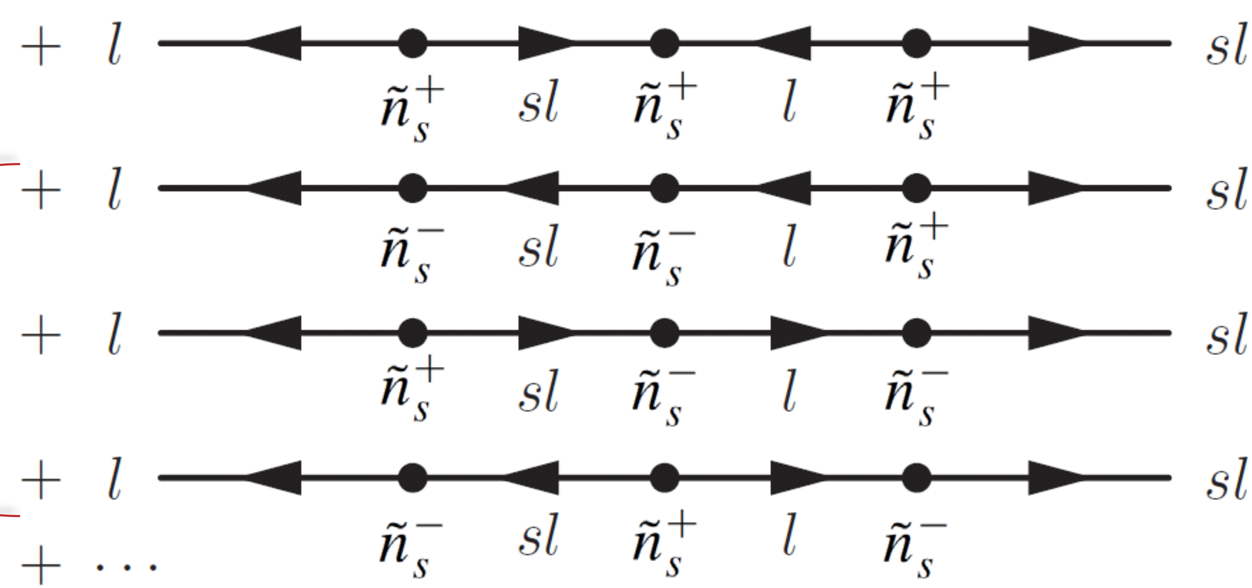
The $\tilde{n}$'s can be thought of as single-site fermion lattice densities. As such, they have the properties of *idempotence* and *co-nilpotence*.

$$(n^{\pm}_{c,s})^2 = n^{\pm}_{c,s}$$

$$n^{\pm}_{c,s} n^{\mp}_{c,s} = 0$$

Since the *spin sector* decoupled from the tunneling problem (spin-charge separation), the property of co-nilpotence restricts the ways of dressing vertexes:





Co-nilpotence:
These three terms **vanish identically!**

Some Finer Details

$$:\psi_\nu^\dagger \psi_\nu := \frac{1}{2\pi}\partial\phi_\nu$$

$$\psi_\nu^\dagger \psi_\nu = e^{i\phi_\nu} e^{-i\phi_\nu}/2\pi a$$

These two need to be consistent,
the OPE of the second one shows how.
It is an expansion on *density fluctuations*!

With BdB, one is usually concerned with a particle-hole symmetric starting point. Which is akin to half filling. But it is possible to change that by *shifting the bosons*.

For the junction, this is equivalent to considering different Boundary Conditions
We are lead to consider anti-periodic BCs (i.e., Affleck's "strong-coupling BCs").

As a result, some non-intuitive numerical factors need to be introduced:

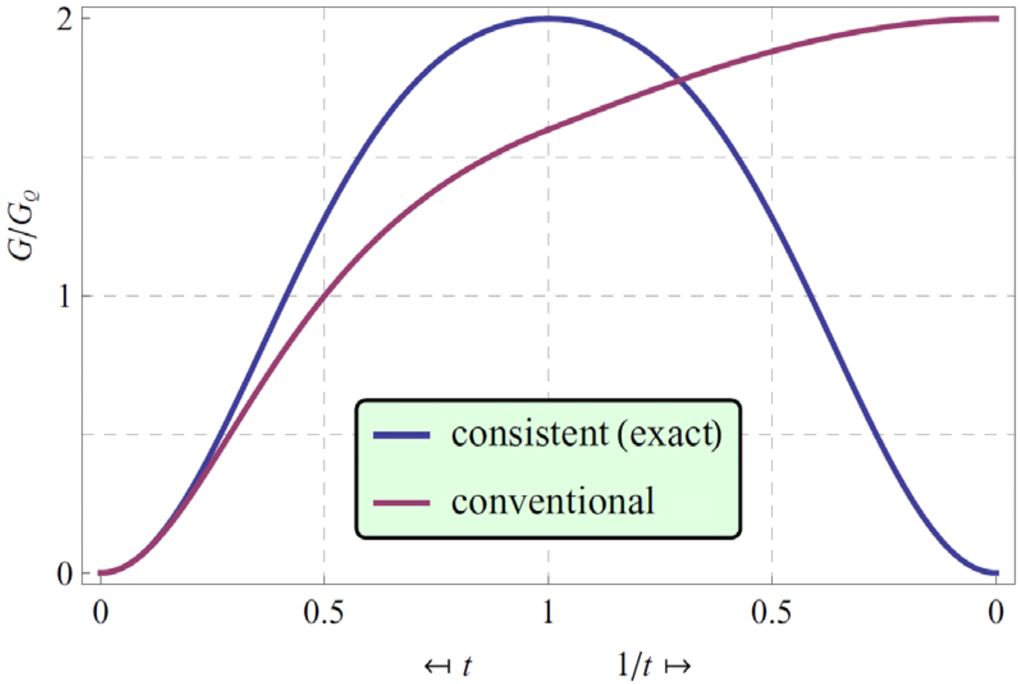
$$2n_{\sigma\ell} \approx \prod_n \sqrt{2}\tilde{n}_{\nu_n} \quad \text{when} \quad 2n_{\sigma\ell} \approx 1,$$

$$2n_{\sigma\ell} \approx \frac{1}{2}\prod_n \sqrt{2}\tilde{n}_{\nu_n} \quad \text{when} \quad 2n_{\sigma\ell} \approx 2$$

For further details on matters of regularization see the papers [PRB 2016]…

Conventional vs. Consistent BdB Approaches

Case study of a (non)-equilibrium junction



Considered a simple junction problem, which is **exactly** solvable both directly and after using BdB transformation

Qualitative discrepancy between conventional and consistent BdB approaches!

Conventional approach yields unphysical results as evident from large t regime.

Key idea

$$\boxed{e^{\pm i\phi_{c,s}/2} e^{\mp i\phi_{c,s}/2} \mapsto \tilde{n}^{\pm}_{c,s}}$$

References:

[1] Series of Papers: Phys. Rev. B **93**, 085440 and 085441 (2016)

Conclusions and Outlook

- Bosonization-deBosonization is subtler than previously thought, but consistency ñ factors save the day and provide guidance in keeping track of boundary conditions and symmetries of the problem
  - Many possible ramifications
    - Other Junction Problems
    - Quantum Impurity Problems
    - Special Boundaries
  - Many possible directions to study the physics of (out-of-equilibrium) strongly correlated (open) quantum systems
- We have already shown that the Non-equilibrium Kondo Problem shows important changes! [next talk]