New Paired-Wavefunction for the Frustrated Antiferromagnetic Spin-Half Chain

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I propose a new paired-wavefunction with a parameter that continuously interpolates from the 1D Jastrow-product to the Majumdar-Ghosh dimer-wavefunction appropriate for the frustrated Heisenberg $S = 1/2$ antiferromagnet. This spin paired-state constructed in $S_z$ basis is an alternative to the well-known resonating-valence-bond basis state for describing the $S = 0$ ground-state with no apparent long-range spin order. Some numerical evidences are presented.

The simplest non-trivial single-particle wavefunction in the first quantized form is the plane wave, $\exp(i \vec{k} \cdot \vec{r})$, corresponding to a free particle in space. For the many-body system the simplest ground-state wavefunction can be constructed by either anti-symmetrizing or symmetrizing the single-particle plane waves depending on the statistics of the particles being considered.

The next non-trivial step is to incorporate the effects of interaction by taking (anti-)symmetric pairwise wavefunction and further (anti-)symmetrizing over all the other remaining variables in the many-body wavefunction. The simplest such wavefunctions are the Jastrow-product and the less well-known BCS paired-wavefunction projected onto the Hilbert space of definite number of particles. Recently, these two-types of wavefunctions have been applied to the fractional quantum Hall states. In this letter I propose a new paired-wavefunction with a parameter that interpolates from the Jastrow-product which is an exact ground-state of the Haldane-Shastry model (HSM) to the Majumdar-Ghosh wavefunction for the frustrated SU(2) Heisenberg spin chain.

One of the main results of this letter is the following wavefunction for the spin chain with $N_a$ sites

$$|\Psi\rangle = \sum_{\sigma} \phi(z, \sigma) e^{i\pi \sum_{j=1}^M m_j |\sigma\rangle}, \quad (1)$$

where $M = N_a/2$ is the total number of down or up spins, the sum is over all the spin configuration $\sigma$ in $S_z$ basis, and $m_i (n_i)$ the integer site index of $i$th down(up) spin. The second factor in the sum corresponds to the Marshall sign. The orbital function $\phi(z, \sigma)$ is given by

$$\phi(z, \sigma) = \text{Det}[f^\dagger(x, y)]$$

$$f(x, y) = (x + y)^{l/4} |x - y|^l,$$

where $z_m = \exp(i2\pi m/N_a)$ and $l$ some integer. Here, $\text{Det}$ denotes determinant of the $M \times M$ matrix $[f(x_i, y_j)]$ while $f(x_i, y_j)$ is a wavefunction for a pair of up- and down-spins. One can consider $\lambda > 0$ as a measure of apparent repulsion between the spin pair.

I summarize some noteworthy features of the wavefunction as follow:

- The wavefunction is a SU(2) spin singlet and an eigenstate of the lattice translation operator with the wavenumber $Q = 2\pi(M - l)/N_a$. Hence, $l = 0$ ($l = M$) corresponds to $Q = \pi$ ($Q = 0$).

- When $\lambda = M - 1$ and $l = 0$ for odd $M$ ($\lambda = M - 2$ and $l = M$ for even $M$) the wavefunction exactly reduces to the following fully Gutzwiller-projected free-fermion wavefunction

$$\phi(z, \sigma) = \prod_{i<j} (z_{n_i} - z_{n_j}) \prod_{i<j} (z_{m_i} - z_{m_j}), \quad (4)$$

which is the exact ground-state of the isotropic SU(2) Haldane-Shastry spin chain. The HSM is known to belong to the same universality class as the Heisenberg spin chain with the nearest neighbor exchange.

- When $\lambda = 1$ it becomes the exact Majumdar-Ghosh wavefunction with definite crystal momentum $Q = \pi$ (for $l = 0$) or $Q = 0$ (for $l = M$),

$$|\Psi\rangle = |A\rangle \mp |B\rangle, \quad (5)$$

where $|A\rangle = (\uparrow \downarrow - \downarrow \uparrow) \cdots (\downarrow \downarrow - \uparrow \uparrow)$ and $|B\rangle = T|A\rangle$. ($T$ is the lattice translation operator.)

- The wavefunction is in the Dyson’s form of the BCS-wavefunction projected onto the Hilbert space of definite particle number. One major difference here is that the power $\lambda$ is positive, reflecting apparent repulsive interaction between the spin pair.

The wavefunction in Eq. (1) is by construction an exact eigenstate of the lattice translation operator with the wavenumber $Q = 2\pi(M - l)/N_a$. Hence, $l = 0$ ($l = M$) corresponds to $Q = \pi$ ($Q = 0$).

$$|\Psi\rangle + \sum_{j=1}^{N_a} \delta_{\sigma_{z,j},1} P_{\sigma_{z,j}j} |\Psi\rangle = 0,$$

where $\delta_{\sigma,1}$ is the Heaviside step function.
where $P^\sigma$ is the spin exchange operator. Using the antisymmetric property and minor expansion of the determinant it is straightforward to show that the singlet requirement reduces to the following condition for some fixed location $z_i^\uparrow$,

$$
\phi(z, \sigma) = \sum_{j=1}^{M} (-1)^{i+j} f(z_j^\uparrow, z_i^\uparrow) M_j \sum_{j \neq \mu, \nu \neq i}^{M} (-1)^{i+j+\mu+\nu} \times \text{sgn}(j-\mu)\text{sgn}(\nu-i) f(z_j^\uparrow, z_\mu^\uparrow) f(z_\nu^\uparrow, z_i^\uparrow) M_j M_\mu M_\nu,
$$

where $M_{ij12...jp}$ is a $(M-p) \times (M-p)$ matrix obtained from the original $M \times M$ matrix by eliminating the columns $t_1, t_2, \ldots, t_p$ and the rows $j_1, j_2, \ldots, j_p$. This condition holds true for any even function $f$ since the second term in Eq. (7) vanishes identically when summed over the dummy indices $j$ and $\mu$ and the first term becomes just a simple minor expansion of the original determinant. Thus, the wavefunction in Eq. (8) with $f$ given by Eq. (3) is a particular case of $SU(2)$ singlet. It is interesting to note that the singlet constraint is naturally resolved with the BCS-like form of wavefunction in the $S_z$ basis, an alternative to the resonating-valence-bond basis.

The pair function $f$ with $\lambda > 0$ in the wavefunction suggests that the interaction between up- and down-spins is of repulsive nature. But, it is somewhat misleading since for the lattice system there could be an arbitrary constant factor $\prod_{l<j}(z_i - z_j)^m$ up to a correction to the phase factor. Thus, even for the apparently repulsive case of $\lambda = M - 1$ (or $\lambda = M - 2$), the wavefunction can be divided by the constant factor with $m = 1$ and be rewritten as

$$
\phi(z, \sigma) \propto \prod_{ij} \text{sgn}(n_i - m_i) \frac{1}{z_{n_i} - z_{m_i}^\uparrow},
$$

where the effective attraction between up- and down-spins (i.e. the short-range antiferromagnetic correlation) is made explicit. It is remarkable that for the case of $\lambda = 1$ there also exists an equivalent alternative form given by

$$
\Psi^l_1 \propto \mathcal{N} \lim_{\kappa \to -\infty} \Psi^l_\kappa,
$$

where $\mathcal{N}$ denotes proper normalization. In this representation the attraction for a spin pair appears to be infinite. While the first state corresponds to the ground-state of the gapless spin liquid where the spinons, the elementary excitations, are unbound and can have arbitrarily low energy (i.e. the effective attraction in this case is not enough to subdue the pair-breaking quantum fluctuation and to induce a gap), the second corresponds to the fully paired or dimerized state with gap in the energy spectrum. I can, thus, infer from the two known cases that as $\lambda$ decreases the effective attraction increases and that the Majumdar-Ghosh limit ($\lambda = 1$) can be viewed as the strongest-possible-pair condensation. In fact the first case can be viewed as the critical point of the frustrated Heisenberg antiferromagnet given in Eq. (10) and any smaller $\lambda$ corresponds to the massive dimerized phase. This transition can be thought of as due to the singlet pair condensation and that the size of the singlet pair fluctuation becomes smaller and smaller as the frustration is increased towards the Majumdar-Ghosh limit.

In order to show more clearly the nature of pairing in the frustrated Heisenberg antiferromagnet I start with the following spin Hamiltonian

$$
H = \sum_{n=1}^{N_a} \bar{S}_n \cdot \bar{S}_{n+1} + \gamma \bar{S}_n \cdot \bar{S}_{n+2},
$$

where $S = 1/2$ and $\gamma > 0$ is the frustration parameter. The Hamiltonian with $\gamma = 0$ corresponds to the Bethe-ansatz solvable model [6]. At $\gamma = 1/2$ the exact doubly degenerate ground-states are the Majumdar-Ghosh wavefunction [7]. When $\gamma$ is greater than a critical value ($\approx 0.241$) the otherwise marginally irrelevant umklapp processes become relevant perturbation to the gapless spin-liquid state and the spin-chain spontaneously dimerizes; and, the critical point is identified with the $\beta^2 \to 8\pi$ limit of the sine-Gordon model [9]. Employing the standard method one can reduce the Hamiltonian to the exactly solvable Luttinger model plus the following umklapp terms expressed with the Jordan-Wigner lattice fermions,

$$
H_u = \sum_{n, \delta = 1, 2} a_{\delta} \psi_{1R}^\dagger(n) \psi_{1L}^\dagger(n + \delta) \psi_{1R}^\dagger(n + \delta) \psi_{1L}^\dagger(n + 2\delta) + \text{Hermitian conjugate},
$$

where $a_1 = 1$ and $a_2 = -\gamma$. The rapidly oscillating modes at the Fermi points have already been factored out from the fermion operators. When the $z$-axis anisotropy is allowed this umklapp term is also responsible for the Néel ordered state [12].

Recently, Wilczek and Nayak interpreted the umklapp term in the two-dimensional Mott-system as pairing interaction of particle and hole and when the order parameter $\langle \psi_{L}^\dagger \psi_{R}^\dagger \rangle$ is a pure imaginary number a BCS-like state rather than the charge-density-wave state is realized [13]. In the spin language their BCS-like state corresponds to the spontaneously dimerised state [7], the charge-density-wave state to the Néel ordered state [12], and their particle-hole pairing to the spin singlet pairing. Furthermore, their BCS-like state through repulsive channel seems consistent with our proposed wavefunction with $\lambda > 0$ which exhibits the apparent repulsive interaction.
The original estimate of the critical frustration $\gamma_c = 1/6$ which can be obtained from Eq. (1) by Taylor expansion of the operators like $\psi(x + \delta)$ is modified to $\gamma_c = 0.277$ if the full quantum operator-product expansion is used. (Numerical estimate of $\gamma_c$ is approximately 0.241.) For estimating $\gamma_c$ it is more convenient to change the dynamical variables to the following canonically conjugate phase fields

$$
\theta(x) = 2\pi \int^x dx' (\rho_R(x') + \rho_L(x')) ,
$$

$$
\phi(x) = \pi \int^x dx' (\rho_R(x') - \rho_L(x')) ,
$$

where $\rho_{R,L}$ are right- and left-density operators and $[\phi(x), \theta(x')] = i\pi \text{sgn}(x - x')$. The original spin SU(2) operators are represented in these fields as $S^\pm(x) \propto \exp(\pm i\phi(x))$ and $S_z(x) \propto \exp(\pm i\theta(x))$. Furthermore, the lattice Jordan-Wigner fermions are decomposed into the right- and left-moving Mandelstam fermions represented in terms of the phase fields as follow

$$
\psi_R(x) = \frac{1}{\sqrt{L}} : e^{i\alpha \phi(x)} : e^{i\beta \theta(x)} : ,
$$

$$
\psi_L(x) = \frac{1}{\sqrt{L}} : e^{i\alpha \phi(x)} : e^{-i\beta \theta(x)} : ,
$$

where $\vdash$ means normal ordering and $\alpha \beta = 1/2$ for the fermionic statistics. In order to obtain the correct anticommutation relations between the right- and left-moving operators the zero-modes of the phase fields are separated as $\theta(x) = \theta_0(x) + \tilde{\theta}(x)$ and $\phi(x) = \phi_0(x) + \tilde{\phi}(x)$ where $\theta_0(x) = \theta_0 + 2\pi N/L$, $\phi_0(x) = \phi_0 + 2\pi J/L$ and $[N, \theta_0] = [J, \theta_0] = i \frac{\pi}{L}$. The operators $\theta_0$, $\phi_0$, $N$, and $J$ are associated with the bulk modes of the 1D fluid and commute with the $q \neq 0$ bosonic modes. ($N$ here is not the number of particles but rather the fluctuations from the mean value $N_0$.) Some care in ordering the operators is needed when contracting the right- and left-moving operators and they are given as follow

$$
\lim_{(x - y) \to m a_0} \psi_R^\dagger(x) \psi_L (y) = \frac{i}{L} \text{sgn}(x - y) \left( m^2 + \lambda^2 \right)^{\tau/2} \times \left( \frac{2\pi a_0}{L} \right)^\tau : e^{-i2\beta \theta(x)} : ,
$$

where $\tau = 2\tilde{\beta}^2 - \tilde{\alpha}^2/2$, $\tilde{\beta} = \beta \exp(\phi)$, $\tilde{\alpha} = \alpha \exp(-\phi)$ and $\phi_0$ is the lattice constant. A similar form appears in Ref. [10] but is missing the important factor $\text{sgn}(x - y)$ and the corrections due to the short-distance cut-off. The dimensionless parameter $\lambda$ is introduced to control the short-distance behavior for normal ordering two exponential operators and, in this linear approximation, is fixed by the filling fraction and is given as $\lambda = 2/(e^C \pi) \approx 0.357$ ($C$ = the Euler’s constant). If $|m| \gg \lambda$ then the control parameter can be dropped from Eq. (14), but if the difference is of the order of the lattice constant it cannot be ignored.

In order to reproduce the correct anticommutation relations at the non-interacting value of the renormalization constant $\exp(-2\varphi) = 1$, I have to set $\beta = 1/2$, $\alpha = 1$ and, thus, $\tau = 0$. More generally, I obtain the following anticommutation relations for the left and right Mandelstam modes

$$
\{\psi_R(x), \psi_L^\dagger(y)\} = \{\psi_L(x), \psi_R^\dagger(y)\} = Z \delta(x - y),
$$

where $Z = (\Gamma(\nu - 1/2)/\sqrt{\pi}(\nu))\lambda^{2-2\nu}$ with $\nu = (\tilde{\alpha}^2 + \tilde{\beta}^2)$. Thus, for the free fermions (i.e. $\exp(\pm \varphi) = 1$) $Z = 1$ or $\nu = 1$. And, this requirement along with the fermion constraint $\alpha \beta = 1/2$ fix the values of $\alpha$ and $\beta$. In the gapless phase of the spin chain, however, $\exp(-2\varphi) = 2^{1/4}$. Thus, $\tilde{\beta}^2 = 1/8$, $\tilde{\alpha}^2 = 2$ and $\tau = -3/4$. The overlap terms $H_u$ given in Eq. (11) can now be contracted to the following form [17]

$$
\left[ 1 - \left( \sqrt{\frac{1 + \lambda^2}{4 + \lambda^2}} + 2 \sqrt{\frac{4 + \lambda^2}{4 + \lambda^2}} \right) \gamma \right] : \cos(2\theta(x)) : ,
$$

where some overall constants have been dropped. The coefficient vanishes when $\gamma \approx 0.277$ and changes sign if $\gamma$ further increases. The difference between this value and the numerical estimate is presumably due to the high energy modes with non-linear dispersion relation near the Brillouin zone boundary.

For half-odd integer spin chains the Lieb-Schultz-Mattis (LSM) theorem dictates that the gap open for both of the two low-energy sectors at the crystal momentum 0 and $\pi$ [18]. And, if the ground-state is doubly degenerate one can construct two linear combinations that are not eigenstates of the lattice translation operator. Therefore, the dimer gap induced by the singlet spin-pairing should also accompany the spontaneously broken translational symmetry. In the presence of holes or in two-dimensional systems, however, the spin paired-state could exist without the broken lattice translational symmetry.

I now numerically demonstrate that the proposed wavefunction given in Eq. (4) is a good trial wavefunction. I do this by taking the overlap of the wavefunction with the exact numerically found ground-state of $N_a = 16$ spin chain given in Eq. (11) with the frustration $\gamma$ ranging from 0 to 1/2 as shown in Table I. Listed in the table are the maximum overlap squared for the sector $Q = 0$ and $Q = \pi$ for four different values of $\lambda$ and the corresponding optimum values of $\gamma$. (For $M$ even (odd) and $\gamma < \gamma_c$ the lowest-energy state in the sector $Q = \pi$ ($Q = 0$) is a $S = 1$ state and the $S = 0$ state is the next lowest for any finite-size system. In all other cases of interest the ground-states for both sectors are spin singlets.) As shown in Table I the overlap squared is very close to one although it somewhat deteriorates in the region $\gamma \approx 0.4$.

In conclusion, I propose a new paired-wavefunction for the frustrated Heisenberg antiferromagnetic spin chain.
The wavefunction continuously interpolates from the gapless spin liquid phase to the fully dimerized phase of Majumdar-Ghosh. From the bosonization method I estimate the critical value of the frustration and further argue that the gap is induced by the singlet pairing in accord with the proposed paired-wavefunction. I also give numerical evidences that show the validity of the paired-wavefunction as ground states of the frustrated spin chain. Details will be published elsewhere [17].

I further speculate that an analog of the trial wavefunction given in Eq. (1) adopted to the 2D lattice (i.e. take $z_j$’s as general complex numbers and use elliptic functions) is a possible ground-state for the 2D frustrated spin system. This $S = 0$ construction in $S_z$ basis is to be contrasted/compared with the RVB states used, for example, by Liang et al [19]. It is also tempting to conjecture that the spin-spin singlet pairing correlation survives the doping of the spin system with small density of holes and that the “built-in” superconductivity naturally arises in some reasonable parameter space. Numerical works are in progress.

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| $Q$ | $\lambda$ | $\gamma$ | $(\text{Overlap})^2$ |
|-----|----------|----------|---------------------|
| 0   | 1        | 1/2      | 1                   |
| 3.0 | 0.44     | 0.9795   |
| 5.0 | 0.29     | 0.9894   |
| 6.0 | 0.15     | 0.9997   |
| $\pi$ | 1        | 1/2      | 1                   |
| 3.0 | 0.41     | 0.9947   |
| 5.0 | 0.29     | 0.9957   |
| 7.0 | 0.18     | 0.9994   |

TABLE I. Square of the overlap of the trial wavefunctions given in the text with the exact $S = 0$ ground-states of the spin-chain with $N_a = 16$ sites at the wave-number $Q = 0$ (or $l = M$) and $Q = \pi$ (or $l = 0$). The frustration $\gamma = 1/2$ corresponds to the Majumdar-Ghosh point and $\gamma = 0$ to the Bethe-ansatz solvable Heisenberg spin chain. The overlaps for $Q = \pi$ are slightly better than those for $Q = 0$ in the intermediate region $0.25 < \gamma < 0.5$.