New method for the quantum ground states in one dimension

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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 several decades, particularly since the discovery of high temperature superconductivity in copper oxides. While we have seen a remarkable progress in rigorous treatment of quantum 1D and classical 2D systems over the last several decades, 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 and then in finite Fermi systems, competing well with the conventional quantum chemistry calculations. More recently, the notion of entanglement from quantum information theory helped a further progress in NRG towards the finite temperature as well as dynamical quantities.

In a recent article, 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. 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. 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.

The Hubbard model is defined by the Hamiltonian,

\[ H = -t \sum_{\sigma,\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \]  

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 \( \sigma \). We take \( t \) as the energy unit. To calculate the ground state of the Schrödinger equation

\[ H\Psi = E\Psi \]  

we follow the following steps.

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

\[ e^{-\beta H}\Psi = e^{-\beta E}\Psi \]  

A well-known observation about (3) is that, starting with a trial wavefunction \( \Psi \) 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. 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,

\[ H = \sum_{\text{bond}} (H_{ij} + H_i + H_j) \equiv \sum_{\text{bond}} H_{\text{bond}} \]
with

\[ H_{ij} = -t \sum_{\sigma, e, j} (c_{i\sigma}^+ c_{j\sigma} + h.c.) \] (5)

\[ H_i = \frac{U}{2} n_i^2 - \mu \left( n_i^+ + n_i^- \right) \] (6)

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

Third, we note a decomposition of the density matrix,

\[ e^{-\beta H} = \Pi_{\text{bond}} e^{-\beta H_{\text{bond}}} + \mathcal{O}(\beta^2) \approx e^{-\beta \sum_{\text{even}} H_{\text{bond}}} e^{-\beta \sum_{\text{odd}} H_{\text{bond}}} \] (7)

This is the simplest Suzuki-Trotter decomposition \([19]\), but it is good enough for \( \beta \to 0 \). In \([8]\), 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,

\[ e^{-\beta H_{\text{bond}}} \approx e^{-\beta H_i} e^{-\beta H_{ij}} \approx \left[ 1 - \frac{\beta U}{2} n_i^2 n_j^2 + \frac{\beta \mu}{2} (n_i^+ + n_i^-) \right] [i \to j] + \beta \sum_{\sigma} \left( c_{i\sigma}^+ c_{j\sigma} + h.c. \right) \]

\[ = \Omega_{\alpha} \otimes \Theta_{\alpha} \] (8)

where and below the repeated indices imply a summation, and \( \Omega_{\alpha} \) takes five operators, \( 1 - \frac{\beta U}{2} n_i^2 n_j^2 \), \( \frac{\beta \mu}{2} (n_i^+ + n_i^-) \), \( c_{i\uparrow}^+, c_{i\downarrow}, c_{i\uparrow}^-, \) and \( c_{i\downarrow} \) and \( \Theta_{\alpha} \) 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 \([8]\) can be written as a operator product of local matrices,

\[ \langle k | e^{-\beta H_{\text{bond}}} | ij \rangle \approx f_{a,ik} \otimes g_{a,jl} \] (9)

where

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

\[ f_2 = \sqrt{\beta t} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \]

\[ g_2 = \sqrt{\beta t} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \]

FIG. 1: Schematic figure of the transfer matrix eigenvalue equation, Eq(3).

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,

\[ \cdots f_{a} \otimes g_{a} \otimes f_{\beta} \otimes g_{\beta} \otimes f_{\gamma} \otimes g_{\gamma} \cdots \] (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,

\[ K \equiv \cdots \otimes f_{a} \otimes f_{\beta} \otimes f_{\gamma} \otimes g_{\gamma} \otimes f_{\delta} \otimes g_{\delta} \otimes f_{\epsilon} \otimes g_{\epsilon} \otimes \cdots \]

\[ = \cdots \Gamma_{\alpha\beta}^1 \otimes \Gamma_{\beta\gamma}^2 \otimes \Gamma_{\gamma\delta}^1 \otimes \Gamma_{\delta\epsilon}^2 \cdots \] (11)

where for notational simplicity, we have raised the indices 1,2 for the two \( \Gamma \) s to their shoulders. Note also that \( \Gamma_{\alpha\beta}^{1,2} \) are 4x4 matrices for each pair of interaction indices \((\alpha, \beta)\). Thus, \( \Gamma_{\alpha\beta}^{1,2} \) are a set of 5\(^2\times4\(^2\) numbers which will be denoted below like \( \Gamma_{\alpha\beta}^{1,2} \), where \((a, b)\) indicates (up,down) interaction channels, whereas \((c,d)\) indicates (left,right) basis states.

Fourth, we write the ground state wavefunction as,

\[ \Psi = \cdots \zeta_{\alpha\beta\gamma}^1 \otimes \zeta_{\beta\gamma\delta}^2 \otimes \zeta_{\gamma\delta\epsilon}^1 \otimes \zeta_{\delta\epsilon\alpha}^2 \cdots \] (12)

on the basis \( \cdot \cdot \cdot |a_1\rangle \otimes |a_2\rangle \otimes |a_3\rangle \otimes |a_4\rangle \cdots \) 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 \([10]\). Consider, for example, a wave function \( \Psi(a_1a_2a_3a_4) \). Regarding this as a matrix of the left index \( a_1 \) and the right index \( a_2a_3a_4 \), SVD (singular value decomposition) gives \( \Psi(a_1a_2a_3a_4) = \sum_\alpha A_{\alpha \beta} \rho_\beta B_{\gamma \delta \epsilon \eta} \). The quantity \( B \) can in turn be regarded as a matrix of the left index \( a_2a_3 \) and the right index \( a_4 \), thus SVD gives \( B_{\gamma \delta \epsilon \eta} = \sum_\beta C_{\gamma \delta \epsilon \eta} \lambda_\beta D_{\gamma \delta \epsilon \eta} \). Likewise, \( D_{\gamma \delta \epsilon \eta} = \sum_\gamma E_{\gamma \delta \epsilon \eta} \Delta_\gamma F_{\gamma \delta \epsilon \eta} \). Putting together,
rewriting \( A_{a_1\alpha} \) as \( A_\alpha(a_1) \), \( C_{a_2\alpha}\gamma \) as \( C_{\alpha\beta}(a_1) \), \( E_{\alpha\beta}\gamma \) as \( E_{\beta\gamma}(a_3) \), and \( F_{\alpha\gamma} \) as \( F_{\gamma}(a_1) \), and appropriately absorbing \( \rho_0 \), \( \lambda_\beta \) and \( \Delta_\gamma \) into the matrices \( A, C, E \) and \( F \), one gets \( \Psi(a_1a_2a_3a_4) = A_\alpha(a_1)C_{\alpha\beta}(a_2)E_{\beta\gamma}(a_3)F_{\gamma}(a_4) \).

For our density matrix with a bipartite structure with translational symmetry, \( \mu_0 \), one arrives at the claimed form. Again for notational simplicity, we have raised the indices 1, 2 for the two \( \zeta \)s to their right shoulders. In quantum information theory, these indices \( \alpha, \beta \) and \( \gamma \) are known as entanglement \( \mu_0 \). Considering only 1 for these indices is a simple mean-field-like approximation for \( \Psi \).

Allowing larger values, one takes into account the effect of correlation with increasing precision. An important note here is that \( \mu_0 \) is not peculiar to the Hubbard model, but rather a general statement for macroscopic quantum ground states with translational symmetry. Putting the above arguments together, the eigenvalue problem \( \zeta \) for \( \beta \rightarrow 0 \) is then written schematically as in Fig. 1. The horizontal lines indicate 4 local basis states, whereas the vertical lines indicate 5 interaction channels connecting nearest neighbor sites for \( \Gamma^{1,2} \) and entanglements for \( \zeta^{1,2} \).

To emphasize the close similarity to our recent analysis of the Isging model, let us call all 4 lines associated with \( \Gamma^{1,2} \) as bonds. Note that Fig. 1 is a slight generalization of Fig. 1 in the 2D Isging model \( \mu_0 \).

Fifth, we follow the procedure in our method for the Isging model, namely we handle the eigenvalue problem \( \zeta \) as a variational problem. We thus maximize the quantity \( \mu_0 = \Psi K \Psi / \Psi \Psi \) by iteration starting with an input state for \( \Psi \). First consider the numerator. A local ingredient of this quantity is, \( A_{\ell'c;mm'f} \equiv \epsilon_{\ell'a}^\ell \Gamma_{\ell'c;mm'f}^{\ell'c;\ell} \Gamma_{g;\ell'c}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma_{\ell'c;\ell}^{\ell} \Gamma}_{

\text{FIG. 2: The ground state energy per site at } U = 8 \text{ vs. the electron number per site, } n = 1 \text{ corresponding to half-filling. From the top, the entanglement } n = 1.46 \text{ (rectangles) and 8 (star, red online). The thick solid line (blue online) is the Bethe Ansatz result \( \zeta \).}
The thick solid line (blue online) is the Bethe Ansatz result \cite{17}.

For $n = 3$ results below. The convergence criterion is $\| \zeta_{\text{old}}^i - \zeta_{\text{new}}^i \| / \| \zeta_{\text{old}}^i \| \leq 5 \cdot 10^{-5}$. When this condition is met, the relative change in the largest eigenvalue $\mu_0$ often hits $10^{-15}$, the machine precision.

Fig. 2 shows the ground state energy at $U = 8$ as a function of the electron concentration, $n = 1$ corresponding to half-filling. With the increase of the entanglement $n = 1, 4, 6$ and 8, our result converges to the Bethe Ansatz result \cite{17}. Fig. 3 shows the local magnetic moment at $U = 8$ as a function of the electron concentration. Again, our calculation converges to the Bethe Ansatz result \cite{17}. Fig. 4 shows the ground state energy per site at half-filling as a function of the Coulomb energy $U$. From the top, the entanglement $n = 1, 2, 3, 5$ (rectangles) and 7 (star, red online). The thick solid line (blue online) is the Bethe Ansatz result \cite{8}.

In conclusion, the essence of the new method shall be summarized and possible future directions be discussed. First, the method is simple, general, not relying on existing methods such as the cluster mean field theories and NRG. It only uses matrix algebra and fully implements translational symmetry. Its application to other quantum systems in one dimension, namely quantum spins, bosons, and fermions with reasonable finite-range interactions and translational symmetry is immediate. Second, extension to thermodynamics with the use of standard procedure from quantum Monte Carlo, namely the quantum transfer matrix and its 90 degree rotation thereby reducing the thermodynamics to a similar eigenvalue problem as treated in this paper, is straightforward. By switching between real and imaginary times, dynam-
ics should be handled as well. Third, and probably the most important and worth repeating the argument in the introduction, extension to the two dimension is also straightforward. In fact, mathematically, the extension from 1D to 2D Hubbard models in our method should go similarly as in our study of the 3D Ising model based on the calculation of the 2D Ising model, the "Russian doll" structure. The only possible complication may arise from the anticommutation algebra in 2D fermions. At present, therefore, it would be safe to say that the extension to 2D bosons and quantum spins is straightforward, but 2D fermions might need a further theoretical thought.

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