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New method for the quantum ground states in one dimension

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Abstract

A simple, general and practically exact method is developed to calculate the ground states of 1D macroscopic quantum systems with translational symmetry. Applied to the Hubbard model, a modest calculation reproduces the Bethe Ansatz results.

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Since the very beginning of the quantum theory, to solve the Schrödinger equation for macroscopic quantum systems has been one of the main tasks of theoretical physics. It would not be an exaggeration to say that, due to lack of such methods, a considerable effort of theoretical physicists has been devoted to the development of a variety of perturbative and approximate methods and numerical simulations. But a desire for powerful non-perturbative methods has grown stronger over the last couple of decades with the list of phenomena played by strongly correlated electrons getting longer, particularly since the discovery of high temperature superconductivity in copper oxides [1]. While we have seen a considerable progress in rigorous treatment of quantum 1D and classical 2D systems over the last several decades [2–9], these rigorous methods are not flexible enough to solve *non-integrable* models in one dimension, nor, most probably, generalizable to higher dimensions. On the other hand, the method of NRG (numerical renormalization group), particularly DMRG (density matrix RG) has seen a remarkable success first in quantum 1D systems [10] and then in finite Fermi systems, competing well with the conventional quantum chemistry calculations [11]. More recently, the notion of *entanglement* from quantum information theory [12] helped a further progress in NRG towards the finite temperature as well as dynamical quantities [13–15].

In a recent Letter, we have developed a simple, general and practically exact method to calculate statistical mechanical properties of macroscopic classical systems with translational symmetry up to three dimensions [16]. We here extend this method to solve the Schrödinger equation for 1D quantum ground states with translational symmetry. As a benchmark model for this development, we consider the Hubbard model. Just like our recent work on the 3D Ising model, our method is *purely algebraic* and other than seeking a convergence in entanglement space, it does not employ any other notions such as NRG, nor make any approximations. Our results for the ground state energy and the local magnetic moment in the 1D Hubbard model agree with the known exact results by Bethe Ansatz [8,17]. An important difference of the present method from the Bethe Ansatz, however, should be emphasized: the new method is not rigorous but mathematically much simpler, general and therefore readily applicable to any quantum spins, fermions and bosons. This is a reflection of the fact that our recent method for the Ising model is applicable to any classical statistical systems with translational symmetry. Yet another but probably the most significant remark here is that the success in 1D Hubbard model should constitute an essential ingredient in the analysis of the 2D Hubbard model by the present method. Again, this is a reflection of the fact that our recent method for the 3D Ising model crucially relies on the successful analysis of the 2D Ising model, we called it the "Russian doll" structure, and the mathematical structure involving the $D = 2, 3$ Ising models and that for the $D = 1, 2$ Hubbard models are essentially identical.

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The Hubbard model is defined by the Hamiltonian,

$$H = -t \sum_{\sigma,\langle ij\rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where t is the transfer integral, a measure of kinetic energy, U is the onsite Coulomb potential and $c_{i\sigma}$, $c_{i\sigma}^\dagger$ are the annihilation and creation operators for electrons at site i and spin σ. We take t as the energy unit. To calculate the ground state of the Schrödinger equation

$$H\Psi = E\Psi \tag{2}$$

we follow the following steps.

First, instead of (2), consider the eigenvalue problem for the density matrix

$$e^{-\beta H}\Psi = e^{-\beta E}\Psi. \tag{3}$$

A well-known observation about (3) is that, starting with a trial wavefunction Ψ which has non-zero overlap with the ground state, only the ground state survives in the limit $\beta \to \infty$. Monte Carlo and NRG simulations are based on this observation [10,18]. Here our idea goes opposite, $\beta \to 0$, and calculate the largest eigenvalue of the operator $1 - \beta H$ and corresponding eigenstate.

Second, we rewrite the Hamiltonian (1) as a sum of a local *bond* Hamiltonian,

$$H = \sum_{\text{bond}} (H_{ij} + H_i + H_j) \equiv \sum_{\text{bond}} H_{\text{bond}}, \tag{4}$$

with

$$H_{ij} = -t \sum_{\sigma,\langle ij\rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}\right), \tag{5}$$

$$H_i = \frac{U}{2} n_{i\uparrow} n_{i\downarrow} - \frac{\mu}{2}(n_{i\uparrow} + n_{i\downarrow}) \tag{6}$$

where the onsite Coulomb term is split into two sites i and j, and the chemical potential μ is introduced to control the electron number per site.

Third, we note a decomposition of the density matrix,

$$\begin{aligned} e^{-\beta H} &= \prod_{\text{bond}} e^{-\beta H_{\text{bond}}} + \mathcal{O}(\beta^2) \\ &\approx e^{-\beta \sum_{\text{even}} H_{\text{bond}}} e^{-\beta \sum_{\text{odd}} H_{\text{bond}}}. \end{aligned} \tag{7}$$

This is the simplest Suzuki–Trotter decomposition [19], but it is good enough for $\beta \to 0$. In (7), following the procedure familiar in quantum Monte Carlo, we have split the entire bonds into two groups: one connecting the sites $(2i, 2i+1)$, the even group, and the other $(2i+1, 2i+2)$, the odd group. Now the local bond density matrix should be further decomposed as,

$$\begin{aligned} e^{-\beta H_{\text{bond}}} &\approx e^{-\beta H_i} e^{-\beta H_j} e^{-\beta H_{ij}} \\ &\approx \left[1 - \frac{\beta U}{2} n_{i\uparrow} n_{i\downarrow} + \frac{\beta\mu}{2}(n_{i\uparrow} + n_{i\downarrow})\right] \cdot [i \to j] \\ &\quad + \beta t \sum_\sigma \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}\right) \\ &\equiv \Omega_\alpha \otimes \Theta_\alpha \end{aligned} \tag{8}$$

where and below the repeated indices imply a summation, and Ω_α takes five operators, $1 - \frac{\beta U}{2} n_{i\uparrow} n_{i\downarrow} + \frac{\beta\mu}{2}(n_{i\uparrow} + n_{i\downarrow})$, $c_{i\uparrow}^\dagger$, $c_{i\uparrow}$, $c_{i\downarrow}^\dagger$, and $c_{i\downarrow}$ and Θ_α likewise operators at site j. Since the local pair density matrix (8) contains even number of creation and annihilation operators, the matrix representation of the density matrix (7) can be written as a operator product of local matrices,

$$\langle lk| e^{-\beta H_{\text{bond}}} |ij\rangle \approx f_{\alpha,ik} \otimes g_{\alpha,jl} \tag{9}$$

where

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

$$f_2 = \sqrt{\beta t} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

$$g_2 = \sqrt{\beta t} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

etc., where four basis states at each site are ordered as $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$. Note that the -1 in the f_2 matrix is due to the fermion anticommutation algebra. Thus the matrix product representation of the even group bonds in the density matrix is,

$$\cdots f_\alpha \otimes g_\alpha \otimes f_\beta \otimes g_\beta \otimes f_\gamma \otimes g_\gamma \cdots \tag{10}$$

and the same expression for the odd group bonds with one lattice shifted from the even group case. Putting together, we have the matrix representation of the density matrix (7) as,

$$\begin{aligned} K &\equiv \cdots \otimes g_\alpha \cdot f_\beta \otimes f_\gamma \cdot g_\beta \otimes g_\gamma \cdot f_\delta \otimes f_\varepsilon \cdot g_\delta \otimes g_\varepsilon \cdot f_\nu \otimes \cdots \\ &\equiv \cdots \Gamma_{\alpha\beta}^1 \otimes \Gamma_{\beta\gamma}^2 \otimes \Gamma_{\gamma\delta}^1 \otimes \Gamma_{\delta\varepsilon}^2 \cdots, \end{aligned} \tag{11}$$

where for notational simplicity, we have raised the indices 1, 2 for the two Γs to their shoulders. Note also that $\Gamma_{\alpha\beta}^{1,2}$ are 4×4 matrices for each pair of interaction indices (α, β). Thus, $\Gamma^{1,2}$ are a set of $5^2 \times 4^2$ numbers which will be denoted below like $\Gamma_{abcd}^{1,2}$, where (a, b) indicates (up, down) interaction channels, whereas (c, d) indicates (left, right) basis states.

Fourth, we write the ground state wavefunction as,

$$\Psi = \cdots \zeta_{\alpha\beta a_1}^1 \otimes \zeta_{\beta\gamma a_2}^2 \otimes \zeta_{\gamma\delta a_3}^1 \otimes \zeta_{\delta\varepsilon a_4}^2 \cdots \tag{12}$$

on the basis $\cdots |a_1\rangle \otimes |a_2\rangle \otimes |a_3\rangle \otimes |a_4\rangle \otimes \cdots$ where a_1, etc., takes 4 states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$. One can derive the form (12) by a successive use of matrix algebra [16]. Consider, for example, a wave function $\Psi(a_1 a_2 a_3 a_4)$. Regarding this as a matrix of the left index a_1 and the right index $\{a_2 a_3 a_4\}$, SVD (singular value decomposition) gives $\Psi(a_1 a_2 a_3 a_4) = \sum_\alpha A_{a_1\alpha} \rho_\alpha B_{\{a_2 a_3 a_4\}\alpha}$. The quantity B can in turn be regarded as a matrix of the left index $\{a_2\alpha\}$ and the right index $\{a_3 a_4\}$, thus SVD gives $B_{\{a_2 a_3 a_4\}\alpha} = \sum_\beta C_{\{a_2\alpha\}\beta} \lambda_\beta D_{\{a_3 a_4\}\beta}$. Likewise,