Exact bosonization for interacting fermions in arbitrary dimensions.

(New route to numerical and analytical calculations)

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Numerical realization: Ervand Kandelaki (RUB Bochum)

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

$$\hat{H} = \sum_p \varepsilon_p \psi_p^+ \psi_p + \frac{V_0}{2} \sum_{p_1, p_2, q; \alpha, \beta} \psi_{p_1,\alpha}^+ \psi_{p_2,\beta}^+ \psi_{p_2-q,\beta} \psi_{p_1+q,\alpha}$$

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

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

$$[\rho, \varphi] = -i$$

ρ -Density fluctuations operator

K-compressibility, N-average density

Importance of long wave length excitations!

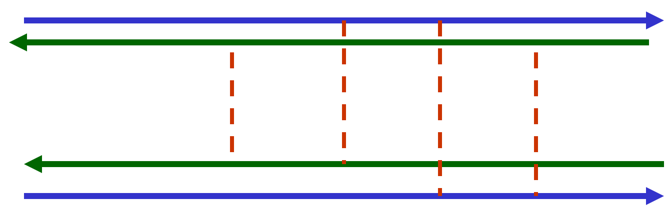
Bosonization: for Tomonaga-Luttinger model (long range interaction) (Luttinger, Tomonaga (196?))

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

Microscopic theory
Haldane (1982)

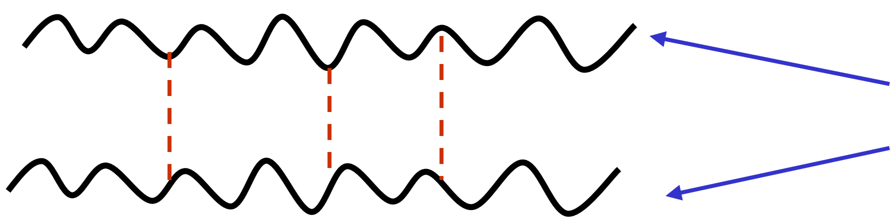
....

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!

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

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 of fermion models onto bosonic ones.
New possibilities for both analytical and numerical computations.

Warning:
Exact in the thermodynamic limit!

Singling out slow modes can still be convenient for analytical calculations.

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

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

$$\Rightarrow$$

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

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

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

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

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

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

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 $Z_f[\phi]$

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

Basis for fermionic MC

↓

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

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

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

$G_{r,r';\sigma}(\tau,\tau')$ -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

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

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

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

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

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

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

The solution in the main approximation.

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

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

⇓

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

Warning: uncertainty at $k = 0, \omega = 0$

However, its contribution is small in the thermodynamic limit!

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

Description with a supersymmetric action and superfields Ψ

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

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

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

Ψ is anticommuting but bosonic(!)

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

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

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)

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

The interaction terms.

$$S_B[\Psi] = -\frac{V_0}{2}\int \delta(\tau-\tau_1)\Psi_{r,r}(R)\theta^*\left(\Psi_{r,r}(R_1)\theta_1^* + 2i\Pi_r(R_1)\right)d\sigma d\sigma_1 dR dR_1$$

$$S_I = \frac{V_0}{2}\sum_r \int \delta(\tau-\tau_1)\Pi_r(R)\Pi_{r'}(R_1)d\sigma d\sigma_1 dR dR_1$$

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

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.

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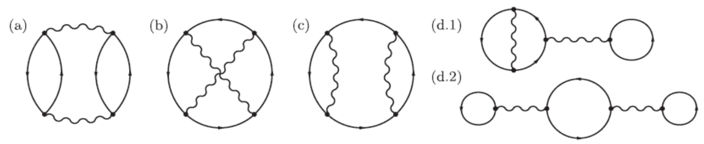

FIG. 4: Diagrams for the second order in the fermion language. Interesting low-energy contributions are only due to diagrams (a) and (b) whereas diagram (c) just renormalize the chemical potential. To check the equivalence of the bosonized model to the original fermion one, we must check, however, that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

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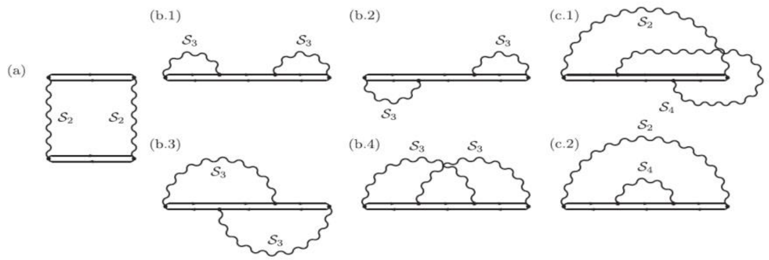


FIG. 5: Second order diagrams describing perturbation series of the superfield theory. Contributions come from $\langle \mathcal{S}_2{}^2 \rangle$ [(a)], $\langle \mathcal{S}_3{}^2 \rangle$ [(b.1)-(b.4)], and $\langle \mathcal{S}_2 \mathcal{S}_4 \rangle$ [(c.1),(c.2)].

Green functions.

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

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

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

$$\omega_n = 2\pi n$$

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

Necessity to exclude some states.

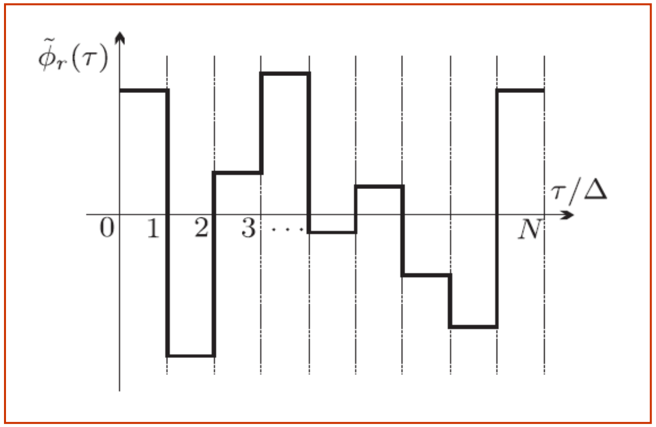
Monte Carlo for the bosonic model

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

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

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

Typical Hubbard-Stratonovich field



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

However, a good agreement is expected for physical Z.

Partition function

$$Z = \int Z_b[\phi] \exp\left[-\frac{1}{2V_0}\int_0^\beta \phi^2(r,\tau)\right] D\phi \qquad Z_b[\phi] = Z_0 \exp\left[-\sum_{r,\sigma}\int_0^1\int_0^\beta \phi_r(\tau) A_{rr}(z)\, du\, d\tau\right]$$

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: The solution for A is not unique and one should select one of them (not necessarily corresponding to the original one).

Regularization

Remove all solutions of the homogeneous equation (pseudoinversion).

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

$$B_{r,r'} = -u n_{r,r'}\left(\phi_r(\tau) - \phi_{r'}(\tau)\right)$$

$$\hat{M}_{r,r'} A_{r,r'} = B_{r,r'}$$

⇓

Tikhonov regularization → $\left(\hat{M}^T \hat{M} + \gamma^2\right) A_{r,r'} = \hat{M}^T B_{r,r'}$ $\gamma \to 0$

Writing a positive real $Z_b[\phi]$ that differs from the original fermionic one but the final results are expected to converge for large systems.

Essential reduction of the computation time is still possible.

1. The size of the matrices to be inverted is $N_s^2 \times N_t$
   (N_s -number of sites, N_t -number of time slices)

However, this can be reduced working in $N_s \times N_t$ space.
The limit $\gamma \to 0$ can be taken from the beginning.

2. Hybrid Monte-Carlo can be efficiently implemented
(is not fully used yet).

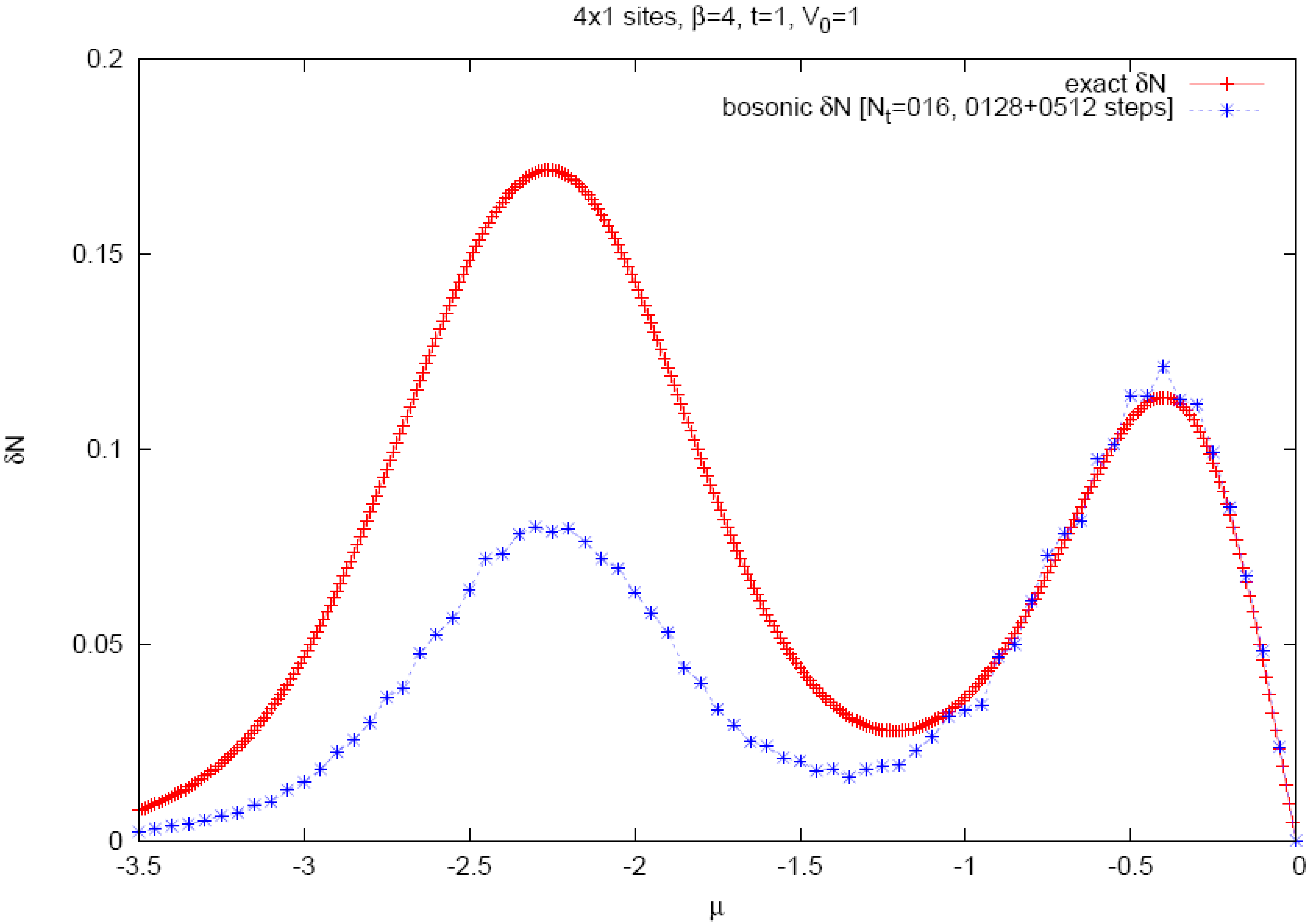
However, exact calculation is still possible for any size of the system using re-weighting.

$$\frac{\left\langle A[\phi] Z_f[\phi] \right\rangle_\phi}{\left\langle Z_f[\phi] \right\rangle_\phi} = \frac{\left\langle \left(A[\phi] \frac{Z_f[\phi]}{Z_b[\phi]} \right) Z_b[\phi] \right\rangle_\phi}{\left\langle \frac{Z_f[\phi]}{Z_b[\phi]} Z_b[\phi] \right\rangle_\phi}$$

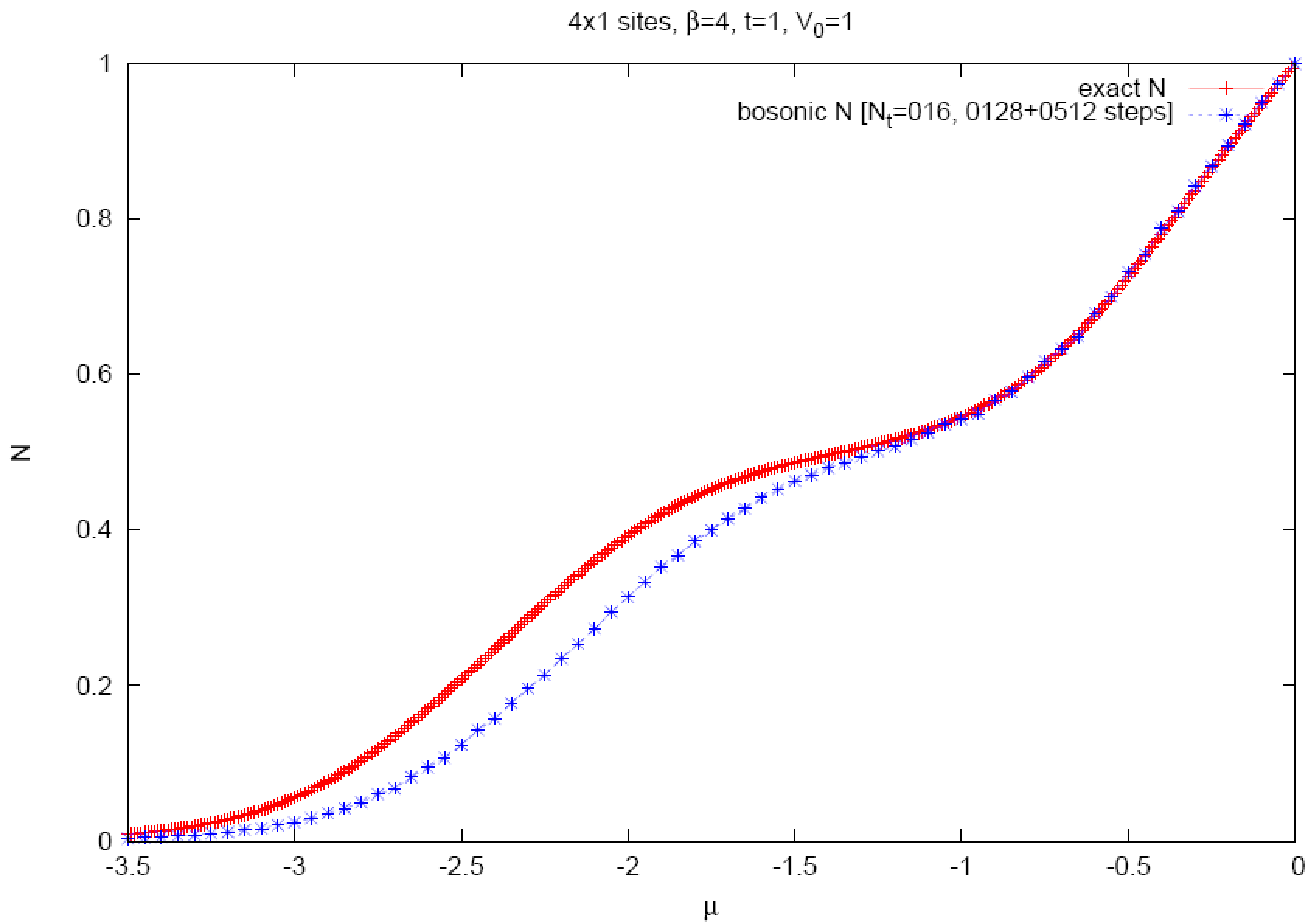
Averaging with positive $Z_b[\phi]$ instead of $Z_f[\phi]$!

Hubbard model:

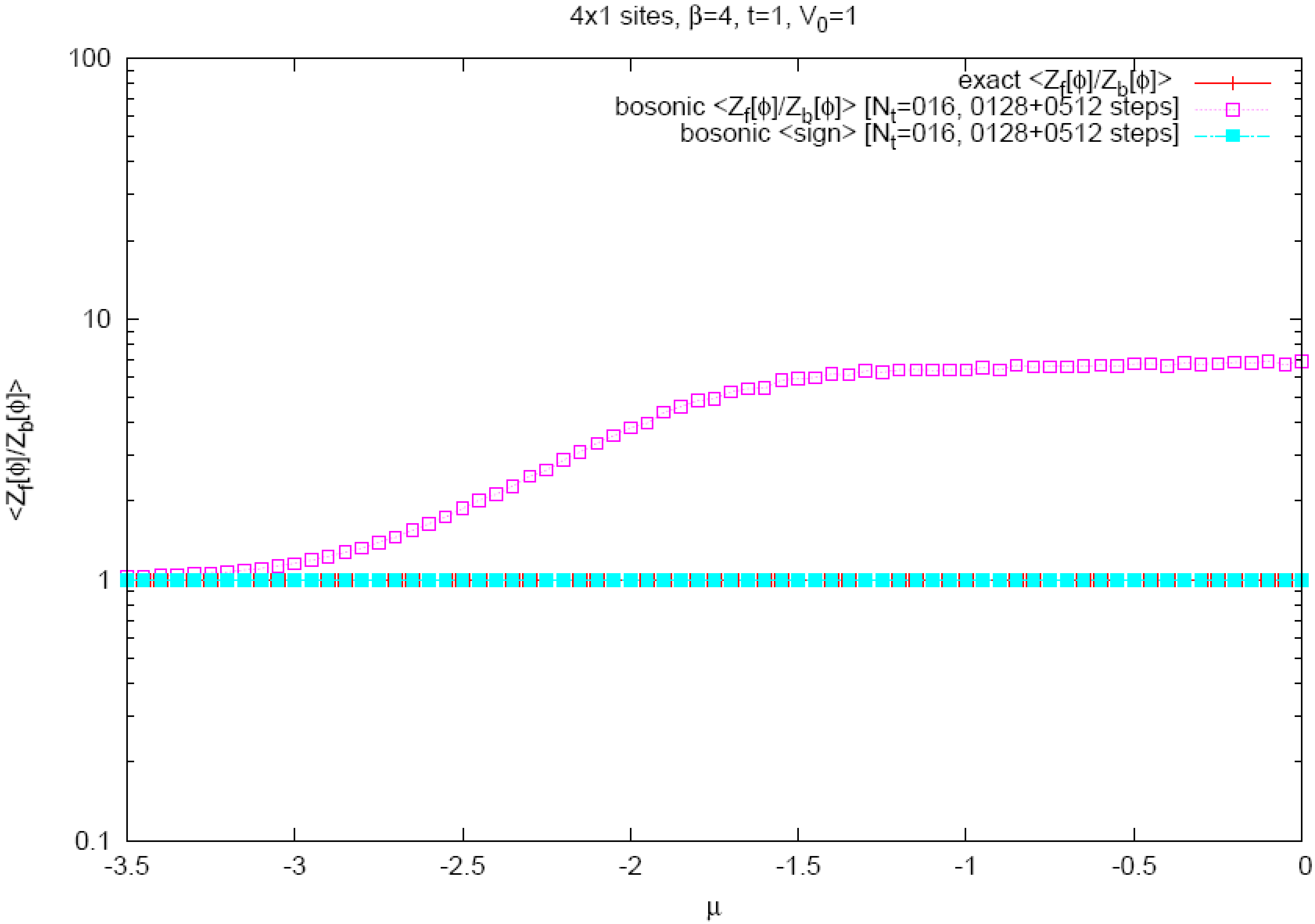
$t = 1$ ⇨ $V_0 = 4$ =band width



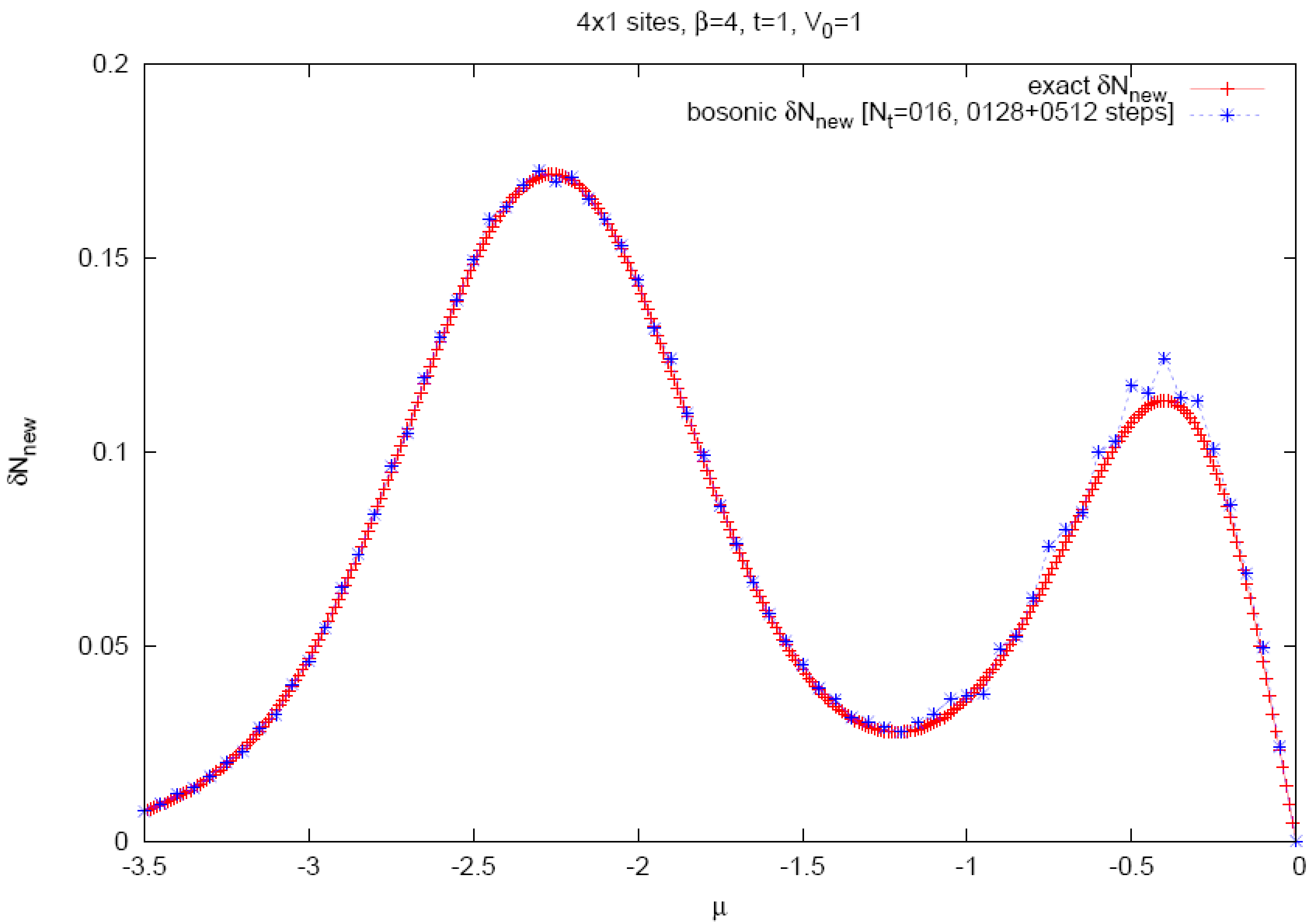
4x1 sites, β=4, t=1, V_0=1
exact δN
bosonic δN [N_t=016, 0128+0512 steps]
δN
μ
0.2
0.15
0.1
0.05
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0



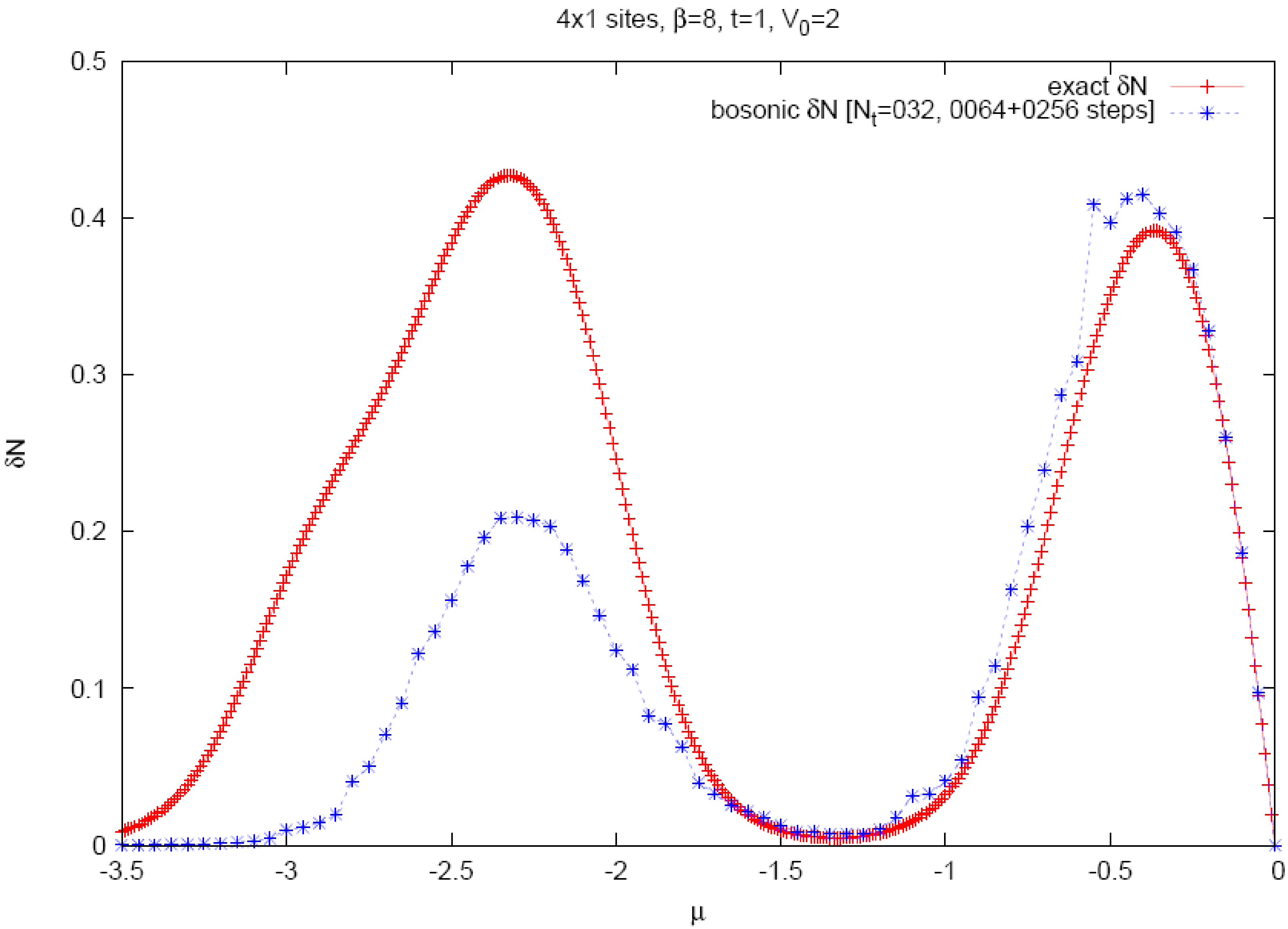
4x1 sites, β=4, t=1, V0=1
exact N
bosonic N [Nt=016, 0128+0512 steps]
N
μ
1
0.8
0.6
0.4
0.2
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0



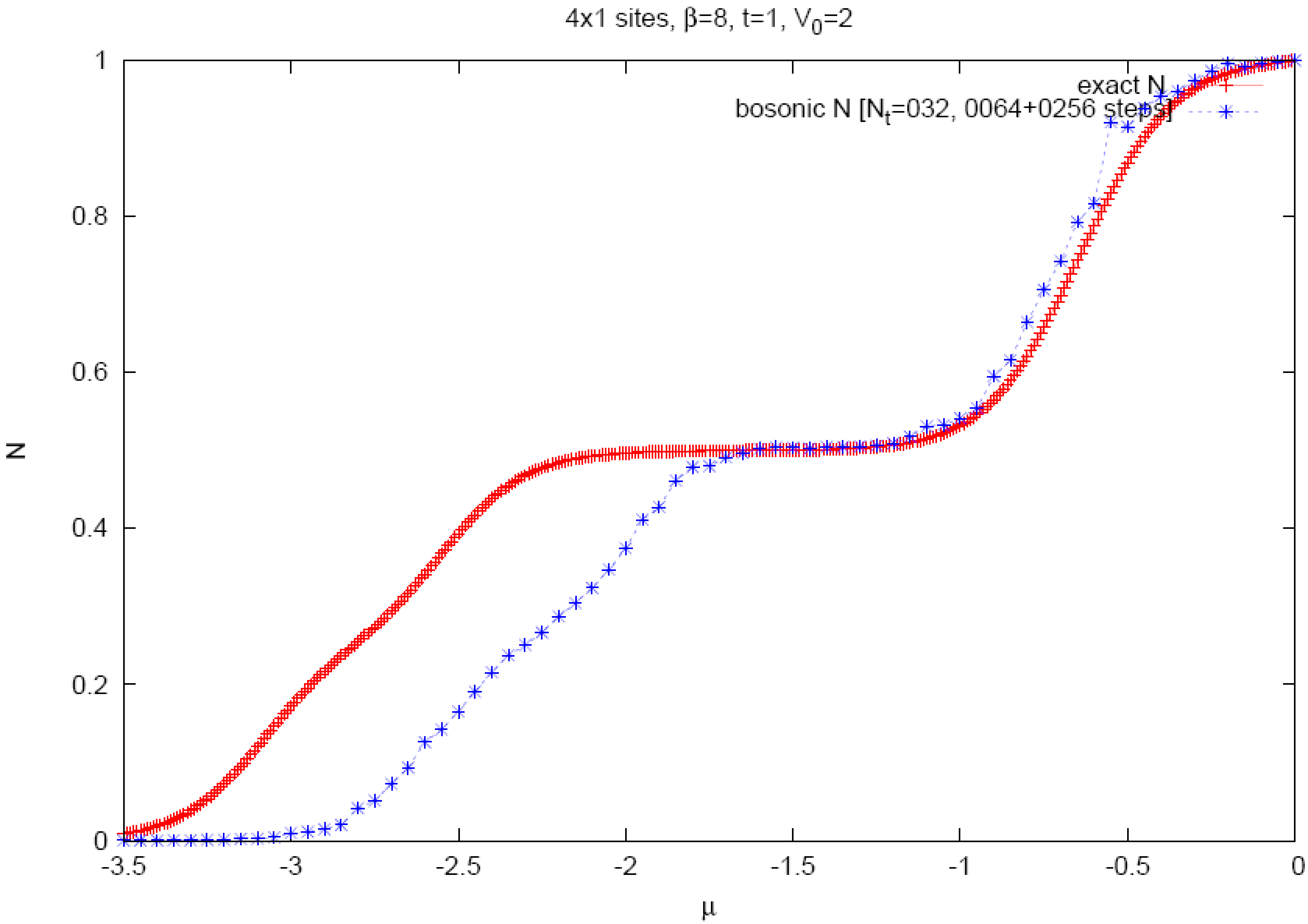
4x1 sites, β=4, t=1, V0=1
exact <Zf[ϕ]/Zb[ϕ]>
bosonic <Zf[ϕ]/Zb[ϕ]> [Nt=016, 0128+0512 steps]
bosonic <sign> [Nt=016, 0128+0512 steps]
<Zf[ϕ]/Zb[ϕ]>
μ
100
10
1
0.1
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0

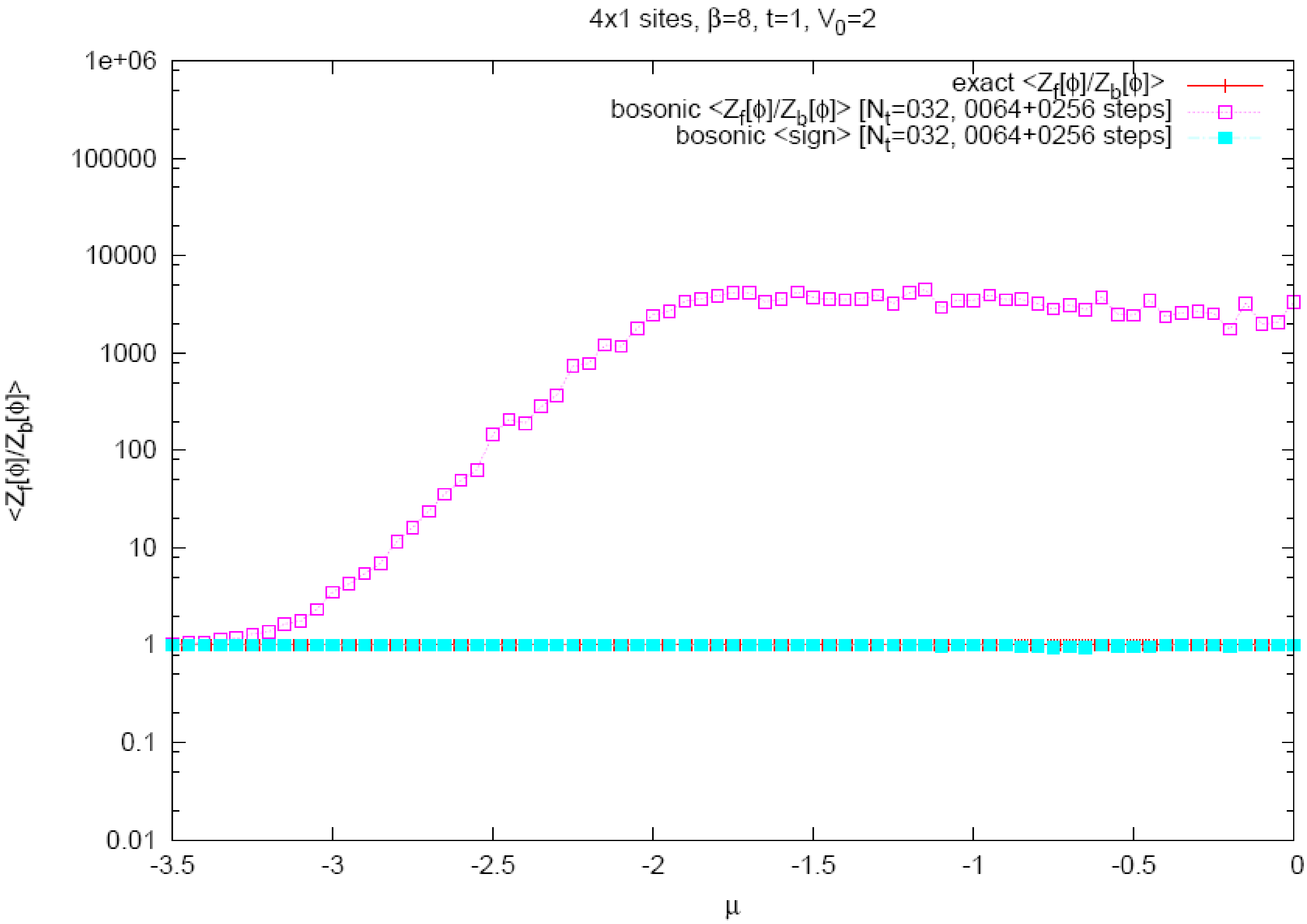


4x1 sites, β=4, t=1, V0=1
exact δNnew
bosonic δNnew [Nt=016, 0128+0512 steps]
δNnew
μ
0.2
0.15
0.1
0.05
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0

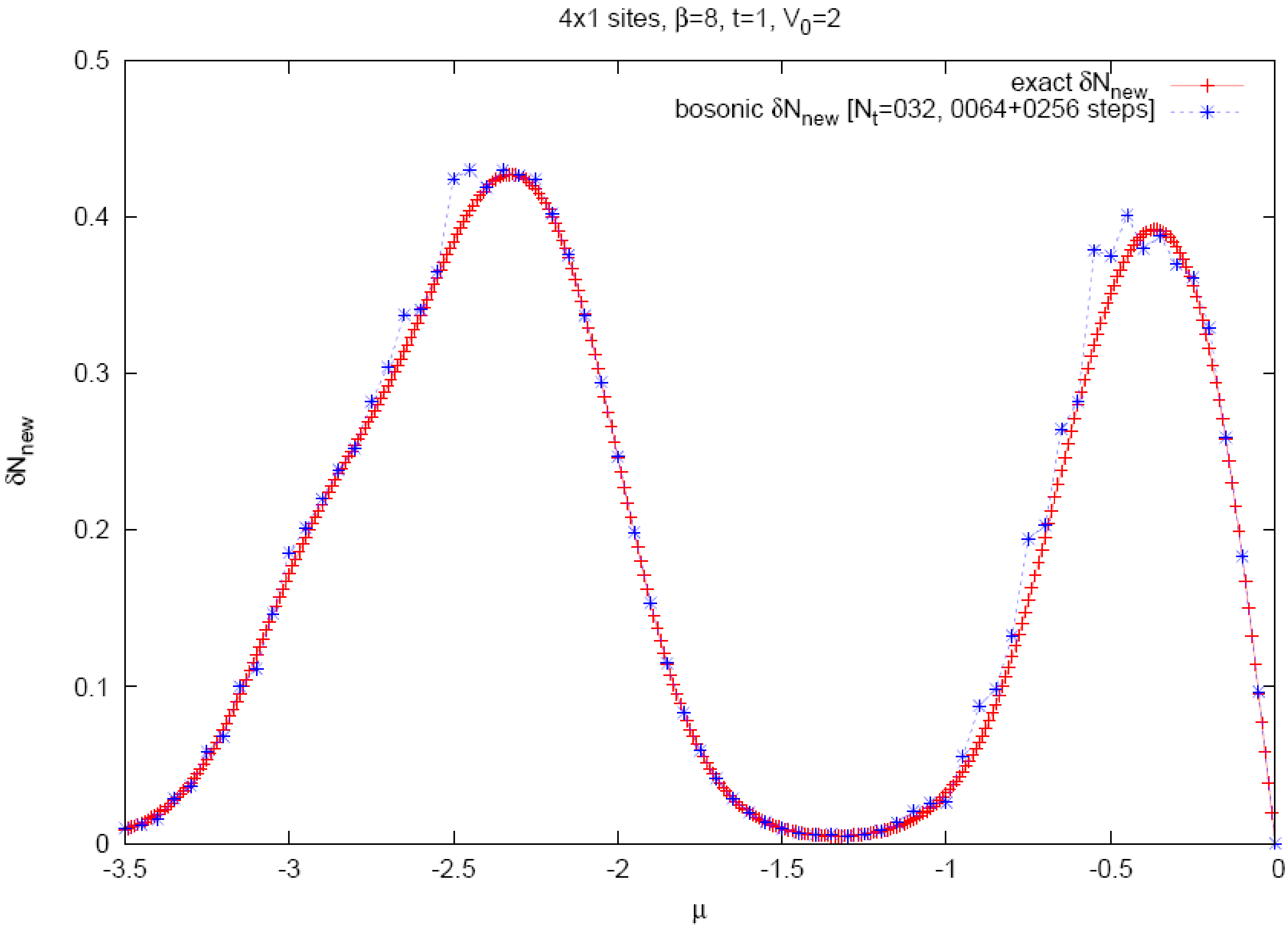


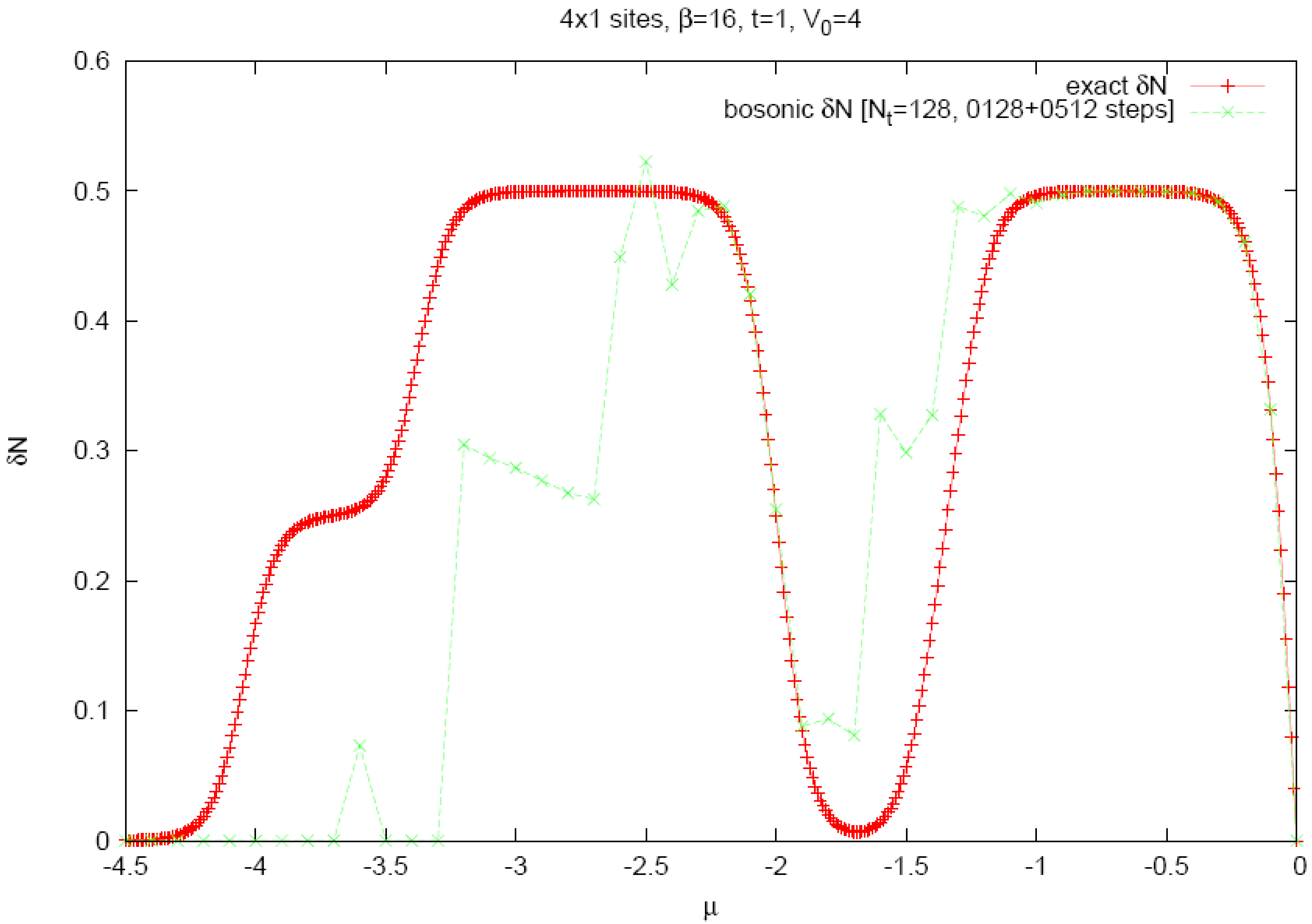
4x1 sites, β=8, t=1, V_0=2
exact δN
bosonic δN [N_t=032, 0064+0256 steps]
δN
μ
0.5
0.4
0.3
0.2
0.1
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0


4x1 sites, β=8, t=1, V_0=2
exact N
bosonic N [N_t=032, 0064+0256 steps]
N
μ
1
0.8
0.6
0.4
0.2
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0

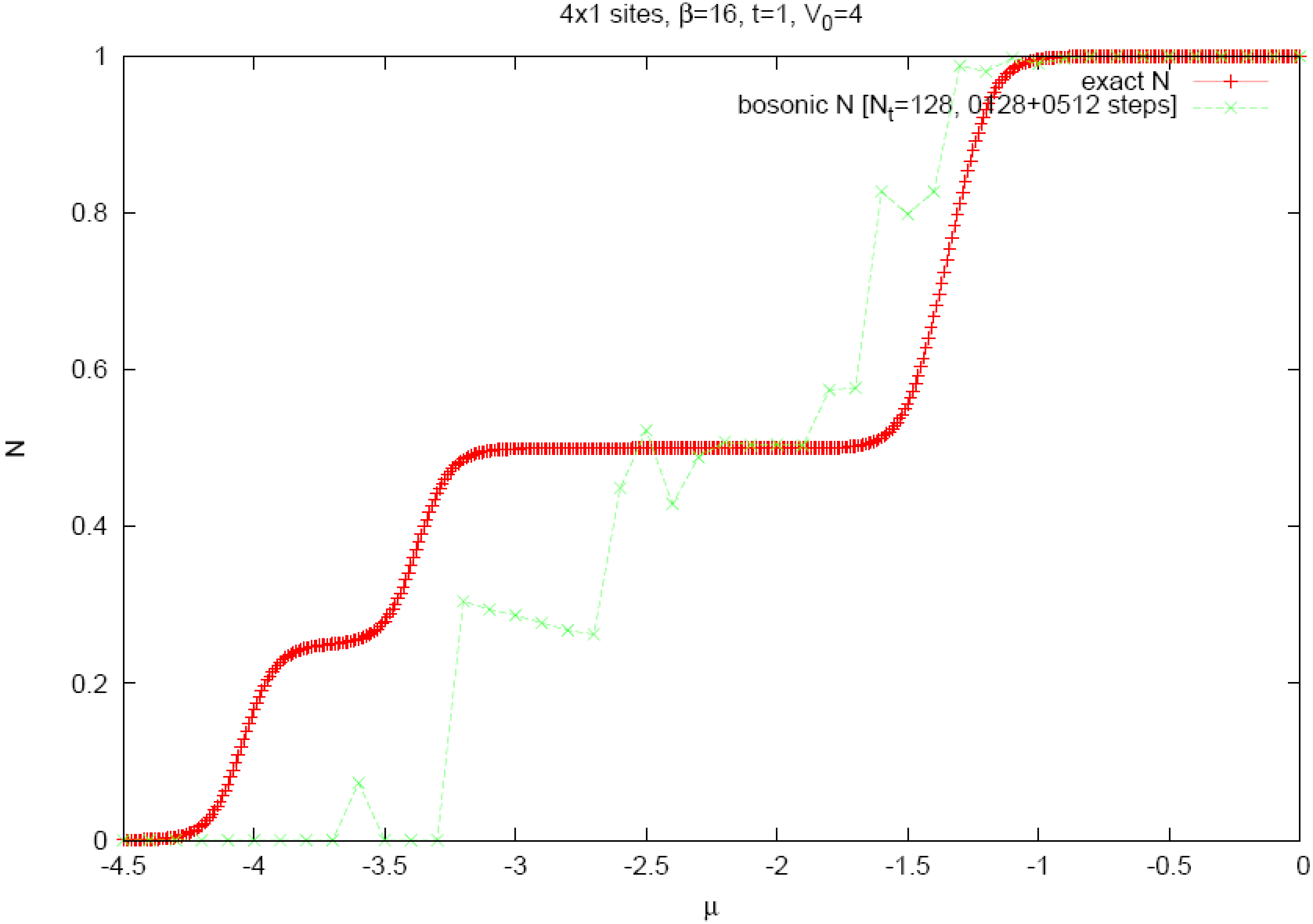


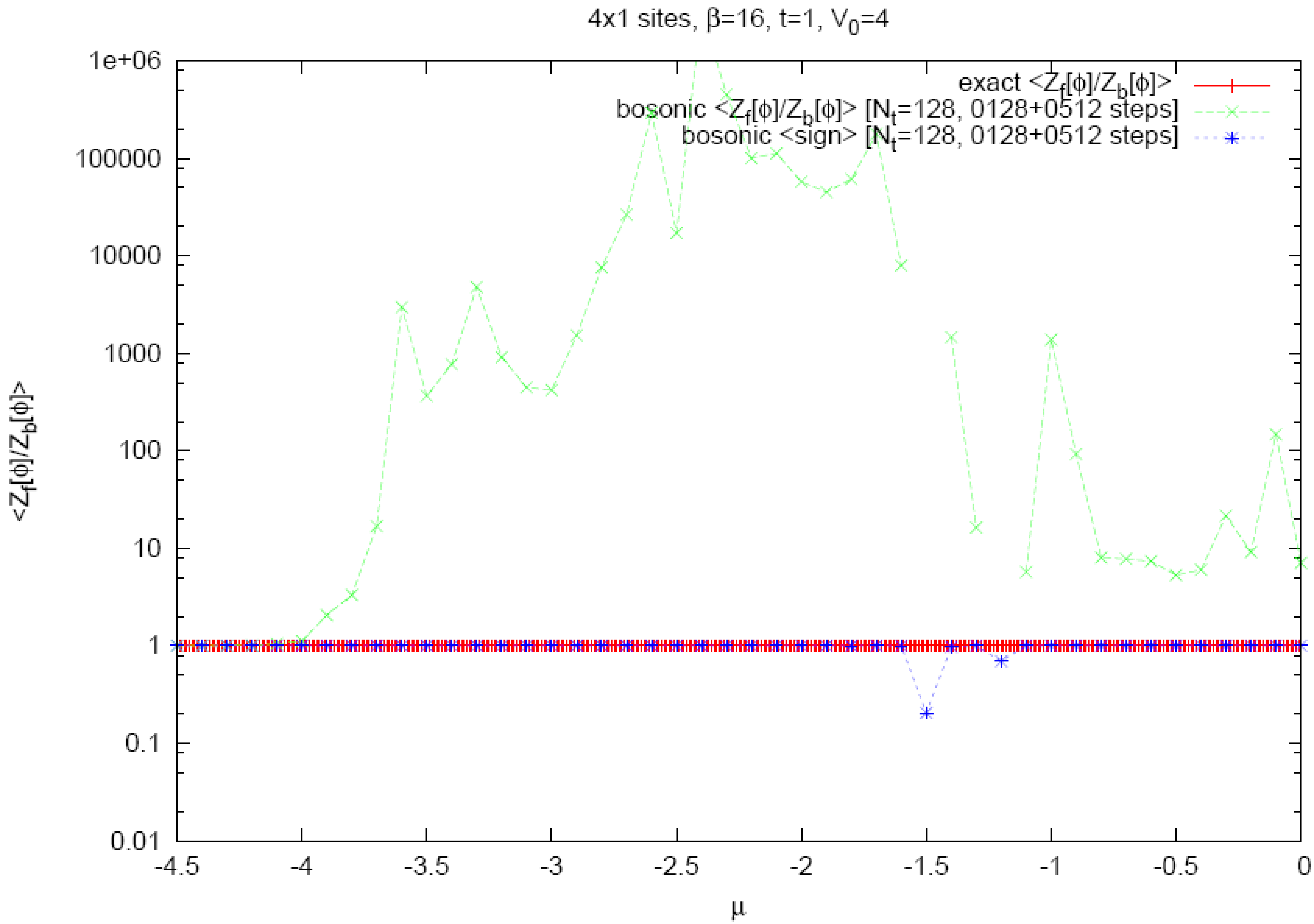
4x1 sites, β=8, t=1, V0=2
exact <Zf[ϕ]/Zb[ϕ]>
bosonic <Zf[ϕ]/Zb[ϕ]> [Nt=032, 0064+0256 steps]
bosonic <sign> [Nt=032, 0064+0256 steps]
1e+06
100000
10000
1000
100
10
1
0.1
0.01
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0
μ
<Zf[ϕ]/Zb[ϕ]>


4x1 sites, β=8, t=1, V0=2
exact δNnew
bosonic δNnew [Nt=032, 0064+0256 steps]
δNnew
μ
0.5
0.4
0.3
0.2
0.1
0
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0



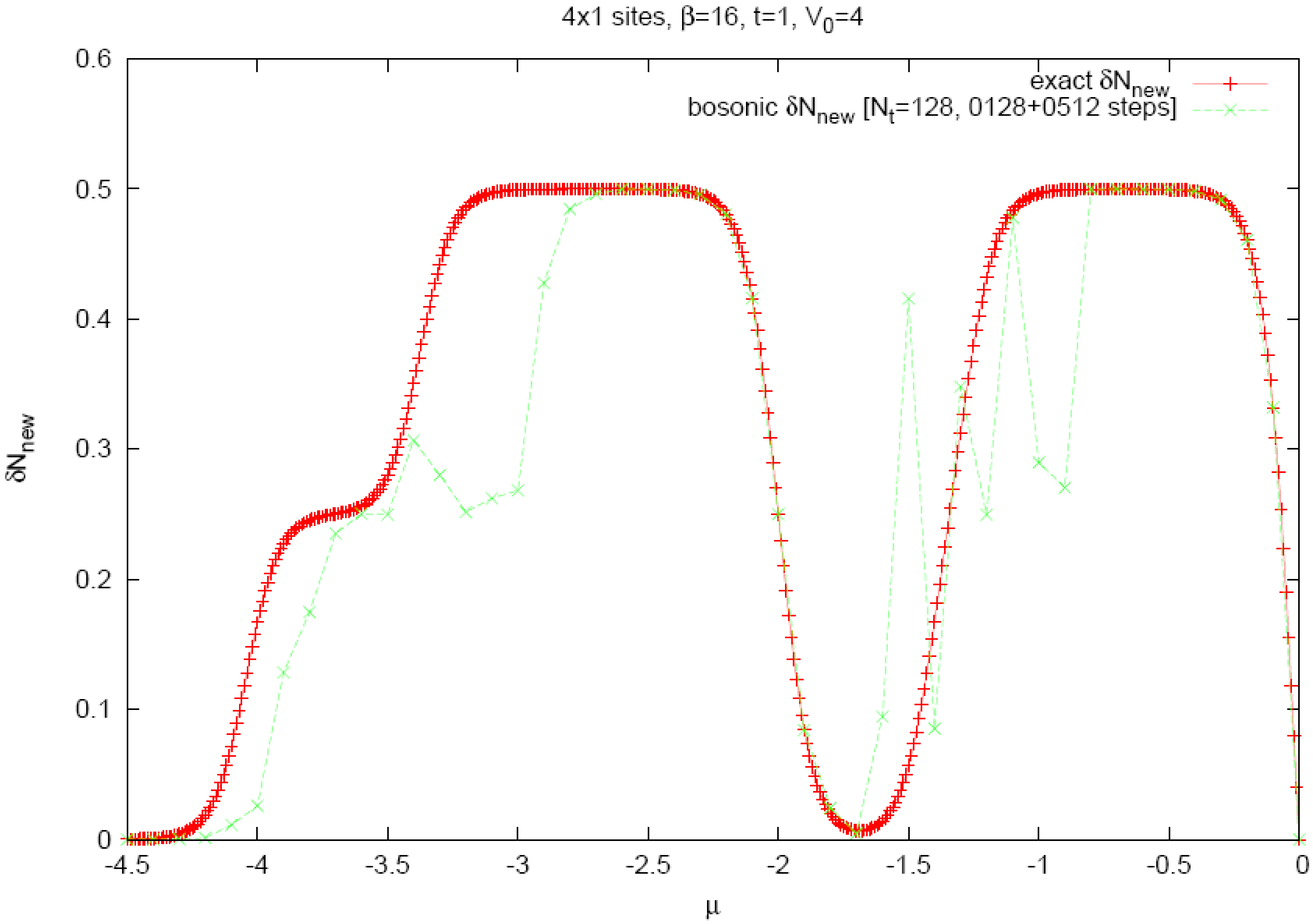
4x1 sites, β=16, t=1, V0=4
exact δN
bosonic δN [Nt=128, 0128+0512 steps]
δN
μ
0.6
0.5
0.4
0.3
0.2
0.1
0
-4.5
-4
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0


4x1 sites, β=16, t=1, V_0=4
exact N
bosonic N [N_t=128, 0128+0512 steps]
N
μ
1
0.8
0.6
0.4
0.2
0
-4.5
-4
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0



4x1 sites, β=16, t=1, V0=4
exact <Zf[φ]/Zb[φ]>
bosonic <Zf[φ]/Zb[φ]> [Nt=128, 0128+0512 steps]
bosonic <sign> [Nt=128, 0128+0512 steps]
<Zf[φ]/Zb[φ]>
μ
1e+06
100000
10000
1000
100
10
1
0.1
0.01
-4.5
-4
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0

Considerable fermionic sign problem ($10^{-1} - 10^{-2}$) in the region near $\mu \approx -1$.



A considerable reduction of the computation time is expected from using the hybrid Monte-Carlo procedure (in the process of debugging now).

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