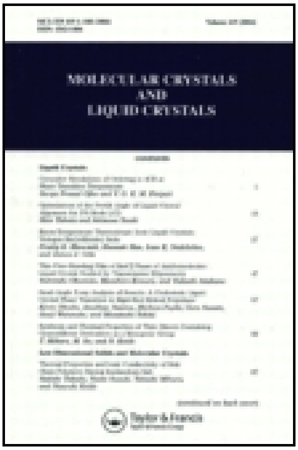

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Shoji Yamamoto [a], Akira Takahash [a b] & Hideo Fukutome [a]
[a] Department of Physics, Kyoto University, Kyoto, 606, Japan
[b] Department of Physics, Faculty of Liberal Arts, Yamaguchi University, Yamaguchi, 753, Japan
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RESONATING HARTREE-FOCK THEORY OF A ONE DIMENSIONAL ELECTRONIC SYSTEM

SHOJI YAMAMOTO, AKIRA TAKAHASHI[†] AND HIDEO FUKUTOME
Department of Physics, Kyoto University, Kyoto 606, Japan
[†]*Department of Physics, Faculty of Liberal Arts, Yamaguchi University, Yamaguchi 753, Japan*

Abstract The electronic structure of the one dimensional (1D) Hubbard model is calculated by the resonationg Hartree-Fock (Res HF) method. As local fluctuations in the spin density wave (SDW) in the half filled case, we consider a soliton-antisoliton pair making quantum translational and breathing motions, i.e, breathers. The breather explains 76.5% ($U = 3$) and 70.1% ($U = 4$) of the ground state correlation energy, which is better than the result of the Gutzwiller method, and gives low energy excited states with the symmetries and energetic ordering characteristic in polyenes. The fluctuations by the breather also explain the spin and density correlations.

INTRODUCTION

In spite of vigorous studies of 1D electronic systems, the natures of the fluctuations and their physical consequences are still left inexplicable because of large quantum fluctuations characteristic in 1D systems. We present in this paper a new approach to the problem[1] based on the Res HF method,[2] where a wave function with large quantum fluctuations are approximated by a superposition of non-orthogonal Slater determinants (dets) which are collectively different from each other and correspond to low energy local minima of the HF equation. Applying it to the 1D half filled Hubbard model whose exact solution is known,[3] we show that a diradical and zwitterionic breather in the SDW, which consists of a neutral and charged soliton-antisoliton pair, respectively, is a good picture of the quantum fluctuations in this model.

SDW BREATHERS IN THE 1D HUBBARD MODEL

We consider a periodic chain with equidistant N sites. The Hubbard Hamiltonian of the chain (in the unit of transfer energy) is

$$H = \sum_{m}\{-\sum_{\sigma}(a^{\dagger}_{m+1\sigma}a_{m\sigma} + a^{\dagger}_{m\sigma}a_{m+1\sigma}) + U(N_{m\uparrow} - \frac{1}{2})(N_{m\downarrow} - \frac{1}{2})\}, \tag{1}$$

where $a_{m\sigma}$ and $a^{\dagger}_{m\sigma}$ are the annihilation and creation operators of the electron at m-th site and with spin σ and $N_{m\sigma} = a^{\dagger}_{m\sigma}a_{m\sigma}$. In the half filled case, the HF ground state is the SDW with a long range order (LRO). As units of quantum fluctuations to destroy the SDW LRO, we employ soliton solutions of the HF equation.

In a periodic chain with even sites, solitons are produced in pair of a soliton (S) and an antisoliton ($\bar{S}$) whose distance $R_{S\bar{S}}$ between S and $\bar{S}$ can change (Figure 1). A single soliton is a low energy HF solution, while an S-$\bar{S}$ pair at a given $R_{S\bar{S}}$ is usually not a static HF solution unless $R_{S\bar{S}}$ is large enough. Therefore, to obtain Slater dets of S-$\bar{S}$ pairs at small $R_{S\bar{S}}$ we can use an approximation to make the densities in the Fock operator by connecting the densities of S and $\bar{S}$ at

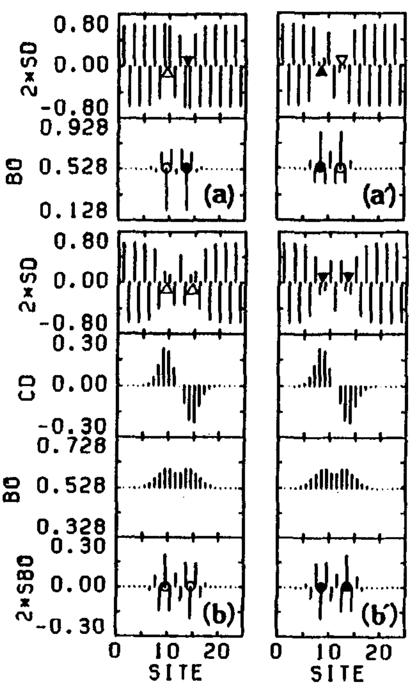

FIGURE 1 Structures of S^0-$\bar{S}^0$ pairs at $U = 3$. $S_1^{0\uparrow}$-$\bar{S}_2^{0\downarrow}$ (a) and $S_2^{0\uparrow}$-$\bar{S}_1^{0\downarrow}$ (a') with $R_{S\bar{S}} = 4$. S_1^{+}-$\bar{S}_1^{-}$ (b) and S_2^{+}-$\bar{S}_2^{-}$ (b') with $R_{S\bar{S}} = 5$.

the middle of $R_{S\bar{S}}$ and to solve once the eigenvalue equation of this Fock operator. We show in Figure 1 examples of S-$\bar{\text{S}}$ pair made by this way. The S-$\bar{\text{S}}$ pairs producible from the SDW are diradical pairs $S^{0\uparrow}$-$\bar{S}^{0\downarrow}$ and $S^{0\downarrow}$-$\bar{S}^{0\uparrow}$ and zwitterionic pairs S^+-$\bar{S}^-$ and S^--$\bar{S}^+$. Since the SDW solitons have two interface types, denoted S_1 and S_2, in which the two SDW phases are interfaced at sites where the alternating components of the SD are positive and negative, respectively, each of the S-$\bar{\text{S}}$ pair has four interface types.

We can construct wave functions of a resonating breather making quantum breathing and translational motions by superposing Slater dets of an S-$\bar{\text{S}}$ pair with different $R_{S\bar{S}}$ and positions as

$$|\Psi^K\rangle = \sum_m e^{imK} \sum_{ij\sigma l} |S_i^\sigma(m)\bar{S}_j^{-\sigma}(m+l)\rangle c_{ijl}^{K\sigma}, \tag{2}$$

where $|S_i^\sigma(m)\bar{S}_j^{-\sigma}(m+l)\rangle$ is the Slater det of the S-$\bar{\text{S}}$ pair at the position m with $R_{S\bar{S}} = l$ and the interface types of i and j and σ denotes the spin $\sigma = \pm 1/2$ for the diradical pair or the charge $\sigma = \pm 1$ for the zwitterionic pair. The superposition coefficients $c_{ijl}^{K\sigma}$ are variationally determined.

We show in the following electronic properties of periodic chains in which a resonating breather is produced in the SDW. The breather can take both the types, diradical and zwitterionic, with certain probabilities.

CORRELATION ENERGY DUE TO THE BREATHERS

The fluctuations by the resonating breathers bring about a correlation stabilization of the Res HF ground state energy E^{RH}/N (per site) relative to the SDW energy E^{SDW}/N. Since the Res HF method is a variational approximation the amount of the correlation energy $E_{\text{corr}}^{\text{RH}}/N = (E^{\text{SDW}} - E^{\text{RH}})/N$ gives an indication how good is the theory. Therefoer, we define the quantity κ as the fraction of the correlation energy explained by the Res HF method, $\kappa = 100 \times E_{\text{corr}}^{\text{RH}}/E_{\text{corr}}^{\text{ex}}$ (%), where $E_{\text{corr}}^{\text{ex}}/N = (E^{\text{SDW}} - E^{\text{ex}})/N$ and E^{ex}/N is the exact ground state energy in the half filled case of the Lieb and Wu solution.[3]

We show in Table I, the values of E^{ex}/N, E^{SDW}/N, E^{RH}/N and κ at $U = 3$ and 4. To see the breather concentration (y) dependences of κ, the latter three quantities are indicated at $N = 12$ ($y = 8.3\%$) and $N = 20$ ($y = 5\%$).

Table I Correlation energy due to the breathers.

U	E^{ex}/N	N	E^{SDW}/N	E^{RH}/N	κ (%)
3	−1.440038	12	−1.334829	−1.415291	76.5
		20	−1.345094	−1.407061	65.3
4	−1.573729	12	−1.469089	−1.542470	70.1
		20	−1.469105	−1.530352	58.5

At $y = 8.3\%$, the present theory can explain 76.5% ($U = 3$) and 70.1% ($U = 4$) of the exact correlation energy. On the other hand, the Gutzwiller method applied to the 1D Hubbard model can explain 70% ($U = 3$) and 47% ($U = 4$) of the correlation energy.[4] Thus the Res HF method regarding breathers in the SDW as important quantum fluctuations gives better variational wave function than the Gutzwiller method.

RESONON LEVELS OF THE BREATHERS

The breathers give excited states with finite gaps from the ground state that are called the breather resonons.[5] The wave function of a breather with $K = 0$ in the form of Eq.(2) has the C_2 symmetry against its center. The diradical breather gives series of spatially symmetric singlet ^1A and antisymmetric triplet ^3B states, while the zwitterionic breather gives ^1A and ^1B states.

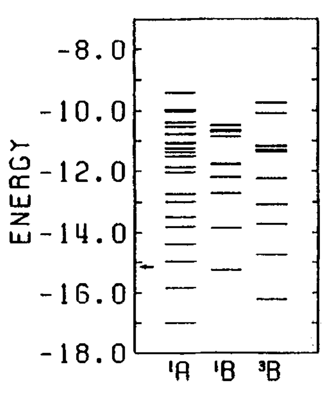

FIGURE 2 Breather resonon levels.

We show in Figure 2 the resonon levels of the breathers for $U = 3$ in the chain with $N = 12$. The lowest excited levels have the symmetries and energetic ordering $^3B < {}^1A < {}^1B$ where the lowest optically allowed state ^1B is slightly below the edge of the interband transition of the SDW gap, which is indicated by the arrow in Figure 2. This situation is similar to the excited states in polyenes.[6]

SPIN AND DENSITY CORRELATION FUNCTIONS

The HF ground state has the SDW LRO. However, it is destroyed by quantum fluctuations in the true ground state. A resonating breather effectively destroys the SDW LRO because it reverses the SDW phase in the region between S and $\bar{S}$ and also has dips in the regions at S and $\bar{S}$.

We show in Figure 3(a) the spin correlation functions

$$L_{spin}(l) = \langle\Psi^0|\mathbf{S}(0)\cdot\mathbf{S}(l)|\Psi^0\rangle / \langle\Psi^0|\Psi^0\rangle \qquad (3)$$

at $U = 3$ and 4 in the Res HF ground state in the chain with $N = 12$.

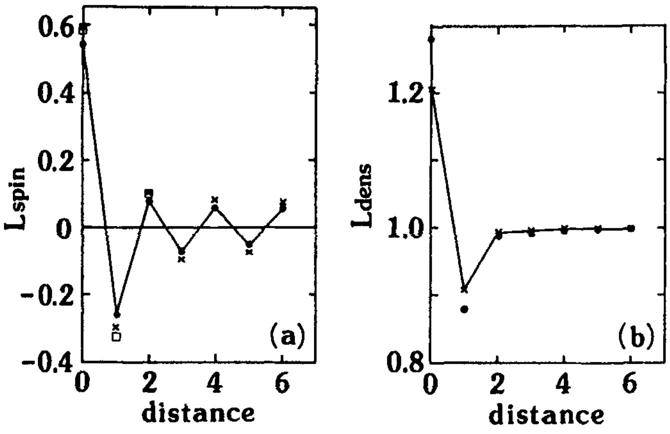

FIGURE 3 Spin (a) and density (b) correlation functions are shown at $U = 3$ (•) and 4 (×). In (a) the exact spin correlation function in the chain with $N = 6$[7] is also shown at $U = 4$ (□).

The spin correlation function rapidly decreases with l in the short range $l \leq 2$ and turns out to be slowly decreasing in the longer distances. At $U = 4$, the value of the Res HF spin correlation function at $l \leq 2$ are in good agreement with the exact results in $N = 6$,[7] indicating that the fluctuations by the breathers are determining the short range decrease of the spin correlation function. The long range tail behavior of a correlation function is considered to be dominated by the fluctuations due to gapless excitations such as magnons[8] that are neglected in the present calculations.

We show in Figure 3(b) the density correlation functions

$$L_{\mathrm{dens}}(l) = \langle \Psi^0 | N(0) \cdot N(l) | \Psi^0 \rangle / \langle \Psi^0 | \Psi^0 \rangle \tag{4}$$

at $U = 3$ and 4 in the Res HF ground state in the chain with $N = 12$. Here $N(l) = \sum_\sigma a_{l\sigma}^\dagger a_{l\sigma}$. As is expected in the Hubbard chain, the density correlation function rapidly converges toward the value one, indicating the ground state of the Hubbard chain is almost homopolar. This tendency is more remarkable for larger U.

We have developed the Res HF theory of the half filled 1D Hubbard model employing the picture which regards the diradical and zwitterionic breathers as the important units of local quantum fluctuations. Figure 8 shows that our wave function gives quantitatively reliable short range correlation. We stress again that the Res HF method, as for the ground state correlation, provides a good approximation of the 1D Hubbard model better than the Gutzwiller method. It also gives low lying excited states which are very important in 1D molecules such as polyenes and polyacetylene. From the above results, we are sure that our theory provides a promising systematic approach to electronic structures of quasi-1D systems.

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