Exact bosonization for interacting fermions in arbitrary dimensions.

(New route to numerical and analytical calculations)

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Bosonization: mapping of electron models onto a model describing collective excitations (charge, spin excitations, diffusion modes, etc).

Origin of the word: 1D electron systems.

A general fermionic Hamiltonian

$$\hat{H} = \sum_{p} \varepsilon_p \psi^{+}_{p} \psi_{p} + \frac{V_0}{2} \sum_{p_1, p_2, p_3; \alpha, \beta} \psi^{+}_{p_1, \alpha} \psi^{+}_{p_2, \beta} \psi_{p_2 - q, \beta} \psi_{p_1 + q, \alpha}$$

Fermionic anticommutation realtions.

$$\left\{ \psi^{+}_{p}, \psi_{p'} \right\} = \delta_{p, p'}$$

$$\left\{ \psi_{p}, \psi_{p'} \right\} = \left\{ \psi^{+}_{p}, \psi^{+}_{p'} \right\} = 0$$

However, there are also bosonic variables.

$$\rho_k = \sum_{p} \psi^{+}_{p} \psi_{p+k}$$

$$\psi \propto \exp(i\phi)$$

Can one reformulate the model in terms of the bosonic variables?

The main idea: writing the electronic operators ψ as

$$\psi \propto \exp(i\varphi)\exp\left(i\int \rho dx\right)$$

A simple Hamiltonian H

$$H = \int [K\rho^2 + N(\nabla\varphi)^2]dx \qquad [\rho, \varphi] = -i$$

ρ -Density fluctuations operator

K-compressibility, N-average density

Importance of long wave length excitations!

Bosonization: for Tomonaga-Luttinger model (long range interaction) (Luttinger, Tomonaga (196?))

The most general form conjectured by K.E. & A. Larkin (1975)

Microscopic theory Haldane (1982)

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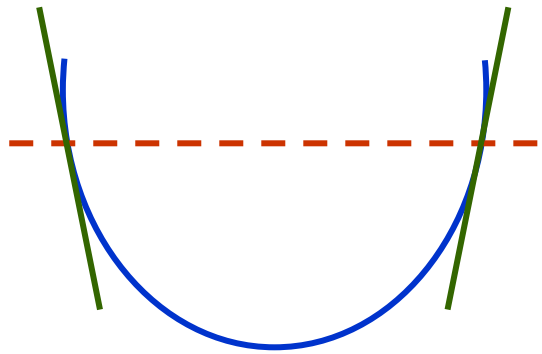
Assumptions:

1. The system is one dimensional.
2. The spectrum is linear.

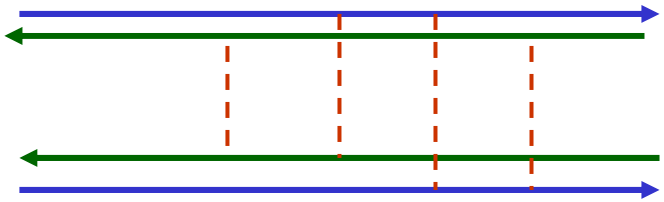
$\varepsilon(p)$



Fermion correlation functions are expressed using

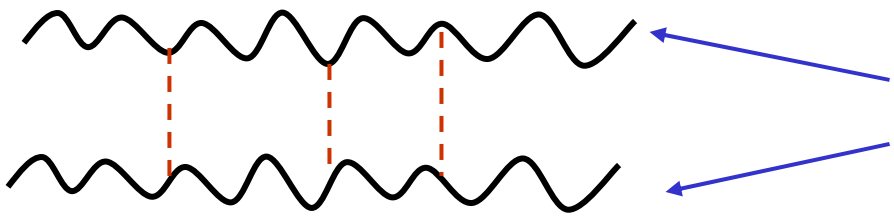
$$\psi \propto \exp(i\varphi)\exp\left(i\int \rho dx\right)$$

Formal replacement of electron Green functions by propagators for collective excitations!



Very often direct expansions with electronic Green functions are not efficient (infrared divergences, high energy cutoffs respecting symmetries).

Equivalent representation



Spin excitations

Transformation from electrons to collective excitations: Bosonization

Why should one bosonize the electronic systems?

A. General interest to description of low temperature behavior. Main contribution comes for the collective excitations and it may be more convenient to have the corresponding bosonic fields.

B. Monte Carlo simulations are difficult for the fermions. The computation time grows exponentially with the inverse temperature 1/T, interaction V and the size of the system N.

Difficulties in Monte Carlo simulations for fermionic systems: negative sign problem ⟹ exponential growth of the computation time with the size of the system.

Negative Sign Problem

$$\langle A \rangle = \frac{Tr[A\exp(-\beta H)]}{Tr(-\beta H)} = \frac{\sum_i A_i p_i}{\sum_i p_i}$$

Random choice of A_i

Fermionic sign problem arises when one of $p_i < 0$

Standard MC procedure

$$\langle A \rangle = \frac{\sum_i A_i p_i}{\sum_i p_i} = \frac{\sum_i (A_i \operatorname{sgn} p_i)|p_i| / \sum_i |p_i|}{\sum_i (\operatorname{sgn} p_i)|p_i| / \sum_i |p_i|} = \frac{\langle Asign \rangle_{|p|}}{\langle sign \rangle_{|p|}}$$

Exponentially increasing time due to the cancellation problem in sign!

$$\langle Asign \rangle_{|p|} \approx \langle sign \rangle_{|p|} \approx \exp(-c\beta N) \quad \Longrightarrow \quad \delta A \propto \exp(c\beta N)$$

Can one bosonize in higher dimensions?

Earlier attempts:

A. Luther 1979: Special form of Fermi surface (square, cube, etc.). Almost 1D.

F.D.M. Haldane 1992: Patching of the Fermi surface, no around corner scattering

Further development of the patching idea:

A. Houghton & Marston 1993; A.H. Castro Neto & E. Fradkin 1994;
P. Kopietz & Schonhammer 1996; Khveshchenko, R. Hlubina, T.M. Rice 1994 et al; C. Castellani, Di Castro, W. Metzner 1994……

Main assumption of all these works: long range interaction.

I.L. Aleiner & K. B. Efetov 2006, Method of quasiclassical Green functions supplemented by integration over supervectors

Logarithmic contributions to specific heat and susceptibility are found. Good agreement with known results in 1D. No restriction on the range of interaction but not a full account of effects of the Fermi surface curvature in d>1.

In all the approaches only low energy excitations were considered: no chance for using in numerics.

Present work: Exact mapping fermion models onto bosonic ones.
New possibilities for both analytical and numerical computations.

Warning:
Exact in the continuous time thermodynamic limit!

Starting Hamiltonian H

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$$

$$Z = Tr \exp(-\hat{H}/T)$$

$$\hat{H}_0 = -\sum_{r,r';\sigma} t_{r,r'} c^+_{r\sigma} c_{r'\sigma} - \mu \sum_{r,r';\sigma} c^+_{r\sigma} c_{r\sigma}$$

The interaction, tunneling and dimensionality are arbitrary!

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{r,r';\sigma,\sigma'} V_{r,r'} c^+_{r\sigma} c^+_{r'\sigma'} c_{r'\sigma'} c_{r\sigma}$$

Small simplification of the formulas

$$V_{r,r'} = \delta_{r,r'} V_0, \qquad V_0 > 0 \quad \Rightarrow$$

$$\hat{H}^{(0)}_{\text{int}} = -\frac{V_0}{2} \sum_r \left(c^+_{r,+} c_{r,+} - c^+_{r,-} c_{r,-} \right)^2$$

$$\mu' \to \mu - V/2$$

Hubbard-Stratonovich Transformation with a real field $\phi(\tau)$

$$Z = Tr_{\bar{c},c}\left[-\beta\hat{H}_0\right]T_\tau \exp\left(-\int_0^\beta \hat{H}_{\text{int}}(\tau)d\tau\right)$$

$$\hat{H}_{\text{int}}(\tau) = \exp(\hat{H}_0\tau)\hat{H}_{\text{int}}\exp(-\hat{H}_0\tau)$$

$$\bar{c} = \exp(H_0\tau)c^+\exp(-H_0\tau)$$

Decoupling of the quartic interaction

$$T_\tau \exp\left(-\int_0^\beta \hat{H}_{\text{int}}(\tau)d\tau\right) = \int T_\tau \exp\left(\sum_{r,\sigma}\int_0^\beta \sigma\phi_r(\tau)\bar{c}_{r,\sigma}(\tau)c_{r,\sigma}(\tau)d\tau\right)\exp\left[-\frac{1}{2V_0}\sum_r\int_0^\beta \phi^2(r,\tau)d\tau\right]D\phi$$

$$\phi(\tau) = \phi(\tau+\beta), \qquad \beta = 1/T$$

Fermions in an "external field"

$$Z = \int Z_f[\phi] \exp\left[-\frac{1}{2V_0} \sum_r \int_0^\beta \phi^2(r,\tau) d\tau \right] D\phi$$

$$\hat{\varepsilon}_r f_r = -\sum_{r'} t_{r,r'} f_{r'}$$

$$Z_f[\phi] = \exp\left[\int_0^\beta Tr_{r,\sigma} \ln\left(-\partial/\partial\tau - \hat{\varepsilon}_r + \sigma\phi_r(\tau) + \mu' \right) d\tau \right]$$

Another representation for $Z_f[\phi]$

$$Z_f[\phi] = \det_{r,\sigma}\left[1 + T_\tau \exp\left(-\int_0^\beta \left(\hat{\varepsilon}_r - \sigma\phi_r(\tau) - \mu' \right) d\tau \right) \right]$$

Unpleasant feature of $Z_f[\phi]$: non-locality in time

Further transformations are desirable!

Derivation of the model (main steps):

$$Z_f[\phi] = Z_0 \exp\left[\sum_{r,\sigma}\int_0^\beta\int_0^1 \sigma\phi_r(\tau)\left[G_{r,r;\sigma}(\tau,\tau+0) - G^{(0)}_{r,r;\sigma}(\tau,\tau+0)\right]d\tau du\right]$$

$G^{(0)}{}_{r,r';\sigma}(\tau,\tau') = \left[G_{r,r';\sigma}(\tau,\tau')\right]_{\phi=0}$ is the Green function of the ideal Fermi gas

$$\left(-\frac{\partial}{\partial\tau} - \hat{\varepsilon}_r + \sigma u\phi_r(r) + \mu'\right)G_{r,r';\sigma}(\tau,\tau') = \delta_{r,r'}\delta(\tau-\tau')$$

$$G_{r,r';\sigma}(\tau,\tau')\left(\frac{\partial}{\partial\tau'} - \hat{\varepsilon}_{r'} + \sigma u\phi_{r'}(r) + \mu'\right) = \delta_{r,r'}\delta(\tau-\tau')$$

$G_{r,r';\sigma}(\tau,\tau')$ -fermionic Green function in the external field.

Boundary conditions

$$G(\tau,\tau') = -G(\tau+\beta,\tau') = -G(\tau,\tau'+\beta)$$

Reformulating the theory in terms of bosonic fields $A_{r,r'}(\tau)$

$$A_{r,r'}(\tau) = G^{(0)}_{r,r'}(\tau, \tau+0) - G_{r,r'}(\tau, \tau+0)$$

Bosonic periodic boundary conditions: $A(\tau) = A(\tau+\beta)$

Then, the "partition function" $Z[\phi]$ is

$$Z_b[\phi] = Z_0 \exp\left[-\sum_{r,\sigma} \int_0^1 \int_0^\beta \phi_r(\tau) A_{rr}(z) du d\tau \right]$$

$$z = \{\tau, \sigma, u\}$$

$$n_{r,r'} = G^{(0)}_{r,r'}(-0)$$ -Fourier transform of the Fermi distribution n(p)

$$n(p) = \frac{1}{e^{\beta(\varepsilon(p)-\mu')} + 1}$$

(Almost) Final equation for A

$$\left(\frac{\partial}{\partial\tau}+\hat{\varepsilon}_r-\hat{\varepsilon}_{r'}-\sigma u\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)\right)A_{r,r'}(z)=-un_{r,r'}\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)$$

$$z=\{\tau,\sigma,u\}$$

First check assuming that $\phi_r(\tau)$ is small

$$A_{r,r'}(\tau)=T\sum_{\omega}\int A_p(k,\omega)e^{-i\omega\tau+ip(r-r')+ik(r+r')/2}\frac{d^d p d^d k}{(2\pi)^{2d}}$$

$$\left(-i\omega+\varepsilon(p+k/2)-\varepsilon(p-k/2)\right)A_p(k,\omega)=-u\phi(k,\omega)\left(n(p+k/2)-n(p-k/2)\right)$$

Left hand side of the equation for A: similarity with the Boltzmann equation.

The solution in the main approximation.

$$Z = Z_0 \int \exp\left[-\frac{T}{2} \sum_{\omega} \int |\phi(k,\omega)|^2 \left(V_0^{-1} + \int \frac{n(p-k/2) - n(p+k/2)}{i\omega + \varepsilon(p-k/2) - \varepsilon(p+k/2)} \frac{d^d p}{(2\pi)^d} \right) \frac{d^d k}{(2\pi)^d} \right] D\phi$$

$$Z = Z_0 \exp\left[-\frac{T}{2} \sum_{\omega} \int \frac{d^d k}{(2\pi)^d} \ln\left[1 + V_0 \int \frac{n(p-k/2) - n(p+k/2)}{i\omega + \varepsilon(p-k/2) - \varepsilon(p+k/2)} \frac{d^d p}{(2\pi)^d} \right] \right]$$

Random phase approximation: First order of expansion in the interaction between collective modes.

Chances to construct a field theory for the bosonic interacting excitations!

Two Directions of Research (next lectures)

1. Analytical.
   Construction of (almost) supersymmetric field theory for description of interacting collective modes.

2. Numerical. Writing a Monte Carlo program. Hopes to overcome the sign problem.

Analytical calculations:

BRST (Becchi, Rouet, Stora, Tyutin)

-possibility of integration over the auxiliary field before doing approximations

How to calculate $B[A_0]$ if A_0 is the solution of the equation $F(A)=0$?

A well known trick: $$B[A_0]=\int B(a)\delta(F(a))\left|\det\left(\frac{\partial F}{\partial a}\right)\right|da$$

Next step: $$\delta(F(a))=C\int\exp(ifF(a))df$$

$$\det\left(\frac{\partial F}{\partial a}\right)=\int\exp[\rho(\partial F/\partial a)\sigma]d\sigma d\rho$$

σ,ρ -Grassmann variables

The main ideas

Grassmann anticommuting variables χ :

$$\{\chi_i, \chi_j\} = 0 \qquad \chi_i^2 = 0$$

Integrals (Berezin 1961):

$$\int \chi_i d\chi_i = 1 \qquad \int d\chi_i = 0$$

All other integrals are repetitions of these two.

Any function of the Grassmann variables is a polynomial !

Example: $\exp(-\chi a \eta) = 1 - \chi a \eta$

Vectors

$$\vec{\chi} = (\chi_1 \quad \chi_2 \quad \dots \quad \chi_n)$$

Quadratic forms

$$\vec{\chi} A \vec{\eta} = \sum_{i=1}^{n} \chi_i A_{ik} \eta_k$$

Some integrals.

$$\int \exp(-\chi a \eta) d\chi d\eta = \int (1 - \chi a \eta) d\chi d\eta = a$$

$$\int \exp(-\vec{\chi} A \vec{\eta}) \prod_{i=1}^{n} d\chi_i d\eta_i = \det A$$

Not $(\det A)^{-1}$ as for conventional variables!

An immediate consequence.

If F(A)=0, where F and A are matrices, one can write a function $B(A_0)$ of the solution A_0 as

$$B(A_0) = \int B(a) \delta(F(a)) Det \left| \frac{\partial F}{\partial a} \right| da$$

$$= \int B(a) \exp[iTr(XF(a))] \exp[-Tr\chi(\partial F / \partial a)\eta] d\chi d\eta$$

The basis of the BRST supersymmetric representation.

Description with a supersymmetric action and superfields Ψ

$$\left(\frac{\partial}{\partial\tau}+\hat{\varepsilon}_r-\hat{\varepsilon}_{r'}-\sigma u\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)\right)A_{r,r'}(z)=-un_{r,r'}\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)$$

Introducing new Grassmann variables θ,θ^* and Ψ superfields

$$\Psi_{r,r'}(R)=a_{r,r'}(z)\theta+f^T_{r,r'}(z)\theta^*+\eta_{r,r'}(z)+\eta^+_{r,r'}(z)\theta^*\theta$$

$$R=\left\{\tau,\sigma,u,\theta,\theta^*\right\}$$

Ψ is anticommuting (!)

The "partition function" $Z[\phi]$ as the functional integral over Ψ

$$Z[\phi]=Z_0\exp\left(S_{ss}[\Psi]-S_{sb}[\Psi]\right)$$

$$S_{ss}[\Psi]=\frac{i}{2}\sum_{r,r'}\int \Psi_{r',r}\left(\frac{\partial}{\partial\tau}+\hat{h}_{r,r'}\right)\Psi_{r,r'}dR$$

$$\hat{h}_{r,r'}=\hat{\varepsilon}_r-\hat{\varepsilon}_{r'}-\sigma u\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)$$

$$S_{sb}[\Psi]=-\sum_r\int\sigma\phi_r(\tau)\Psi_{r,r'}\theta^* dR+i\sum_{r,r'}\int\sigma n_{r,r'}\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)\Psi_{r,r'}\theta u dR$$

Why had one to try to represent the function $Z[\phi]$ in such a form?

Gaussian averaging over ϕ can immediately be performed!

$$Z=\int Z_b[\phi]\exp\left[-\frac{1}{2V_0}\int_0^\beta\phi^2(r,\tau)\right]D\phi$$

Final superfield theory (still exact).

$$Z = Z_0 \int \exp\left(-S[\Psi]\right) D\Psi$$

$$S[\Psi] = S_0[\Psi] + S_B[\Psi] + S_I[\Psi]$$

Z_0 -partition function of the ideal Fermi gas

$$S_0[\Psi] = \frac{i}{2} \sum_{r,r'} \int \left[\Psi_{r',r} \left(\frac{\partial}{\partial \tau} + \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} \right) \Psi_{r,r'} \right] dR$$

$S_0[\Psi]$ is the bare action
(fully supersymmetric)

The interaction terms.

$$S_B[\Psi] = -\frac{V_0}{2}\int \delta(\tau-\tau_1)\Psi_{r,r}(R)\theta^*\left(\Psi_{r,r}(R_1)\theta_1^* + 2i\Pi_r(R_1)\right)\sigma\sigma_1 dRdR_1$$

$$S_I = \frac{V_0}{2}\sum_r \int \delta(\tau-\tau_1)\Pi_r(R)\Pi_{r'}(R_1)\sigma\sigma_1 dRdR_1$$

$$\Pi_r(R) = u\sum_{r'}\left[\left(\Psi_{r',r}(R) - n_{r,r'}\theta\right)\left(\Psi_{r,r'}(R) - n_{r,r'}\theta\right)\right]$$

The terms S_0 and S_I are invariant under the transformation of the fields : Ψ

$$\Psi_{r,r'}\left(\theta,\theta^*\right)\mapsto \Psi_{r,r'}\left(\theta+\kappa,\theta^*+\kappa^*\right)-\kappa n_{r,r'}$$

(Almost) supersymmetry transformation.

κ,κ^* -anticommuting variables

What to calculate?

Logarithmic contributions exist in any dimensions and they can be studied by RG. Reduction of the exact model to a low energy one is convenient. Variety of phenomena for, e.g., cuprates and other strongly correlated systems can be attacked in this way.

Second order perturbation theory in both fermionic and bosonic representations.

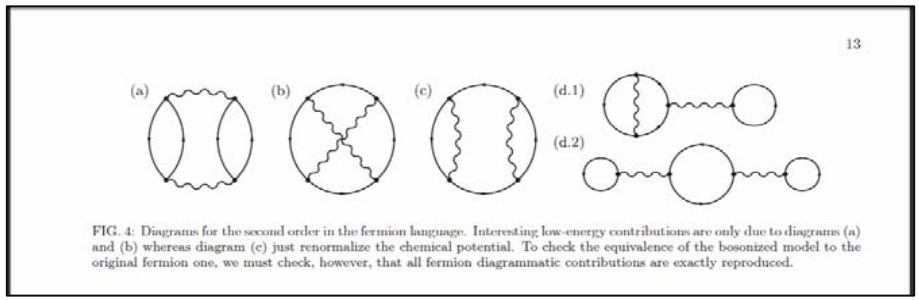


FIG. 4: Diagrams for the second order in the fermion language. Interesting low-energy contributions are only due to diagrams (a) and (b) whereas diagram (c) just renormalize the chemical potential. To check the equivalence of the bosonized model to the original fermion one, we must check, however, that all fermion diagrammatic contributions are exactly reproduced.

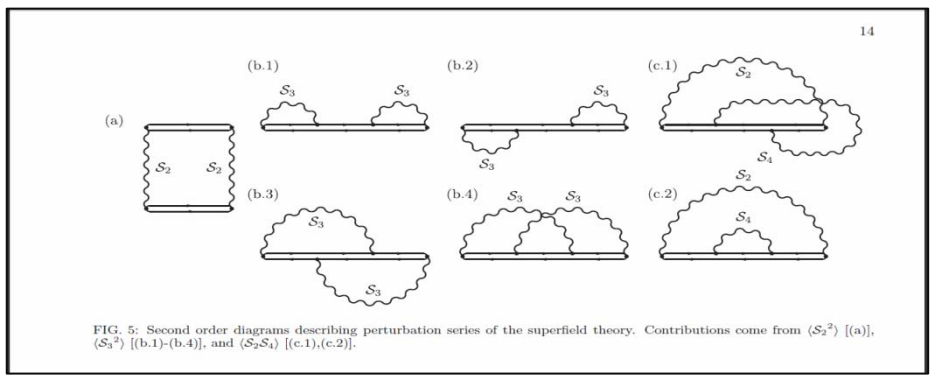


FIG. 5: Second order diagrams describing perturbation series of the superfield theory. Contributions come from $\langle S_2^2 \rangle$ [(a)], $\langle S_3^2 \rangle$ [(b.1)-(b.4)], and $\langle S_2 S_4 \rangle$ [(c.1),(c.2)].

Green functions.

$$\frac{1}{i\varepsilon_n - \varepsilon(p) + \mu}, \qquad \varepsilon_n = 2\pi\left(n + \frac{1}{2}\right)$$

$$n = 0, \pm 1, \pm 2, \pm 3 \ldots$$

$$\frac{1}{-i\omega_n + \varepsilon\left(p + \frac{k}{2}\right) - \varepsilon\left(p - \frac{k}{2}\right)}$$

Fermionic diagram (c) from bosonic b.1, b.2, c.2

$$\omega_n = 2\pi n$$

Necessity to introduce a bath and exclude some states.

Introducing the bath $$V_{r,r}^{total} = \begin{cases} V_0, & r < R \\ 0, & r > R \end{cases}$$

Fourier transform $$V^{total}(q, q_0) = \sum_{r,r'} V_{r,r'} e^{-iq_0(r+r')/2 - iq(r-r')}$$ ⇒ Translational invariance is broken!

Introducing a small parameter γ to exclude the solutions of the homogeneous equation (coinciding states in the diagrams).

$$\begin{pmatrix} \gamma & \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} + \partial/\partial\tau \\ \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} - \partial/\partial\tau & -\gamma \end{pmatrix} \Gamma_{r,r';r_1,r_1'}(\tau, \tau_1) = \delta_{r,r_1}\delta_{r',r_1'}\delta(\tau - \tau_1)$$

The introduced error is of order 1/N

The function Y is not universal and depends on a cutoff function f.

Final result by RG
(from Aleiner and Efetov (2006))

$$\chi(\theta) = -\mu_d \gamma_b(\theta) \ln\left[\max\left\{\theta, T/\varepsilon_0\right\}\right]$$

$$\delta c_{d=2} = -\frac{3\zeta(3)T^2}{\pi\varepsilon_F^2}\left\{\left[\gamma_b^\rho\right]^2 + \frac{3\gamma_b^2\left\{\ln\left[1+\chi(T)\right]\right\}^2}{2\left[\chi(T)\right]^2}\right\}; \quad (7.37a)$$

$$\delta c_{d=3} = -\frac{3\pi^4}{10}\left(\frac{T}{\varepsilon_F}\right)^3 \times\left\{\left[\gamma_b^\rho\right]^2 \ln\frac{\varepsilon_F}{T} + \frac{3\gamma_b}{2\mu_3}\int_0^{\chi(T)}\frac{dz}{z^2}\left[\mathrm{L}i_2(-z)\right]^2\right\}; \quad (7.37b)$$

$$\mathrm{L}i_2(x) = \sum_{k=1}^{\infty} x^k/k^2$$

Polylogarithm function

Logarithms found for the first time by the bosonization.

1d case

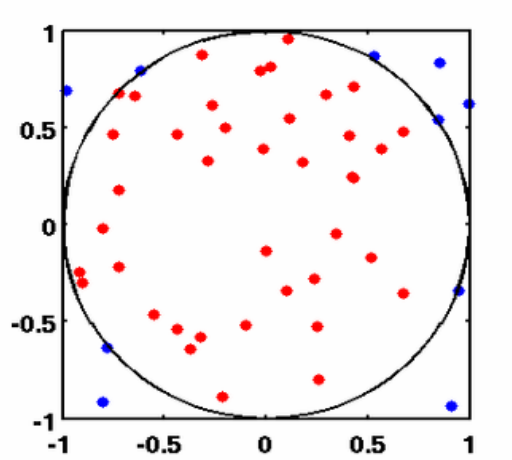
$$\delta\Omega_3(T) = -\frac{\pi T^2}{16 v_F}\left[\frac{2\gamma_b}{1+2\gamma_b \ln\frac{\epsilon_F}{T}}\right]^3$$

Agreement with Lukyanov (1998),

Excellent check of the validity of the method.

Monte Carlo method for statistical physics.

The main feature: probabilistic method of calculations



Calculation of π

General advantage: a drastic reduction of the computation time!

Example: Ising model.

$$Z = \sum_{\{s\}} \exp\left[-\beta \sum_{i,j} J_{ij} s_i s_j \right], \qquad \beta = 1/T$$

Sum over 2^N configurations

The same for an average.

$$K_{kl} = \frac{\sum_{\{s\}} s_k s_l \exp\left[-\beta \sum_{i,j} J_{ij} s_i s_j\right]}{\sum_{\{s\}} \exp\left[-\beta \sum_{i,j} J_{ij} s_i s_j\right]}$$

Again, the number of configurations in the sum is 2^N

How can the Monte Carlo method help?

Replacement of the sum over all configurations by the following sum:

$$K_{kl} = \frac{\sum_{\{s\}} s_k s_l P\{s\}}{\sum_{\{s\}} P\{s\}}, \qquad P\{s\} = \frac{\exp\left[-\beta \sum_{i,j} J_{ij} s_i s_j\right]}{\sum_{s} \exp\left[-\beta \sum_{i,j} J_{ij} s_i s_j\right]}$$

The partition function Z does not enter the average for K!
But why is it good?

P{s} is the probability distribution

Finding P{s} can be much faster than computing Z (the number of steps is proportional to N^{α} and not to 2^{N}).

Metropolis algorithm for finding P{s}

The algorithm is designed to generate a set of M configurations of the system $\xi_1, \xi_2, \xi_3, \ldots \xi_M$ such that

$$\lim_{M\to\infty} \frac{M_{\xi}}{M} = P(\xi)$$

$P(\xi)$ -is a given probability and M_{ξ} is the number of configurations ξ

Step 1: Pick a configuration ξ_n

Step 2: Pick trial configuration ξ_t and compute the probability ratio $R = \frac{P(\xi_t)}{P(\xi_n)}$. Pick a random number 0<p<1.

Make $\xi_{n+1} = \xi_t$ if p<R. Otherwise, make $\xi_{n+1} = \xi_n$

Step 3: Go to 2 replacing ξ_n by ξ_{n+1}

Step 3 is repeated M times, where M is a sufficiently large number.

The algorithm evolves any arbitrary distribution towards the equilibrium distribution where $\frac{M_\xi}{M} = P(\xi)$

As a result: $\langle A \rangle \approx \overline{A} = \frac{1}{M} \sum_\xi M_\xi A(\xi)$

However, all $P(\xi)$ must be positive to proceed with the MC method (trivial for the Ising model but generally not so for fermionic $Z_f[\phi]$

$$Z_f[\phi] = \exp\left[\int_0^\beta Tr_{r,\sigma} \ln\left(-\partial/\partial\tau - \hat{\varepsilon}_r + \sigma\phi_r(\tau) + \mu'\right) d\tau \right]$$

What can one do in this situation? Making a positive weight

$$\langle A \rangle = \frac{\sum_i A_i p_i}{\sum_i p_i} = \frac{\sum_i (A_i \operatorname{sgn} p_i)|p_i| / \sum_i |p_i|}{\sum_i (\operatorname{sgn} p_i)|p_i| / \sum_i |p_i|} = \frac{\langle Asign \rangle_{|p|}}{\langle sign \rangle_{|p|}}$$

However, one encounters a big problem: the average sign vanishes

$$\langle Asign \rangle_{|p|} \approx \langle sign \rangle_{|p|} \approx \exp(-c\beta N) \quad \Rightarrow \quad \delta A \propto \exp(c\beta N)$$

The computation time grows exponentially ⇒ no advantage of using Monte Carlo method.

One can try to convert the fermions into bosons hoping that the sign problem disappears for the latter.

Another representation for $Z_f[\phi]$

$$Z_f[\phi] = \det_{r,\sigma}\left[1 + T_\tau \exp\left(-\int_0^\beta (\hat{\varepsilon}_r - \sigma\phi_r(\tau) - \mu')d\tau\right)\right]$$

Basis of auxiliary field Monte Carlo simulations
(Blankenbecler, Scalapino, Sugar (1981))

Procedure: subdividing the interval $0 \le \tau \le \beta$ into time slices and calculation for each slice recursively.

The function $Z_f[\phi]$ is positive for slowly varying HS field ϕ
However, $Z_f[\phi]$ can in such a procedure be both positive and negative if ϕ strongly fluctuates:  sign problem!
Not convenient for analytical calculations either.

Good news: $Z[\phi]$ can exactly be obtained from a bosonic model!

What is exact and what is not in this derivation?

Examples of exact and approximate transformations.

$$\int_0^\infty \cos ax^2 dx = \frac{1}{\sqrt{2}} \int_0^\infty e^{-ax^2} dx$$

$$\sum_{i=1}^\infty \cos ax_i^2 (\Delta x) \neq \frac{1}{\sqrt{2}} \sum_{i=1}^\infty e^{-ax_i^2} (\Delta x)$$

Difficulty of a numerical computation depends on the analytical representation!

(Almost) Final equation for A

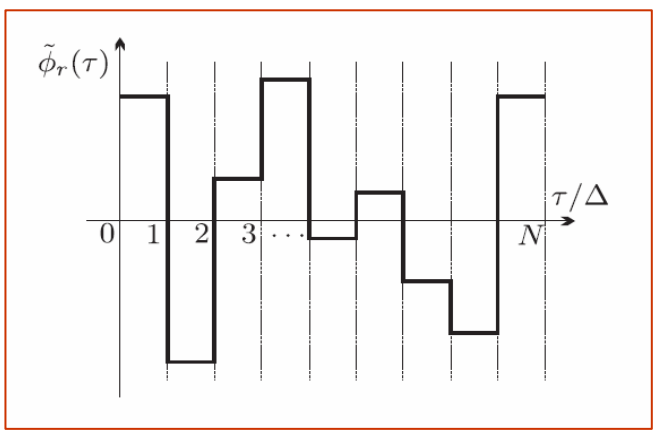
$$\left(\frac{\partial}{\partial\tau}+\hat{\varepsilon}_r-\hat{\varepsilon}_{r'}-\sigma u\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)\right)A_{r,r'}(z)=-un_{r,r'}\left(\phi_r(\tau)-\phi_{r'}(\tau)\right)$$

$$z=\{\tau,\sigma,u\}$$

The functions $\phi_r(\tau)$ and $\phi_{r'}(\tau)$ are taken at the same time!

Exact for smooth functions $\phi_r(\tau)$ but a big difference for typical functions arising in MC procedure!

Typical Hubbard-Stratonovich field



$$Z_b[\phi]\neq Z_f[\phi]$$

Partition function

$$Z = \int Z_b[\phi] \exp\left[-\frac{1}{2V_0} \int_0^\beta \phi^2(r,\tau) \right] D\phi$$

$$Z_b[\phi] = Z_0 \exp\left[-\sum_{r,\sigma} \int_0^1 \int_0^\beta \phi_r(\tau) A_{rr}(z) du d\tau \right]$$

Boundary conditions

$$\phi_r(\tau) = \phi_r(\tau + \beta), \qquad A_{r,r'}(\tau) = A_{r,r'}(\tau + \beta)$$

Purely bosonic problem! Linear (almost separable) real equation for A

However: spurious solutions A for certain configurations ϕ exist and a regularization is necessary!

Regularization

Introduction of a bath with non-interacting electrons and excluding spurious solutions of the equation for A by doubling the size of the matrices A and introducing a small parameter γ

The bosonization is exact in the thermodynamic continuous time limit but is approximate for the piece-wise function!

Writing a positive real $Z_b[\phi]$ that differs from the original fermionic one.

Final formula for $Z_b[\phi]$ (suitable for numerics)

$$Z_b[\phi] = Z_0 \exp\left[-\frac{1}{2} \sum_{r,r_1,r_1'} \int_0^\beta \int_0^\beta d\tau d\tau_1 \phi_r(\tau) n_{r_1,r_1'} Tr\left[(\Gamma\Phi\Lambda_1)^{-1} \ln\left(1-(\Gamma\Phi\Lambda_1)^2\right) \right]_{\{r,r\},\{r_1,r_1'\}}^{\tau,\tau_1} \right]$$

The function Γ is the solution of the equation

$$\begin{pmatrix} \gamma & \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} + \partial/\partial\tau \\ \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} - \partial/\partial\tau & -\gamma \end{pmatrix} \Gamma_{r,r';r_1,r_1'}(\tau,\tau_1) = \delta_{r,r_1}\delta_{r',r_1'}\delta(\tau-\tau_1)$$

$$\Phi_{r,r'}(\tau) = \phi_r(\tau) - \phi_{r'}(\tau)$$

$$\Lambda_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

γ is the regularizer that should be taken as small as necessary

$Z_b[\phi]$ is real and positive: solution of the sign problem (?)

Perturbation theory:

expanding in $\phi_r(\tau)$ and subsequent integration over this field.

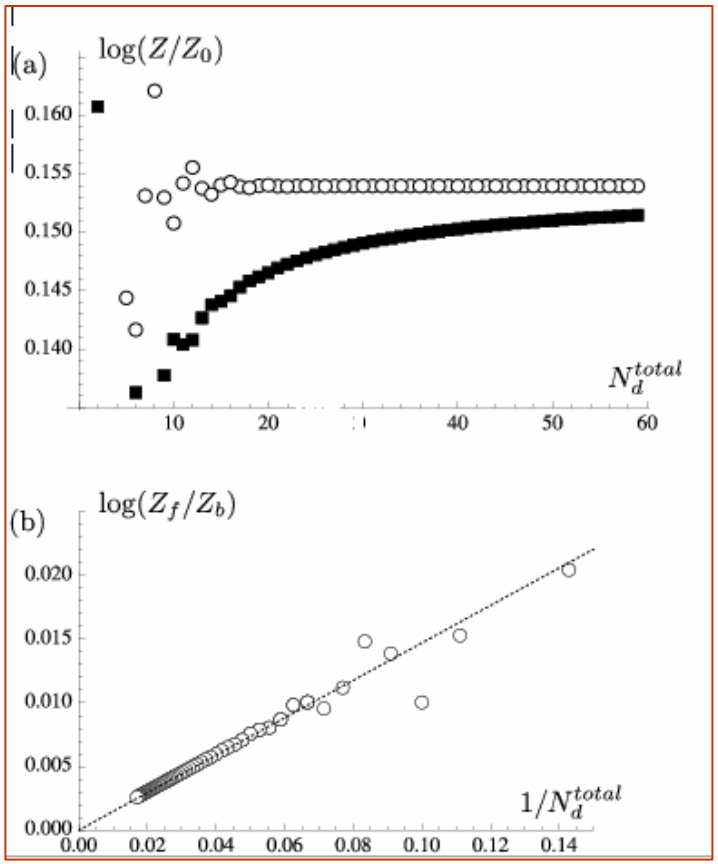
Main order:

$$Z = Z_0 \exp\left[-\frac{T}{2} \sum_{\omega} \int \frac{d^d k}{(2\pi)^d} \ln\left[1 + V_0 \int \frac{n(p-k/2) - n(p+k/2)}{i\omega + \varepsilon(p-k/2) - \varepsilon(p+k/2)} \frac{d^d p}{(2\pi)^d} \right] \right]$$

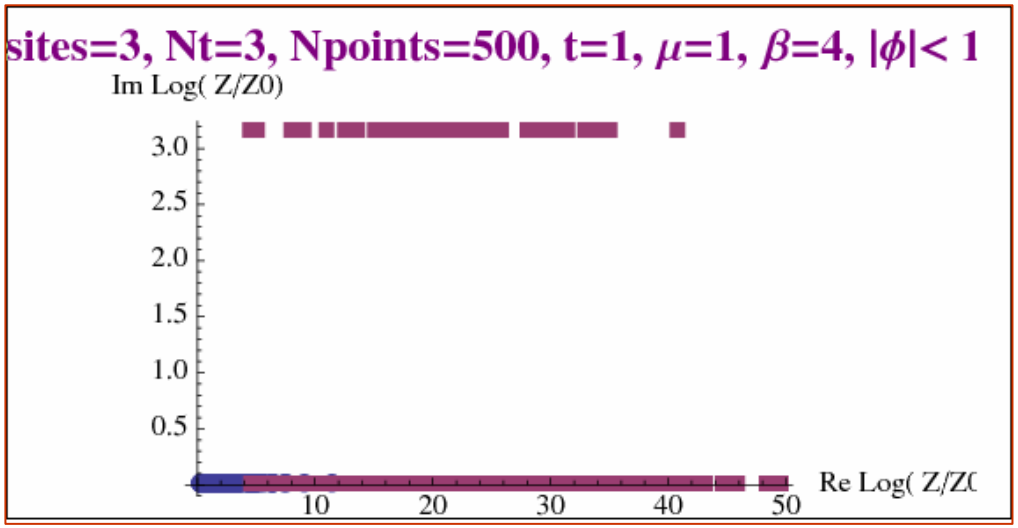
RPA-like formula

(first order in the expansion in collective excitations).

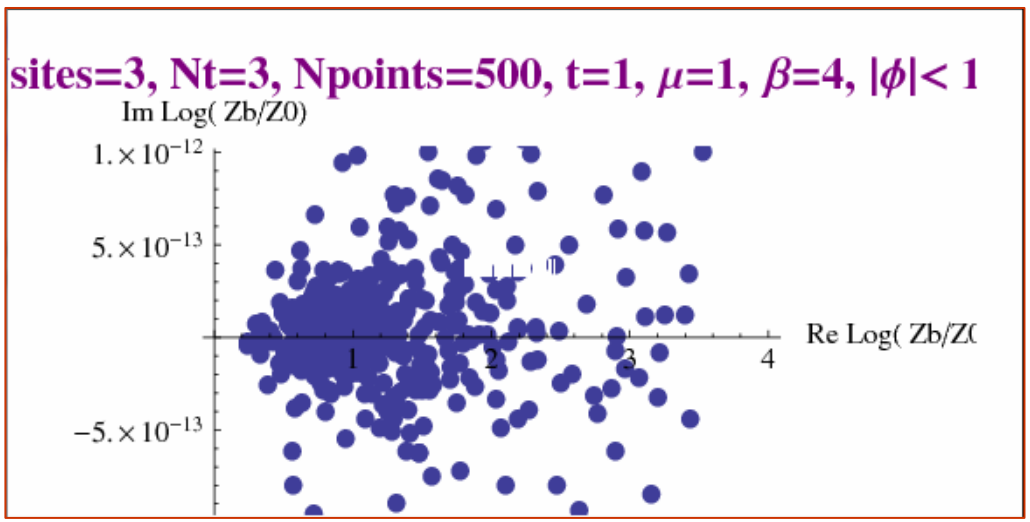
Numerical comparison of $Z_b[\phi]$ and $Z_f[\phi]$



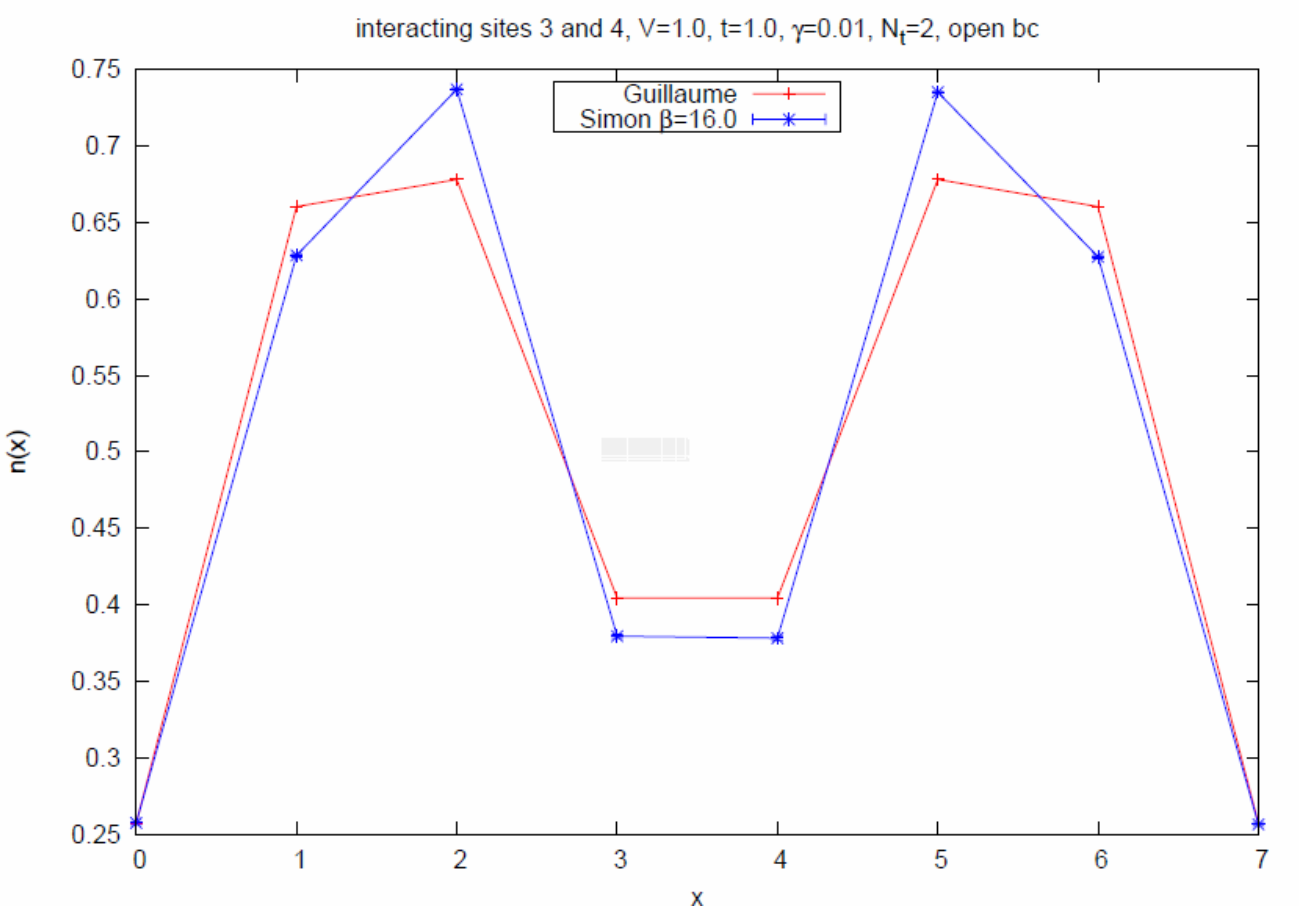
Fermionic and bosonic representations for two sites model for a static HS field ($\gamma = 10^{-2}$).



Fermionic representation
(two sites and one site bath,
three time slices,
500 random configurations).
Sign problem!

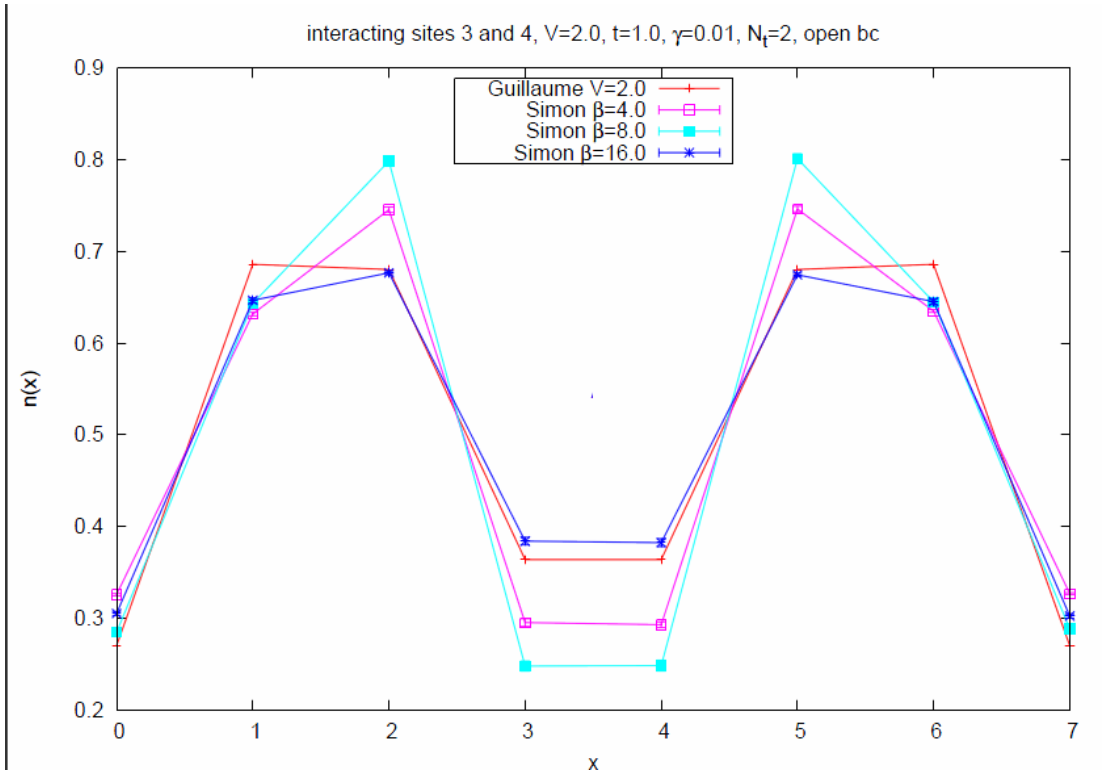


Bosonic representation
(the same parameters).
No sign problem!



First comparison of the bosonization MC with DMRG for the local number of particle n(x)

(Low temperature limit is most difficult for MC but DMRG gives results for zero temperature in 1D only)



The same for a stronger interaction.

A lot of hopes….

Conclusions.

The model of interacting fermions can be bosonized in any dimension for any reasonable interaction.

Can the bosonization be the key to the ultimate solution of the sign problem?
Can one solve non-trivial models (e.g., models for high temperature cuprates or for quantum phase transitions) using the supersymetric model for collective excitations?

To be answered