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QUANTUM FLUCTUATIONS TO DESTROY THE ANTIFERROMAGNETIC SPIN ORDER IN THE ONE DIMENSIONAL HALF FILLED HUBBARD MODEL

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Abstract Quantum fluctuations in the one dimensional half filled Hubbard model are investigated with the resonating Hartree-Fock method with the orbital optimization. The optimized Slater determinants include an inhomogeneous spin density wave and configurations accommodating some neutral soliton pairs. The short and long range spin orders are destroyed by quantum translational and breathing motions of soliton pairs and gapless Gaussian type fluctuations, respectively. Our calculation suggests that the lowest singlet and triplet excitation branches are the translational modes of breathing neutral soliton pairs dressed with the Gaussian type fluctuations.

INTRODUCTION

Molecular magnets often make quasi one dimensional (1D) structures. However a pure 1D electronic system cannot have a magnetic long range order (LRO) owing to its large quantum fluctuations. If we understand the nature of the quantum fluctuations, then we can know what kind of weak 3D interactions effectively suppress them. Such a knowledge will be useful to design quasi 1D molecular magnets.

As a test case to study quantum fluctuations in a 1D electronic system, we consider the half filled 1D Hubbard model. The Hartree-Fock (HF) ground state of this model has a magnetic LRO of a spin density wave (SDW). The SDW has topological soliton excitations. We consider that soliton pairs making translational and breathing motions are the basic units of fluctuations in this system.[1,2] To confirm this physical picture, we investigated this model with the resonating HF (Res HF) method which was proposed by one of the authors.[3] Since the exact solutions of the 1D Hubbard model are known, we can check the validity of the new approximation.

The Res HF method approximate quantum fluctuations by superposing non-orthogonal Slater determinants (S det) such as $|\Psi\rangle = \sum_f |f\rangle C_f$. A $|f\rangle$ has a LRO and other $|f\rangle$'s contain fluctuations in them. Both C_f and orbitals in $|f\rangle$ are determined variationally to minimize the expectation value of the energy. This method can treat large quantum fluctuations. By analyzing the optimized $|f\rangle$'s we

can elucidate the physical nature of the quantum fluctuations.

CALCULATIONAL METHODS

The 1D Hubbard Hamiltonian is given by

$$H = \sum_{m=1}^{N} \{ - \sum_{\sigma} (a^{\dagger}_{m+1\sigma} a_{m\sigma} + a^{\dagger}_{m\sigma} a_{m+1\sigma}) + U a^{\dagger}_{m\uparrow} a^{\dagger}_{m\downarrow} a_{m\downarrow} a_{m\uparrow} \}, \tag{1}$$

where $a^{\dagger}_{m\sigma}$ and $a_{m\sigma}$ are the creation and annihilation operators of an electron with spin σ at m-th site. H and the on-site Coulomb energy U are scaled by the transfer integral. We consider the half filled $N = 4l + 2$ chain with the periodic boundary condition, $a^{\dagger}_{N+1\sigma} = a^{\dagger}_{1\sigma}$. We restrict S dets to the type of different orbitals for different spins, $|f\rangle = \prod_{a=1}^{n\uparrow} f^{\dagger}_{a\uparrow} \prod_{a=1}^{n\downarrow} f^{\dagger}_{a\downarrow} |0\rangle$. A half-filled and $S_z = 0$ state ($n_{\uparrow} = n_{\downarrow} = 2l + 1$) is considered. The optimized $|f\rangle$'s usually break all the translation, reflection and spin inversion symmetries of the Hamiltonian. We determine $|\Psi\rangle$ so as to recover the symmetries. Thus the symmetry adapted Res HF state is given as

$$|\Psi_k\rangle = \sum_{f=1}^{N_S} |f^{\mathrm{P}}_k\rangle C_f, \quad |f^{\mathrm{P}}_k\rangle = \sum_{m=0}^{N-1} \cos(km) T^m (1 + R)(1 \mp I_S)|f\rangle, \tag{2}$$

where T is the operation to translate $|f\rangle$ by one site, R is the C_2 rotation in the D_N symmetry of the system and I_S is the spin inversion. The operations $1 - I_S$ and $1 + I_S$ select even and odd total spins, respectively, and are used as approximate spin projections. If we take $k = 0$ and $1 - I_S$, we get the ground state.

We optimize C_f and $|f\rangle$ with a direct minimization algorithm developed recently. The detail of the algorithm will be given elsewhere.[4] The former works[1,2] did not optimize $|f\rangle$'s. As trials we use S dets of the SDW and neutral soliton pairs. We observe, however, large deformation from the trials such as spontaneous creations of soliton pairs during the optimization process. We note that the orbital optimization incorporates Gaussian fluctuations because the second variation used in it has RPA like matrix elements.

RESULTS

Correlation Energy of the Ground State

Since the Res HF approximation is a variational method, we can check its goodness by examining the fraction of the ground state correlation energy, κ =

TABLE I. Fraction κ (%) of the ground state correlation energy explained by the Res HF and Gutzwiller methods.

		U					
N	N_S	1	2	3	4	6	8
14	1	96.1	83.7	67.9	49.4		
	2		94.2	83.7	70.4		
	4	99.6	97.8	92.4	85.3		
	6	99.9	99.1	95.8	90.0		
	12				96.7	90.9	87.7
	15						90.7
	21						94.6
18	4			85.5			
22	4		92.4	78.7			
RHF-GW [6]				70	47	×	×
SDW-GW [7]			~85	78	77	59	50

$(E_{\rm HF} - E_{\rm ResHF})/(E_{\rm HF} - E_{\rm exact})$, explained by it. We show in Table I the values of κ for various N and N_S. The exact energies are taken from the finite version of the Lieb-Wu solution.[5] We find that the Res HF approximation can explain more than 90 % of the exact correlation energies in all the correlation regimes. It gives much better κ than the Gutzwiller method.[6,7] The smaller the U is, the more effective our method is and the larger κ is obtained with small number N_S of the generating S dets. For $U \leq 2$ and $N = 14$, our approximation gives more than 99% of the correlation energy with only $N_S = 6$. This result is encouraging since the Coulomb interactions of many real systems such as conducting polymers and halogen bridged transition-metal 1D complexes are in this regime. In the strong correlation regime with U=8 we need $N_S = 15$ to explain more than 90% of the correlation energy. However, the number of independent S dets with $S_z = 0$ is $({}_N C_{n/2})^2$. For $N = 14$ and $n = 14$ it is equal to 11,778,624. Hence we can explain most of the correlation energy with very few S dets.

The fraction κ decreases as the system size is enlarged unless we increase N_S. This is because more S dets are necessary to keep the density of soliton pairs

constant and to take into account their relative motions in longer chains. It is, however, satisfactory that we can explain more than 80% of the correlation energy with small N_S for the systems with $N = 18$, 22 to which exact diagonalization is not applicable.

Structures of the Slater Determinants Generating the Res HF Wave Function

In order to elucidate the physical picture of the quantum fluctuations in this model, we examine the structures of the optimized S dets generating the Res HF state. We show in FIGS. 1 and 2 the net and alternating components [8] of the spin density (NSD and ASD) and the bond order (NBO and ABO) of the S dets in the case of $N_S = 6$ for $N = 14$ and $U = 4$ and 2. No charge densities and spin bond orders are present in all the S dets showing that the ground state is homopolar.

The S det in FIG. 1a represents a non-uniform SDW. Those in FIG. 1b, c and d represent states with one neutral soliton (S) pair with S–S distance $R_{SS} = 2$, 4 and 6, respectively. The centers of S's are zero points of the ASD and marked by dots. The resonance among these S dets expresses a breathing S–S pair (breather). The S dets in FIGS. 1e and f contain two S–S pairs with R_{SS}=2. The second pair is considerably deformed and its NSD is small. The resonance between these S dets expresses the relative motion of the two S–S pairs. The contribution from configurations with multiple S–S pairs is important even in this short chain.

We see from FIG. 2 that the number of the S dets with two S–S pairs are increased at the small $U = 2$. This is consistent with the HF result that the creation energy of a S at $U = 2$ is smaller than that at $U = 4$.[2] The S det in FIG. 2f with 4 S's may be regarded as a complex of a triplet S–S pair and two S's with the opposite spin around it.

The numerals in FIGS. 1 and 2 show the probability to find the symmetry adapted bases $|f_0^P\rangle$ in the Res HF state, $|\langle f_0^P|\Psi_0\rangle|^2/|\langle f_0^P|f_0^P\rangle|^2$. The probability of the SDW type S det (FIGS. 1a, 2a) becomes small as U is increased.

For $N_S \leq 4$, we find only S dets with one or two S–S pairs. No SDW like S det is obtained. This shows that the fluctuations owing to S–S pairs is the most important feature in the true ground state.

The widths of the solitons in the orbital optimized states are narrow localizing only on two sites and independent of U in contrast to the HF S's with increasing width with decreasing of U.[1] It is noteworthy that, in all correlation regimes, all the symmetries are broken in all the optimized S dets.

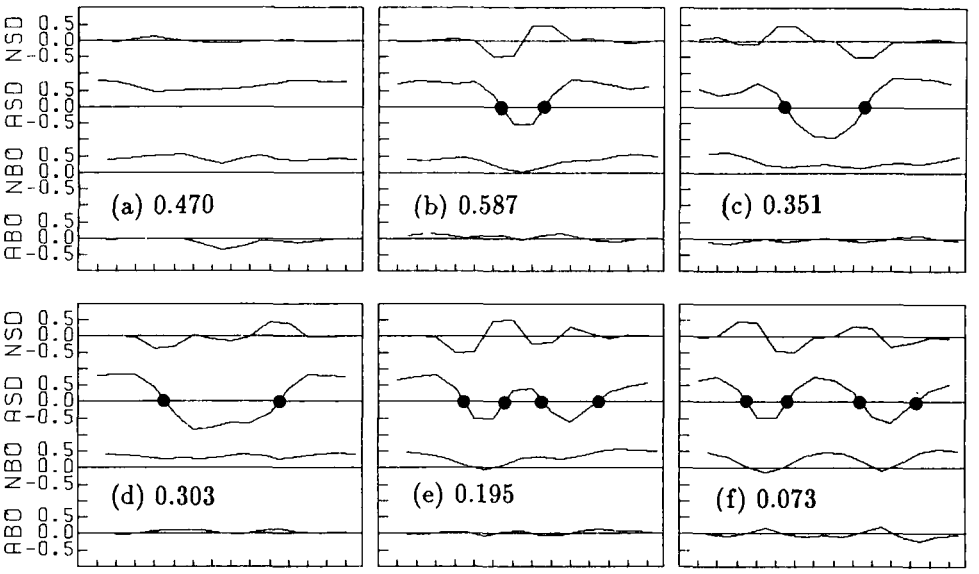

FIGURE 1 Structures of the optimized S dets generating the Res HF ground state in the approximation with $N_S = 6$ for $U = 4$ and $N = 14$.

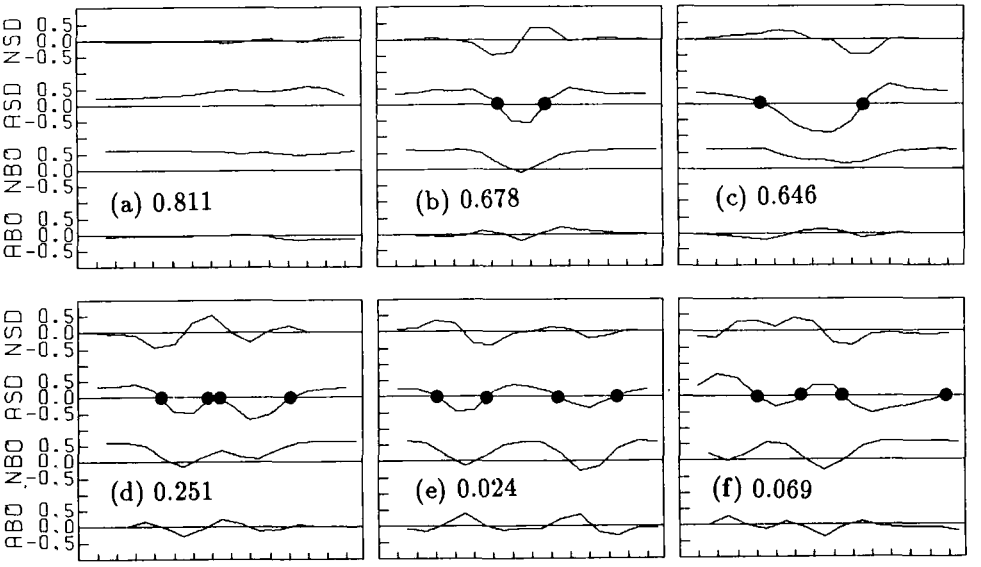

FIGURE 2 Structures of the optimized S dets for $U = 2$. The other conditions are the same as FIG. 1.

Spin Correlation Function

We show in FIGS. 3a and b the spin correlation function $L(l) = \langle\Psi_0|\mathbf{S}(0)\cdot\mathbf{S}(l)|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle$ in the case of $N_S = 6$ for $N = 14$ and $U = 4$ and 2. Our results are compared with the exact result for $N = 6$ and $U = 4$ [9] (o), the exact long range behavior $\sim(-1)^l l^{-3/2}\ln l^{1/2}$ [10,11] scaled at our $L(2)$ (- - -) and the previous Res HF result without orbital optimization (×) [1]. The present approximation succeeds to reproduce both of the rapid and gradual decreases in the short and long distances, respectively. The short range rapid decrease is due to the translational and breathing motions of soliton pairs.[1] The long range gradual decrease is due to the Gaussian fluctuations related to gapless excitations.[10,11] The orbital optimization is necessary to explain it. The calculated total spins $\langle\Psi_0|S^2|\Psi_0\rangle$ for $U = 2$ and 4 are 0.004 and 0.327, respectively. Thus contaminations of higher spin states in the Res HF states are very small at U=2 and about 16 % at $U = 4$.

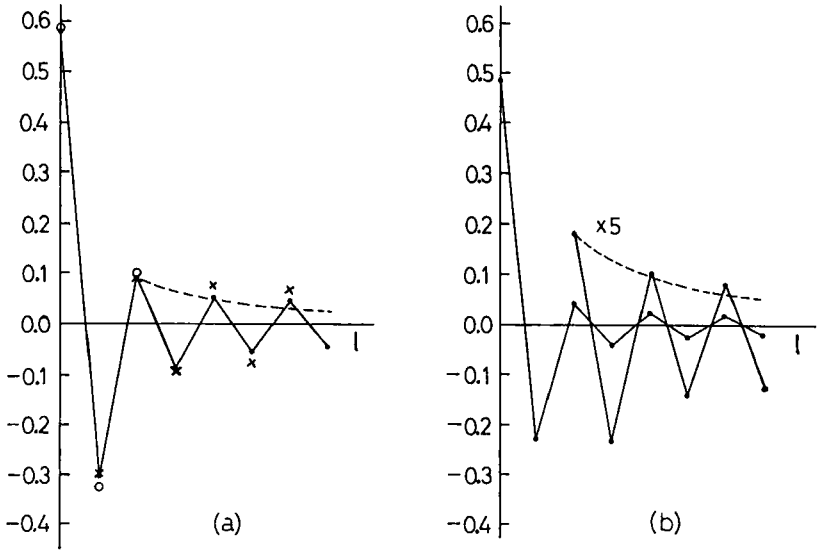

FIGURE 3 Spin correlation function $L(l)$ for $U = 4$ (a) and $U = 2$ (b).

Excited States

We at last calculate by eq.(1) the k dispersions of the lowest lying singlet and triplet excitations. The S dets are optimized at each k. At $k = 0$ and π, we can also get the optimized states which belong to the representation A_2 and B_2 by

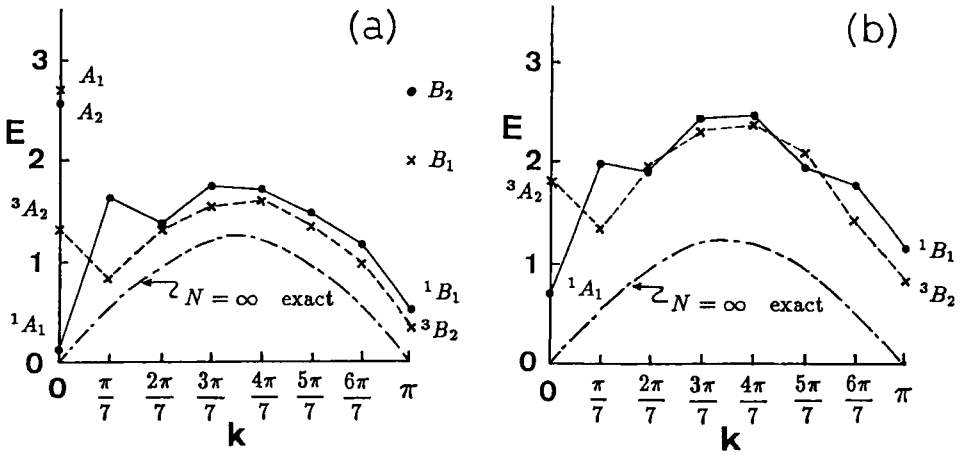

FIGURE 4 k dispersions of the lowest excited states for $N = 14$ and $U = 4$ given by the Res HF method with six S dets optimized at every k (a) and with three HF S dets without orbital optimization (b).

adopting the projection $1 - R$ in stead of $1 + R$.

We show in FIG. 4a the optimized dispersion of the lowest singlet (•) and the triplet (×) excitations in the case of $N_S = 6$ for $N = 14$ and $U = 4$, and compare them with the exact dispersion of the homopolar excitation in the infinite chain (----).[12] Both of the branches well reproduce the sin like behavior. The anomaly in the singlet state at $k = \pi/7$ was observed in the exact excitations in the finite version of the Lieb-Wu solution.[13]

FIGURE. 4b shows the dispersions calculated with three HF S dets which contain only one S–S pair with $R_{SS} = 2$, 4 and 6. It is important that the sin like dispersions are already produced in this simple approximation, indicating that the sin like profiles in the k dispersions arise from translational and breathing motions of one S–S pair. The energy stabilization of the dispersions in Figs. 4a from 4b are due to inclusions of four S states and Gaussian type fluctuations incorporated by the orbital optimization. Namely, low lying spin excitations are produced by moving S–S pairs dressed with Gaussian type fluctuations.

DISCUSSION

As seen in this paper, the spin order in the half filled 1D Hubbard model is

destroyed by the quantum fluctuations owing to S–S pairs making translational and breathing motions which are dressed with Gaussian type fluctuations. If we find weak 3D interactions that effectively suppress the fluctuations, we will get quasi 1D antiferro-magnets with a high transition temperature.

The Res HF method has been shown to give good results for the ground state correlation energy, the spin correlation function and the low lying excited states. It gives a concrete picture about large quantum fluctuations in a 1D system. It, therefore, will be a powerful method to study 1D electronic systems.

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