Correlation functions in 1D Hubbard model

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Hubbard model

Model of high-T superconductivity and Mott transitions was proposed by J. Hubbard (also M. Gutzwiller and J. Kanamori) in 1963.

$$H = -t \sum_{\substack{j=-L \\ \alpha=\uparrow,\downarrow}}^{L} (\psi^\dagger_{j\alpha}\psi_{j+1\alpha} + \psi^\dagger_{j+1\alpha}\psi_{j\alpha}) - hN + 2BS_z + U \sum_{j=-L}^{L} n_{j\uparrow}n_{j\downarrow}$$

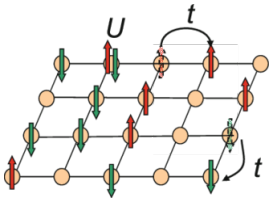
where $\psi_{j,\alpha}$ are either bosons either *fermions* (we consider the latter case)

$$\psi_{j\alpha}\psi^\dagger_{j'\alpha'} + \psi^\dagger_{j'\alpha'}\psi_{j\alpha} = \delta_{jj'}\delta_{\alpha\alpha'} \qquad n_j = n_{j\uparrow} + n_{j\downarrow}$$

S_z is a total magnetization, B – magnetic field, N – particles number and h is a chemical potential

Tight-binding approximation

- Each site corresponds to the ion
- Particles are valence electrons
- Hopping parameter t is a probability of tunneling between sites
- U is the on-site Coulomb repulsion
- Intersite interaction: neglected! (see, however, extended Hubbard)



Each site contains one of the possibilities (Pauli principle!)

$$|0\rangle, \quad |\uparrow\rangle, \quad |\downarrow\rangle, \quad |\uparrow\downarrow\rangle$$

- Bonus: AdS/CFT

Model was extensively studied extensively (the list is to long to be given here even partially)

- A. Altland, B. Simons, "Interaction effects in the tight-binding system"
- F. H. L. Essler *et. al.*, "The one-dimensional Hubbard model"
- D. Baeriswyl *et. al.*, "The Hubbard Model"
- A. Montorsi, "The Hubbard Model" (Collection of reprints)
- Shastry, Omedilla, Wadati, ... (integrability)
- de Leeuw, Beisert, Frolov (AdS/CFT)

Exact solution

For simplicity 1D version of model is widely studied (and periodicity is assumed). It was discovered by Lieb and Wu that model could be solved explicitly in 1D. *Exact many-particle eigenfunctions* and *spectrum* of the system were found

- The exact microscopical solution is given in terms of particles of two types
- *The first type* is describing motion of N electrons in the system of size L
- *The second type* describes the motion of M spin waves in the system of size N
- Obviously, these two degrees of freedom are not independent

Bethe vectors

Eigenvectors are traditionally called *Bethe vectors* and they are nothing but *linear combinations of plane waves* (2 types of plane waves in our case) with coefficients fixed from the Hamiltonian

$$|\psi\rangle = \frac{1}{N!} \sum_{x_1,\ldots,x_N=1}^{L} \sum_{a_1,\ldots,a_N=\uparrow,\downarrow} \psi(\mathbf{x};\mathbf{a}|\mathbf{k},\boldsymbol{\lambda})|\mathbf{x},\mathbf{a}\rangle$$

where $|\mathbf{x};\mathbf{a}\rangle$ are Fock space vectors and

$$\psi(\mathbf{x};\mathbf{a}|\mathbf{k},\boldsymbol{\lambda}) = \sum_{P\in\Sigma^N} \sum_{Q\in\Sigma^M} \mathrm{sign}(PQ) F_{PQ}(\mathbf{k},\boldsymbol{\lambda}) e^{i\left(\sum_j^N k_j x_{Pj} + \sum_k^M \lambda_k a_{Qk}\right)}$$

Bethe ansatz solution

In a periodic system of size L momentums of particles are given by *Bethe equation*

$$e^{ik_jL} = \prod_{\ell=1}^{M} S_1(\lambda_\ell, \sin k_j), \qquad j = 1, \dots, N$$

$$\prod_{j=1}^{N} S_1(\lambda_\ell, \sin k_j) = \prod_{m\neq\ell}^{M} S_2(\lambda_\ell, \lambda_m), \qquad \ell = 1, \dots, M$$

Where scattering matrix elements between are given by

$$S_1(x, y) = \frac{x - y - iU/t}{x - y + iU/t}, \qquad S_2(x, y) = \frac{x - y - 2iU/t}{x - y + 2iU/t}$$

Correlation functions and observables

Green-Kubo theorem

In the *linear response approximation* kinetic coefficients $\{\sigma\}$ can be calculated via the correlataion functions

$$\sigma(q,\omega) \sim \int_0^\infty dt\, e^{i\omega t} \left\langle \left[J^\dagger(q,t), J(q,0) \right] \right\rangle_\beta$$

where $\{\omega, q\}$ are the frequency and the momenta and $[\cdot\,,\cdot\,]$ is a commutator

The problem is reduced to the computation of correlation functions

$$\langle J^\dagger(x,t) J(0,0) \rangle_\beta = \sum_n e^{-\beta E_n} \langle n | J^\dagger(x,t) J(0,0) | n \rangle$$

Large coupling limit

In large coupling limit $U \to \infty$ states with double occupancies are effectively prohibited since they possess infinity energy. Only possibilities $|0\rangle, \quad |\uparrow\rangle, \quad |\downarrow\rangle$ are allowed in each site
Under this condition *we are dealing with effectively free model*
The simplest evidence are equation of spectrum

$$e^{ik_a L} = e^{i(M+1)M}, \quad a = 1, \dots N$$
$$e^{i\lambda_b N} = (-1)^{M+1}, \quad b = 1, \dots M.$$

Spin-charge separation

Spin-charge basis

In the new basis of *spinless fermions* c_j where *charge and spin degrees of freedom are "separated"*

$$|f\rangle = c_{j_1}^\dagger \dots c_{j_N}^\dagger |0\rangle, \qquad |\ell\rangle = |\alpha_1, \dots, \alpha_N\rangle$$

The total wavefunction is given by

$$|\mathbf{j}, \boldsymbol{\alpha}\rangle = |f\rangle \otimes_f |\ell\rangle, \qquad j_1 < j_2 < \dots < j_N.$$

The subscript f in $\otimes_f$ indicates a constraint in the tensor product $\otimes$:
the number of spinless fermions N in the charge part $|f\rangle$, determines the number of sites of the spin chain in the spin part $|\ell\rangle$.

Spinless fermions

In a basis of free fermioins we arrive to *free Hamiltonian*

$$H = -\sum_{j=-\infty}^{\infty} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) - hN + 2BS_z$$

Within spin-charge separation computation of correlation functions simplifies

$$\langle \cdots \rangle_T = \frac{1}{Z} \sum_{N=0}^{\infty} \sum_{f,\ell} \Big(\langle \ell | \otimes_f \langle f | \Big) e^{-\beta H} \cdots \Big(| f \rangle \otimes_f | \ell \rangle \Big)$$

Remark: physical operators should be translated to the new basis too

One point correlation function example

Local magnetization $s_z(j,t)$ can be expressed via 1-point correlation of free spinless fermions with a shifted energy

$$E \longrightarrow \tilde{E} = E - Nh - N\beta^{-1}\log[2\cosh(\beta B)]$$

Artifact, the system remembers about the spin! Then

$$\langle s_z(j,t)\rangle_T = -\frac{\tanh(\beta B)}{2}\frac{\sum_{N=0}^{\infty}\sum_{\mathbf{k}} e^{-\beta\tilde{E}_{\mathbf{k}}}\langle\mathbf{k}|n_j|\mathbf{k}\rangle}{\sum_{N=0}^{\infty}\sum_{\mathbf{k}} e^{-\beta\tilde{E}_{\mathbf{k}}}}$$

Farther computation is done like in free spinless fermions

Magnetization

In thermodynamic limit $L \to \infty$, $N \to \infty$, $M \to \infty$, $L/N = Density$, $M/L = Magnetization$

$$\langle s_z(x,t)\rangle_T = \langle s_z(0,0)\rangle_T = -\frac{\tanh(\beta B)}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\rho(k),$$

where $\rho(k)$ is a Fermi-Dirac distribution with the modified energies

$$\rho(k) = \frac{1}{e^{\beta\tilde{\varepsilon}(k)}+1} = \frac{2\cosh(\beta B)}{2\cosh(\beta B)+e^{\beta[\varepsilon(k)-h]}}$$

Two-point correlation functions

Spin densities correlator in the thermodynamic limit is given by

$$\langle s_z(x,t) s_z(0,0)\rangle_\beta = \sigma_0(x,t) + \sigma_1(x,t)$$

$$\sigma_1(x,t) \sim \int_{-\pi}^{\pi} \frac{d\lambda}{2\pi} \frac{\hat{S}\mathcal{F}_\lambda(x,t)}{1-\cos\lambda}, \qquad \sigma_0(x,t) \sim \tanh^2(\beta B) \frac{\hat{S}\mathcal{F}_\lambda(x,t)}{1-\cos\lambda}\Big|_{\lambda=0}$$

$\hat{S}f(x) = 2f(x) - f(x+1) - f(x-1)$ is a discrete analog of the second derivative

$\mathcal{F}_\lambda$ is a *Fredholm determinant with a modified sine-kernel* (old result for free fermions!)

Correlation function via generalized hydrodynamics

$$\partial_t Q_\ell(x,t) + \partial_x J_\ell(x,t) = 0, \qquad \ell = 1, 2, \ldots$$

Drude weight D *and Onsager matrix* $\mathcal{L}$ are defined as (sub)leading terms

$$D = \lim_{\tau\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} ds \int \langle J(x,s) J(0,0) \rangle_\beta \qquad \mathcal{L} = \lim_{\tau\to\infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} ds \int \Big(\langle J(x,s) J(0,0) \rangle_\beta - D \Big)$$

On the other hand D, $\mathcal{L}$ can be expressed via charges correlator $\sigma = \langle q(x,t) q(0,0) \rangle_\beta$
(J. De Nardis *et. al.* (2020), also H. Spohn, B. Doyon)

$$\frac{1}{2} \sum_x x^2 \left(\sigma(x,t) + \sigma(x,-t) \right) = Dt^2 + \mathcal{L}t + o(1)$$

Drude weight

$$\mathrm{D} = \frac{\tanh^2(\beta B)}{4} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \varepsilon'(k)^2 \rho(k)(1-\rho(k))$$

From GHD prediction: E. Ilievski, J. De Nardis (2017), J. De Nardis *et. al.* (2020)

$$\mathrm{D}^{\mathrm{GHD}} = \int dk \rho(k)(1-\rho(k))(v^{\mathrm{eff}}(k))^2 (m^{\mathrm{dr}}(k))^2$$

here *dressed* velocity v^{eff}, magnetization m^{dr}, root density $n(k)$ and particles distribution ρ_p should be computed via microscopic approach. We see the following identification

$$v^{\mathrm{eff}}(k) \leftrightarrow \varepsilon'(k) \qquad\qquad m^{\mathrm{dr}}(k) \leftrightarrow -\tanh(\beta B)/2$$

Diffusion vs ballistic

At $B = 0 \longrightarrow \mathrm{D} = 0$ and the system switches to the diffusive behavior

From the long range analysis $x \to \infty$, $t \to \infty$, $x \sim \sqrt{t}$ diffusion constant could be fixed

$$\langle s_z(x,t) s_z(0,0)\rangle_\beta \sim \int \frac{dq}{2\pi}\rho(q)\frac{e^{-x^2/(2\mathcal{D}t)}}{\sqrt{2\pi\mathcal{D}t}} + \text{Ballistic part}$$

$$\mathcal{D} = \langle s_z\rangle^{-2}\int_{-\pi}^{\pi}|\varepsilon'(q)|\rho(q)(1-\rho(q))\frac{dq}{2\pi}$$

At $T \to \infty$ result for $\mathcal{D}$ coincides with the semi-classical prediction J. Feldmeier *et. al.* (2022)

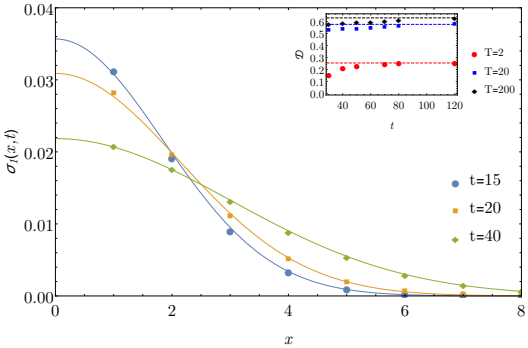


Figure: Diffusive part of the spin-spin correlation function. Solid lines show analytic answer of asymptotic analysis and dots correspond to numeric evaluation of correlators (Fredholm determinants discretization) with parameter $h = 2$, $B = 1$, $T = 2$.
Inset shows the diffusion constant $\mathcal{D}$ after numerical fitting of correlators $B = 0$, $h = 2$ and temperatures according to the legend. Dashed lines show analytic answer

Diffusive behavior

Again, use $\sigma = \langle q(x,t)q(0,0)\rangle_\beta$ and

$$\frac{1}{2}\sum_x x^2\left(\sigma(x,t)+\sigma(x,-t)\right) = Dt^2 + \mathcal{L}t + o(1)$$

The diffusion constant could be computed as

$$\mathfrak{D} = \mathcal{L}/\langle s_z\rangle$$

(J. De Nardis *et. al.* (2020), also H. Spohn, B. Doyon). It coincides with $\mathcal{D}$ only if the ballistic part is absent (i.e. for $B = 0$) when the Drude weight disappears.

Diffusion

GHD prediction of diffusion coefficient

$$\mathcal{D}^{\mathrm{GHD}} = \int dk\, \rho_p(k)(1-n(k))|v^{\mathrm{eff}}(k)| \frac{\partial_B^2 (m^{\mathrm{dr}}(k))^2}{16\langle s_z\rangle^2}\Big|_{B=0},$$

coincides with our prediction

$$\mathcal{D} = \langle s_z\rangle^{-2} \int_{-\pi}^{\pi} |\varepsilon'(q)|\rho(q)(1-\rho(q))\frac{dq}{2\pi}$$

after the proper identification

$$v^{\mathrm{eff}}(k) \leftrightarrow \varepsilon'(k) \qquad\qquad m^{\mathrm{dr}}(k) \leftrightarrow -\tanh(\beta B)/2$$

Conclusions

- Correlators in the dynamical case from exact microscopic approach
- Finite temperature correlators

- More complicated correlators?
- Relaxation dynamics?
- Finite coupling constant?
- Extended Hubbard model(s)?

Perspectives: "real" Hubbard?

- Model takes into account intersite interaction
- Model is integrable only in some particular cases
- Bariev, Alcaraz, Schaschneider, Essler, Korepin, Montorsi,...

$$H = -\sum_{j=1}^{L}\sum_{\sigma=\uparrow,\downarrow}\left[t - X(n_{j,\sigma} + n_{j+1,-\sigma}) + \tilde{X} n_{j,\sigma} n_{j+1,-\sigma}\right]\left(c^{\dagger}_{j,\sigma} c_{j+1,\sigma} + h.c.\right) + U\sum_{j=1}^{L} n_{j,\uparrow} n_{j,\downarrow}$$

$$+\frac{V}{2}\sum_{j=1}^{L} n_j n_{j+1} + \frac{W}{2}\sum_{\sigma,\sigma'=\uparrow,\downarrow} c^{\dagger}_{j,\sigma} c^{\dagger}_{j+1,\sigma'} c_{j,\sigma'} c_{j+1,\sigma} + Y c^{\dagger}_{j,\uparrow} c^{\dagger}_{j,\downarrow} c_{j+1,\downarrow} c_{j+1,\uparrow} + P n_{j,\uparrow} n_{j,\downarrow} n_{j+1}$$

$$+\frac{Q}{2}\sum_{j=1}^{L} n_{j,\uparrow} n_{j,\downarrow} n_{j+1,\uparrow} n_{j+1,\downarrow} + \mu_e \sum_{j,\sigma} n_{j,\sigma}$$