

PERTUBATION THEORY ABOUT SELF-CONSISTENT FIELD SOLUTION IN ONE-DIMENSIONAL HUBBARD MODEL

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The accurate analytical and numerical calculations of the electronic band structure and ground state properties of strongly correlated electrons within the Hubbard model are performed by constructing convergent perturbation theory for general interaction strength and electron concentration. We test the developed perturbation approach about mean field solution in the extreme conditions of one dimensionality for entire parameter space of electron interaction U/t and electron concentration n . The many-body perturbation formalism up to second order about the generalized self-consistent field (GSCF) Hamiltonian goes beyond the range of applicability of standard perturbation theory by incorporating systematically the effect of the random-phase-type perturbation techniques and controlled expansion of the energy functional for general U/t and n . The second order perturbation correction vanishes at small and large U/t limit and performed calculations of the ground state energy show a next to the perfect numerical agreement with the Bethe-ansatz results.

1. Motivation

The analytical theory for the interacting electron gas was first developed by Gell–Mann and Brückner,^{1,2} now known as random phase approximation (RPA), gives the exact values for the correlation energy in the high density-weak coupling regime. However, this method runs into difficulties due to the insufficient treatment of fluctuations. Starting from the weak coupling regime Schrieffer, Wen and Zhang examined the fluctuations around the SDW mean field solution for repulsive Hubbard model using the RPA.^{3,4} This fact gave a rise the hope that the RPA fluctuations might be able to interpolate between the large and small coupling limits.^{3,5,6} However, the low-energy physics is still not properly treated within the traditional mean field with corresponding RPA extensions.⁷

We study the dynamic many body effects of strongly correlated electrons in the periodic lattices by including the effect of fluctuations around the self-consistent solution. It is a combination of the self-consistent approach with systematic use of the effect of the random-phase-type perturbation techniques applied in entire space of electron concentration, magnetic field and U/t for calculation of the ground state properties by comparison with the rigorous results in one and in two dimensions.^{8,9}

Here we initially test the developed perturbational approach up to the second order around so called linearized generalized self-consistent field (GSCF) theory for the repulsive Hubbard model and numerical results in one dimension (1d) are compared with the Bethe-ansatz solution. At large U/t limit the result of second order perturbation vanishes and at small and intermediate U/t range the perturbation theory gives rather good agreement with the Bethe-ansatz result.

2. Results in Linearized GSCF Approach

The GSCF theory for attractive and repulsive interaction has been successfully used in calculating of the ground state properties and electronic structure of many body systems.^{8,9} The GSCF ground state at arbitrary q and $U > 0$ is

$$|0_{\text{GSCF}}\rangle = \prod_k \alpha_{kq\lambda}^+ |0\rangle, \quad (1)$$

where $\alpha_{kq\lambda}^+$ is the quasi-particle operator, k is inside the Fermi-region (“Fermi-sea”), i.e. $\mathcal{E}_{k\lambda}^{(+)}(q) \leq \mu^{(+)}$. The quasi-particle energy spectrum $\mathcal{E}_{k\lambda}^{(+)}(q)$ is determined by

$$\mathcal{E}_{k\lambda}^{(+)}(q) = \frac{\epsilon_k + \epsilon_{k+q} + nU - \lambda \sqrt{(\epsilon_k - \epsilon_{k+q} - 2Us - h)^2 + (\Delta_q^{(+)})^2}}{2}, \quad (2)$$

$\lambda = 1$ (\uparrow) or -1 (\downarrow) with transverse ($\Delta_q^{(+)}$) and longitudinal (s) spin order parameters and the chemical potential $\mu^{(+)}$. The eigenvalue of the GSCF Hamiltonian in the ground state is

$$E_{\text{GSCF}}^{(+)(0)} = \frac{1}{N_{\text{latt}}} \sum_{k,\lambda} \mathcal{E}_{k\lambda}^{(+)}(\mathbf{q}) n_{kq\lambda}^{(+)(0)} + \frac{(\Delta_q^{(+)})^2}{4U} - \frac{n^2 U}{4} + s^2 U, \quad (3)$$

where $n_{kq\lambda}^{(+)(0)}$ means occupation numbers of quasi-particle states. The GSCF eigenvalue $E_{\text{GSCF}}^{(+)(0)}$ provides for energy a simple interpolation scheme between the weak and strong interaction in entire range of U/t , h and all $0 \leq n \leq 1$. The GSCF and exact results coincide in extreme limits of weak and strong interaction. However, instead of a common belief that the mean field approximation is a valid starting point at weak interaction limit, the GSCF numerical results clearly demonstrate qualitative discrepancy for all $n \leq 1$ in prediction of behavior for double occupancy $D^{(+)}$ and kinetic energy E_{kin} at $U/t \ll 1$.⁸ The exact and the GSCF limiting values of $D^{(+)}$ are the same, although the GSCF result barely changes at weak interaction $|U|/t \ll 1$, while the exact result gives a linear dependence. The GSCF theory

also fails in description of the chemical potential $\mu^{(+)}$ at intermediate and strong interaction limit, especially at $n = 1$. In fact the GSCF solution for $\mu^{(+)}$ versus n unstable and has a tendency toward the phase separation, while the exact $\mu^{(+)}$ is everywhere monotonous function on n .

3. Convergent Perturbation Theory

The GSCF theory does not account for the strong dynamic fluctuations around the average values. The traditional perturbation theory about non-interacting Hamiltonian has zero convergent radius and perturbational expansion diverges at large U/t . One can naively think that because U/t can be the largest energy scale for systems of interest, such straightforward expansion of fluctuations about zero order mean field Hamiltonian do not necessary vanish.

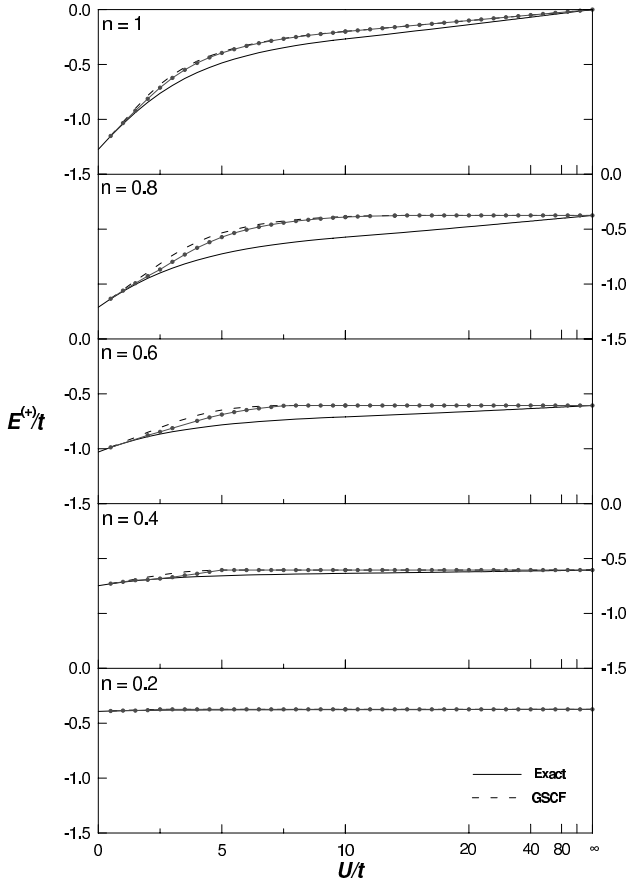


Fig. 1. The ground state energy $E^{(+)}/t$ as a function of U/t for various n in the Bethe-ansatz solution (solid curve), the GSCF approach (dashed curve) and II order perturbation result (dark bullets).

We suggest here convergent perturbation approach beyond the standard linear approximation, using the Bogolyubov-type transformation to the new quasiparticles. The problem can be reduced simply to carefully resorting the contribution of different terms in transformed the GSCF and exact Hubbard models and calculating of the corresponding matrix elements. We consider the GSCF Hamiltonian $H_{\text{GSCF}}^{(+)}$ as a zero order term and take the difference $H_{\text{exact}} - H_{\text{GSCF}}^{(+)}$ as a perturbation. In equilibrium the GSCF self-consistent equations are satisfied and the I order correction is identical to zero, $E^{(+)(1)} = 0$. The next correction to the GSCF result $E_{\text{GSCF}}^{(+)(0)}$ for the ground state energy is II order perturbation term, $E^{(+)(2)}$.

The performed numerical calculations in Fig. 1 of the ground state energy $E^{(+)}/t$ demonstrate next to the perfect numerical agreement with the Bethe-ansatz results at weak and intermediate range of U/t . However the results at large U/t differ from Bethe-ansatz ones. It also should be kept in mind that the comparison with the exact result in 1d is probably a “worst-case” scenario for most approximation theories due to strong quantum fluctuations. This work is a first attempt to develop an accurate and regular perturbation scheme valid in the entire parameter space. We expect that this approach will be even more accurate in higher dimensions, where corresponding fluctuations are suppressed.

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