New method for the quantum ground state in one dimension

Sung Chung

Physics Dept, Western Michigan University,
Kalamazoo Michigan 49008, USA

Solve the Schrödinger equation

- Strong correlation phenomena like High T_c CuO_2

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powerful nonperturbative method

- Rigorous methods in 2D classical, 1D quantum systems
- Exact diagonalization, Monte Carlo ⟶ finite size problem
- Numerical renormalization group ⟶ not yet successful

for macroscopic 2D quantum systems

New method

- We here present a new method to solve the Schrödinger eq. for 1D quantum ground states with translational symmetry
- Our results for ground state energy and local magnetic moment in the 1D Hubbard model agree with the Bethe Ansatz results
- Simple, general and practically exact, without approximations and notions such as NRG

Hubbard model

$$H = -t \sum (c_{i\sigma}^{+} c_{j\sigma} + h.c.) + U \sum n_{i\uparrow} n_{i\downarrow}$$

Schrödinger eq.

$$H\Psi = E\Psi$$

$$\downarrow$$

$$e^{-\beta H}\Psi = e^{-\beta E}\Psi$$

Monte Carlo, NRG : only ground state survives at $\beta \to \infty$

Here $\beta \to 0$

$$(1 - \beta H)\Psi = (1 - \beta E)\Psi$$

$$H = \sum_{even} H_{bond} + \sum_{odd} H_{bond}$$

$$e^{-\beta H} = e^{-\beta \sum_{even} H_{bond}} e^{-\beta \sum_{odd} H_{bond}} + \vartheta(\beta^2)$$

Local density matrix

$$e^{-\beta H_{bond}} \approx \Omega_\alpha \otimes \Theta_\alpha$$

$$\Omega_\alpha = 1 - \frac{\beta U}{2} n_\uparrow n_\downarrow + \frac{\beta \mu}{2}(n_\uparrow + n_\downarrow)$$

$$c_\uparrow^+, c_\downarrow^+, c_\uparrow, c_\downarrow$$

$$e^{-\beta H_{bond}} \approx f_\alpha \otimes g_\alpha$$ on basis $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

$$f_1 = g_1 = \begin{matrix} 1 & 0 & 0 & 0 \\ 0 & \beta\mu/2 & 0 & 0 \\ 0 & 0 & \beta\mu/2 & 0 \\ 0 & 0 & 0 & -\beta U/2+\beta\mu \end{matrix}$$

Matrix product representation of even group bonds

$$\bullet\bullet\bullet\, f_\alpha \otimes g_\alpha \otimes f_\beta \otimes g_\beta \otimes f_\gamma \otimes g_\gamma \,\bullet\bullet\bullet$$

Matrix product representation of density matrix

$$K \equiv \bullet\bullet\bullet g_{\alpha}.f_{\beta} \otimes f_{\gamma}.g_{\beta} \otimes g_{\gamma}.f_{\delta} \otimes f_{\varepsilon}.g_{\delta} \bullet\bullet\bullet$$

$$\equiv \bullet\bullet\bullet \Gamma^{1}_{\alpha\beta} \otimes \Gamma^{2}_{\beta\gamma} \otimes \Gamma^{1}_{\gamma\delta} \otimes \Gamma^{2}_{\delta\varepsilon} \bullet\bullet\bullet$$

Wave function

$$\Psi = \bullet\bullet\bullet \varsigma^{1}_{\alpha\beta}(a_1)\varsigma^{2}_{\beta\gamma}(a_2)\varsigma^{1}_{\gamma\delta}(a_3)\varsigma^{2}_{\delta\varepsilon}(a_4) \bullet\bullet\bullet$$

on basis $\bullet\bullet\bullet |a_1> \otimes |a_2> \otimes |a_3> \otimes |a_4> \otimes \bullet\bullet\bullet$

$|0>, |\uparrow>, |\downarrow>, |\uparrow\downarrow>$

$$\Psi(abcd) = A_{a\alpha} B_{\{bcd\}\alpha}$$

↘

$$C_{\{b\alpha\}\beta} D_{\{cd\}\beta}$$

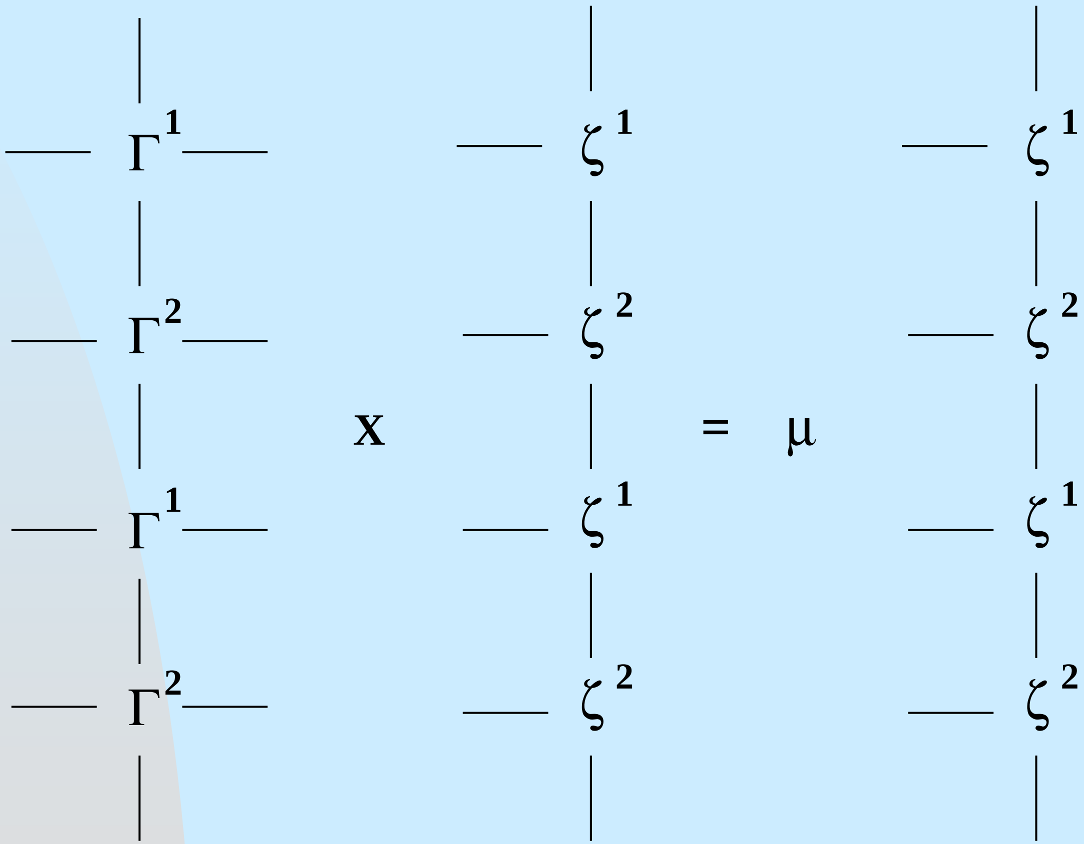
SVD it !

↘

$$E_{\{c\beta\}\gamma} F_{d\gamma}$$

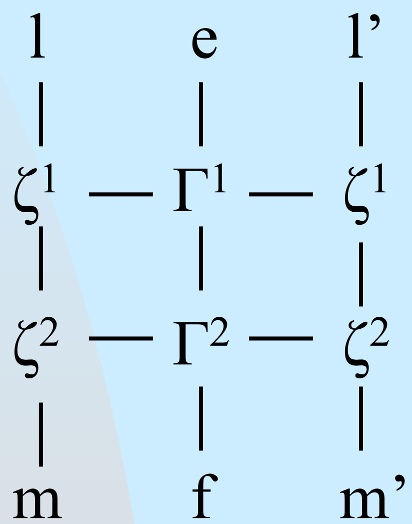
$$= A_{\alpha}(a) C_{\alpha\beta}(b) E_{\beta\gamma}(c) F_{\gamma}(d)$$

Transfer matrix eigenvalue problem



Variational problem

$$\mu = \Psi K \Psi / \Psi\Psi \longrightarrow \max$$



$$= A_{\ell e \ell', mfm'} = R \nu L^{tr}$$

$$\Psi K \Psi = \nu_0 L_0{}^{tr} A R_0 \qquad \Psi\Psi = \rho_0 \tilde{L}_0{}^{tr} B \tilde{R}_0$$

μ contains ζ quadratically

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Generalized eigenvalue problem for ζ

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Back to start until convergence

Ground state properties

$$\langle n_\uparrow \rangle, \langle n_\downarrow \rangle, \langle n_\uparrow n_\downarrow \rangle$$

Kinetic energy per site

Local magnetic moment

Quantities sitting on adjacent sites

$$\left\langle \hat{A}\hat{B} \right\rangle = \Psi \hat{A}\hat{B}\Psi / \Psi\Psi$$

$$= AB \cdot \widetilde{L}_0 \varsigma^1 \varsigma^1 \cdot \varsigma^2 \varsigma^2 \widetilde{R}_0 / \rho_0$$

Parameters used : $\beta = 10^{-6}$ 10^{-7} no difference

Convergence criteria : $\| \zeta_{old} - \zeta_{new} \| / \| \zeta_{old} \| < 5 \times 10^{-5}$

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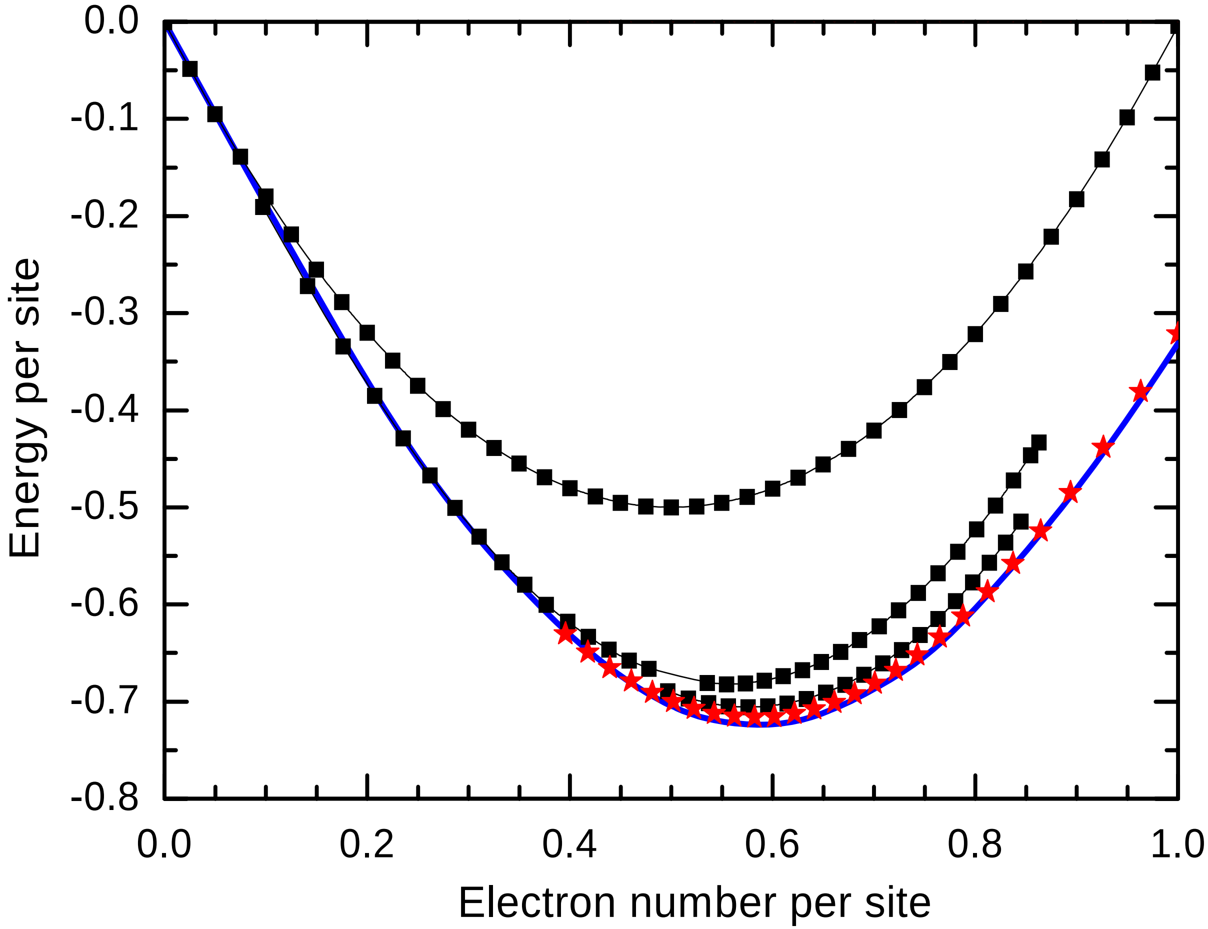
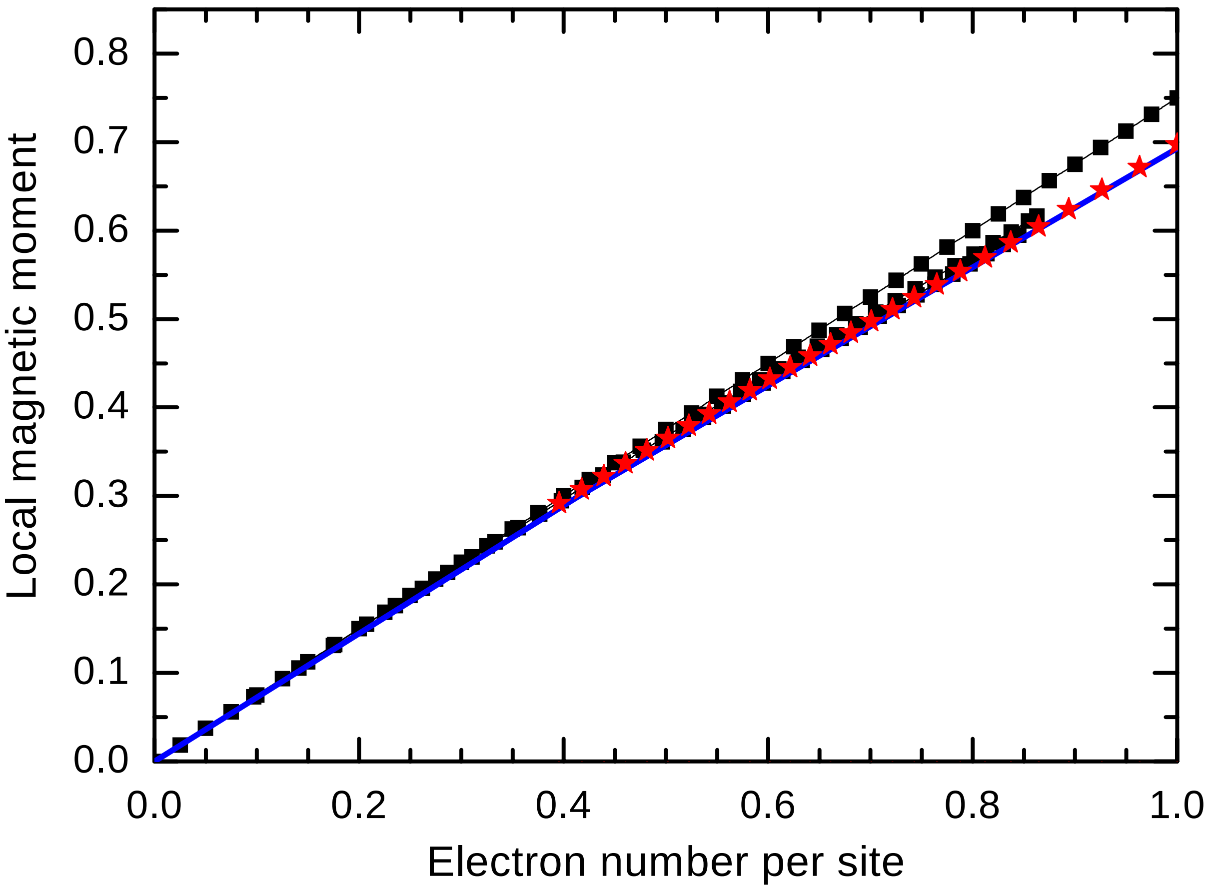
μ_0 10^{-15} accurate

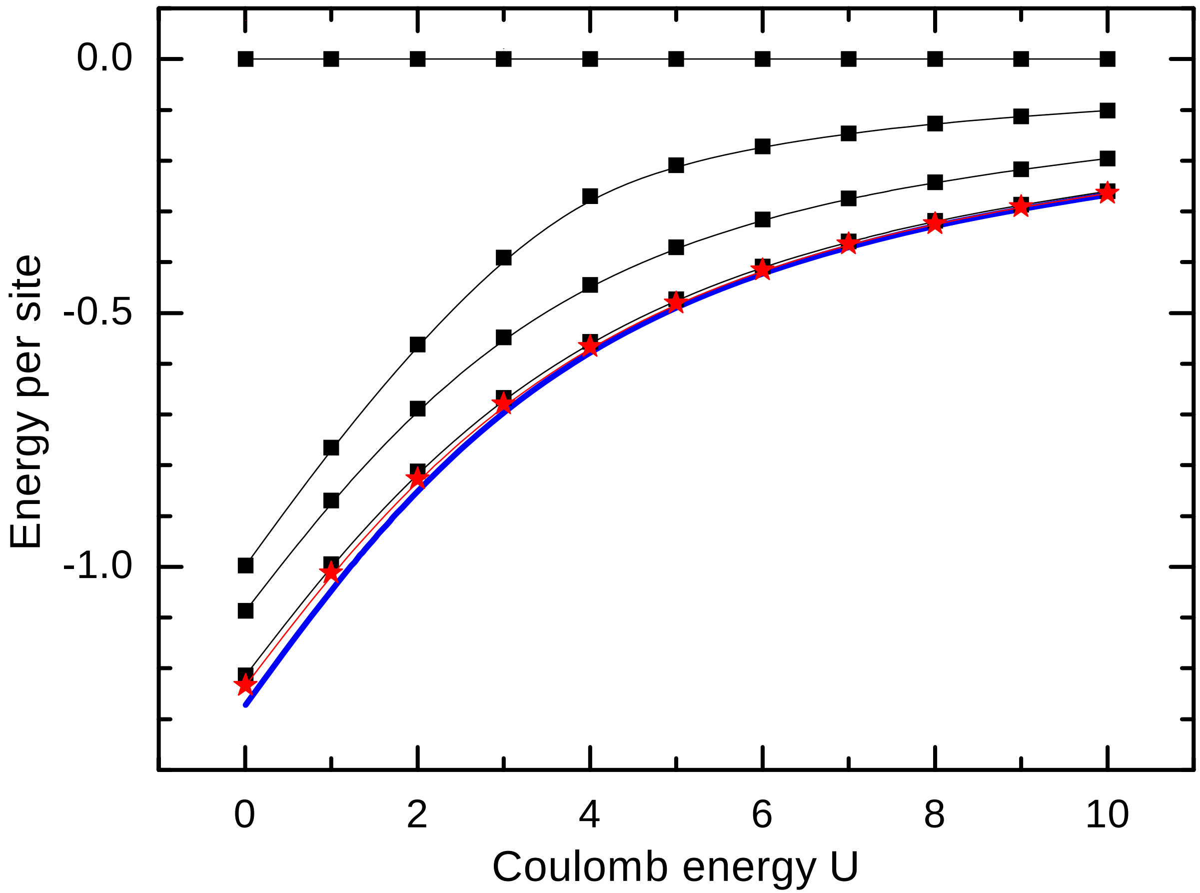
Ground state energy vs electron density at U=8



Local magnetic moment vs electron density at U=8



Ground state energy vs U at half-filling



Slow convergence at U « 1

Entanglement = 10, still 1.4% difference from BA

Kinetic energy → itinerancy

Coulomb repulsion → localization

U → ∞ : our results with entanglement = 1

agree with Bethe Ansatz

Summary

- A new method for the 1D quantum ground states with translational symmetry
- Applied to the 1D Hubbard model, it reproduces the Bethe Ansatz results
- Method is free from any existing notions such as NRG, and readily applicable to any quantum spins, bosons and fermions

Currently underway

- Two dimension
- Thermodynamics, dynamics