

Gutzwiller-Hund wave function for an $S = 1$ linear chain

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We introduce a wave function for a spin-1 Heisenberg linear chain using the strategy of Gutzwiller to project out a spin-1 system out of two copies of the half-filled noninteracting Fermi gas. The projection further involves Hund symmetrization of the spin- $\frac{1}{2}$ particles to produce a spin-1 at each site. The correlation functions in the wave function seem to have the same power-law decay as those of a Bethe-ansatz soluble spin-1 chain. Some exact results for finite length systems are presented.

In this paper, we introduce a generalization of the Gutzwiller idea of projection in the study of an $S = 1$ Heisenberg linear chain. Our motivation is the remarkable efficacy of the idea for $S = \frac{1}{2}$, where the Gutzwiller projection of the free-Fermi gas at half-filling produces a spin wave function that does exceedingly well as a variational wave function¹ for the $S = \frac{1}{2}$ nearest-neighbor Bethe model. It has been shown to have asymptotic power-law correlations with the same character, and exponents² as those of the Bethe chain. Moreover, the wave function is the exact ground state of a long-ranged spin Hamiltonian.^{3,4}

The generalization introduced here uses the notion of symmetric projection, or Hund projection, as a means of coupling two copies of $S = \frac{1}{2}$ systems to produce a spin-1 system. This is a familiar idea in spin systems, and can be used to generate interesting and nontrivial spin-1 wave functions starting from spin- $\frac{1}{2}$ functions. One interesting application of this idea is the construction⁵ of the valence bond states for spin-1 starting from dimerized spin- $\frac{1}{2}$ states.⁶ The question we pose, and partially answer in this paper is, what is the nature of spin correlations in an $S = 1$ system obtained by Hund projecting a pair of $S = \frac{1}{2}$ Gutzwiller spin chains? This question certainly has more tractability than the corresponding question with a pair of Bethe spin- $\frac{1}{2}$ chains, and it may be reasonable to assume that the results have similar characteristics. Of particular interest is the question of power-law falloff of the correlations, as opposed to an exponential decay, which is intimately related to that of a gap in the spectrum of an appropriate Hamiltonian.⁷

We introduce in this work the Gutzwiller-Hund wave functions for spin 1 and carry out the projections explicitly for the case of half-filling. The correlations have been computed numerically by exact enumeration of states for chains up to $L = 18$. A study of the finite-sized effects strongly suggests power-law decay with an exponent which is similar to that of the gapless bilinear-biquadratic spin-1 chain.⁸ Partial analytical results are presented concerning the possibility of finding a Hamiltonian for which our wave function is the exact ground state.

We consider two closely related fermionic tight-binding models in one-dimension (1D) on a chain of

length L , with an orbital degeneracy. There are two kinds of fermions at each site described by destruction operators $c_{n\sigma}$ and $d_{n\sigma}$, where $1 \leq n \leq L$ and $\sigma = \pm 1$, and these hop with kinetic energies

$$\begin{aligned} T_c &= -t \sum_n (c_{n+1\sigma}^\dagger c_{n\sigma} + \text{H.c.}), \\ T_d &= -t \sum_n (d_{n+1\sigma}^\dagger d_{n\sigma} + \text{H.c.}). \end{aligned} \quad (1)$$

The two models considered couple these chains through a Hund's rule coupling in the form

$$H_1 = T_c + T_d - J_{\text{Hu}} \sum_n \mathbf{S}_n(c) \cdot \mathbf{S}_n(d) \quad (2)$$

or a slightly modified coupling

$$H'_1 = T_c + T_d - J'_{\text{Hu}} \sum_n [\mathbf{S}_n(c) + \mathbf{S}_n(d)]^2, \quad (3)$$

where the local spin operators are defined as usual $S_n^\alpha(c) = \frac{1}{2} c_{n\sigma_1}^\dagger \tau_{\sigma_1\sigma_2}^\alpha c_{n\sigma_2}$ and $S_n^\alpha(d) = \frac{1}{2} d_{n\sigma_1}^\dagger \tau_{\sigma_1\sigma_2}^\alpha d_{n\sigma_2}$, with τ 's as the usual Pauli matrices.

The model H'_1 can be considered as a pair of coupled Hubbard models. We will confine ourselves to the cases $J_{\text{Hu}} \geq 0$ and $J'_{\text{Hu}} \geq 0$, which correspond to a tendency to form local spin moments. The model possesses an "orbital reflection positivity" for this sign of the exchange, which causes the suppression of the orbital "triplet" state. It is possible to adapt the ideas of Ref. 9 to this problem and rigorously show that the ground state is an orbital singlet using this positivity. Also, we will confine attention to the "half-filled" case, where the number of "c" and "d" electrons $N_e = N_d = L$. It is clear that, in the limit of large J_{Hu} (or J'_{Hu}), we may ignore the kinetic energy, and we get a "local" energy level scheme where the triplet is at lowest energy ($-J_{\text{Hu}}/4$ and $-2J'_{\text{Hu}}$, respectively) and with a degenerate doublet excited state (0 and $-\frac{3}{4}J'_{\text{Hu}}$, respectively). The kinetic energy mixes up this highly degenerate "ground"-state manifold by exciting virtually into the doublet manifold and results in the usual Heisenberg spin-1 exchange antiferromagnet

$$H_{\text{ex}} = J_{\text{ex}} \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \quad |\mathbf{S}_n| = 1, \quad (4)$$

where $J_{\text{ex}} = 4t^2/J_{\text{Hu}}$ and $J'_{\text{ex}} = 4t^2/(5J'_{\text{Hu}})$. Naive perturbation theory in J_{Hu} of H_1 is, of course, full of low-frequency divergences, but for large J_{Hu} , we should expect an insulator with a charge gap of $O(J_{\text{Hu}})$, described by the spin-1 Heisenberg antiferromagnet, presumably with a gap in the spin sector of $O(J_{\text{ex}})$.⁷

In keeping with the spirit of this work, we study the generalized Gutzwiller-Hund wave function for H_1 or H'_1 in the limit of large J_{Hu} . As discussed earlier, a natural generalization of Gutzwiller's idea is to study the wave function

$$|\Psi_0\rangle = \lim_{\alpha \rightarrow \infty} e^{\alpha \sum_n (c \cdot S_n(d))} |\phi_0\rangle, \quad (5)$$

where $|\phi_0\rangle$ is the composite Fermi-gas wave function

$$\begin{aligned} |\phi_0\rangle &= |\phi_c\rangle \otimes |\phi_d\rangle, \\ |\phi_c\rangle &= \prod_{|k| < k_F} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |\text{vac}\rangle. \end{aligned} \quad (6)$$

The operator in Eq. (5) has the twofold effect of removing double occupation in each of the Fermi gases, followed by a symmetrization. We write the operator as a product of two kinds of projection operators:

$$\lim_{\alpha \rightarrow \infty} e^{\alpha \sum_n (c \cdot S_n(d))} \propto P_H P_G(c) P_G(d), \quad (7)$$

where the Gutzwiller projection operator

$$P_G(c) = \prod_m [1 - n_{m\uparrow}(c) n_{m\downarrow}(c)]$$

and a similar definition for $P_G(d)$, and the Hund projection operator $P_H = \prod_m [\frac{3}{4} + \mathbf{S}_m(c) \cdot \mathbf{S}_m(d)]$. As a prelude let us write $P_G(c)|\phi_c\rangle$ in the form⁴

$$\begin{aligned} P_G(c)|\phi_c\rangle &= \sum_{1 \leq x_1 \leq \dots \leq x_{L/2}} \chi(x_1, x_2, \dots, x_{L/2}) \\ &\quad \times [S_{x_1}^-(c) \cdots S_{x_{L/2}}^-(c)] |F_c\rangle, \end{aligned} \quad (8)$$

where the squared Vandermonde determinant

$$\chi(x_1, \dots, x_{L/2}) = \exp(i\pi \sum x_j) \prod_{i < j} [(i - j)]^2 \quad (9)$$

and the metric function $[[r]] \equiv \sin r\pi/L$, and $|F_c\rangle$ is the fully saturated ferromagnetic reference state $\pi c_{n\uparrow}^\dagger |\text{vac}\rangle$. A similar expression for $P_G(d)|\phi_d\rangle$ holds. In order to carry out the Hund projection, we note the following simple local rules with

$$\begin{aligned} |F\rangle &= |F_c\rangle \otimes |F_d\rangle, \quad P_H|F\rangle = |F\rangle, \\ P_H S_x^-(c)|F\rangle &= \frac{1}{2}[S_x^-(c) + S_x^-(d)]|F\rangle, \end{aligned}$$

and

$$P_H[S_x^-(c)S_x^-(d)]|F\rangle = [S_x^-(c)S_x^-(d)]|F\rangle.$$

Since the resulting state is purely symmetric in the exchange of "c" and "d," we introduce spin-1 operators S_n^α , with $|\mathbf{S}_n \cdot \mathbf{S}_n| = 2$ and $S_n^\pm = (S_n^x \pm iS_n^y)$, identify $|F\rangle$ with the up projection state, thus the rules become $P_H S_x^-(c) \rightarrow (1/\sqrt{2})S_x^-$, $P_H S_x^-(d) \rightarrow (1/\sqrt{2})S_x^-$, $P_H S_x^-(c)S_x^-(d) \rightarrow (S_x^-)^2$. The Hund projection is now easy to perform. We write down the configurations of spin states as a string of S^- 's and S^{-2} 's acting upon the reference $|F\rangle$ state, and sum over all the contributing amplitudes. The Gutzwiller-Hund wave function is written in the form

$$\begin{aligned} |\Psi\rangle_{\text{GH}} &= \sum_{\nu=0}^{L/2} \Psi_\nu(r_1, r_2, \dots, r_{L-2\nu} | t_1 \cdots t_\nu) S_{r_1}^- \cdots S_{r_{L-2\nu}}^- \\ &\quad \times \{S_{t_1}^- S_{t_2}^- \cdots S_{t_\nu}^-\}^2 |F\rangle, \\ 1 \leq r_1 < r_2 < \dots < r_{L-2\nu} \leq L, \\ 1 \leq t_1 < t_2 < \dots < t_\nu \leq L, \end{aligned} \quad (10)$$

with

$$\Psi_\nu(r_1, r_2, \dots, r_{L-2\nu} | t_1 \cdots t_\nu) = (\exp i\pi \sum r_j) 2^\nu (2 - \delta_{\nu, L/2}) \theta^4(t_1 \cdots t_\nu) \left\{ \prod_{i=1}^{\nu} \prod_{j=1}^{L-2\nu} [[t_i - r_j]]^2 \right\} \chi_\nu(r_1 \cdots r_{L-2\nu}), \quad (11)$$

where

$$\theta(\alpha_1, \alpha_2, \dots, \alpha_m) \equiv \prod_{\nu=1}^{\mu} \prod_{\nu'=1}^{\nu} [[\alpha_\nu - \alpha_{\nu'}]], \quad (12)$$

$$\begin{aligned} \chi_\nu(r_1 \cdots r_{L-2\nu}) &= \sum_P \theta^2(r_1, r_{P_2}, \dots, r_{P_{L/2-\nu}}) \\ &\quad \times \theta^2(r_{P_{L/2-\nu+1}} \cdots r_{P_{L-2\nu}}), \end{aligned} \quad (13)$$

where P is a sum over the

$$\begin{bmatrix} L - 2\nu - 1 \\ L/2 - \nu - 1 \end{bmatrix}$$

distinct combinations for writing the arguments in Eq. (13).

A few remarks are appropriate at this state. The phase factor in Eq. (11) is the familiar "Marshall" sign factor, the exact ground state of the nearest-neighbor spin-1 Hamiltonian Eq. (4) has the same phase structure. The wave function Ψ_{GH} is a many-body singlet; we know this from our construction, since we took a singlet, the Fermi wave function, and carried out rotationally invariant projections. A direct verification of the singlet sum rule $S_{\text{tot}}^+ |\Psi_{\text{GH}}\rangle = 0$ is, in fact, possible for $L = 4, 6$, and 8 , but the combinatorial tricks that go into this annihilation become extremely complex. A direct proof can be easily

given using the Weyl representation (see later). The wave function has many features that distinguish it from the considerably simpler wave function of the $S=\frac{1}{2}$ Gutzwiller problem. First, we have the sum over ν in Eq. (10), therefore the number of $(S^-)^2$ is not conserved. Second, the sum involved in Eq. (13) eliminates any possibility of interpreting the modulus squared of the wave function as a classical partition function of a Coulomb gas. Such an analogy, if it exists, simplifies the correlation function calculation enormously. (A configuration receives its contribution in the wave function from several underlying spin- $\frac{1}{2}$ configurations, and we must sum and *then* square.)

We next present the results of a numerical evaluation of the spin-correlation functions in the wave function Eq. (13). These were carried out by exact enumeration of all the states up to $L=18$, and by using the singlet nature of the wave function to write $c(r) \equiv \langle S_0^z S_r^z \rangle = \frac{1}{3} \langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$. For chain length L , the number of distinct correlations that can be measured are $L/2$ in number. In Table I, we present all the distinct correlations for all even chain lengths up to $L=18$. Exact enumeration becomes prohibitively time consuming for $L > 18$ (even on a CRAY), and Monte Carlo methods need to be employed for these. We would need data with L up to 50 or so in order to reach really firm answers and so the conclusions drawn here are tentative. On the basis of the data at hand, we cannot strictly rule out an (infinite volume) correlation length larger than, say, nine lattice constants. The data does, however, strongly suggest power-law decay for the range available.

We have analyzed the data by attempting a fit of the correlations at a given fixed distance, to a power law in the inverse square of the system size. Owing to periodic bc 's, we expect no correction of $O(1/L)$, and a gap in the spectrum would lead to more rapid, in fact, exponential, convergence. We find reasonable convergence, particularly if the shortest chain length is discarded (e.g., $r=3$, we fit $L=8, \dots, 18$). The fits are displayed in Fig. 1. The infinite-size extrapolation of correlations can be attempted for distances up to 7 with these fits, and are presented in the last row of the Table I. The estimates are quoted to the third decimal place but should be regarded as progressively uncertain for larger distances. A

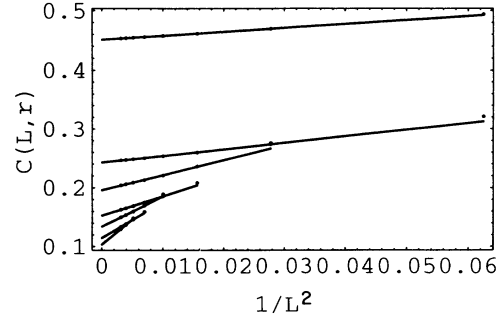


FIG. 1. The correlation function at different separations as a function of $1/L^2$ and a linear fit to $1/L^2$. The fits were obtained by discarding the shortest spin chain at a fixed separation.

simple log-log fit of these extrapolated correlations gives $c(r) = (-1)^r a / r^\eta$, with $a = 0.435$, $\eta = 0.744$, and this fit (on a linear scale) as well as the data are shown in Fig. 2. The fit seems to be very good. We tentatively conclude $\eta = 0.74 \pm 0.04$.

The extrapolated $L \rightarrow \infty$ limit value of the nearest-neighbor correlation for $C(1) = -0.451 \pm 0.002$. It is interesting to note that the exact ground-state energy of the $S=1$ chain gives¹⁰ $C_{\text{HAFM}}(1) = -0.467$. Thus, the wave function, Eq. (10), viewed as a variational wave function for Eq. (4) gives an energy that is $\sim 4\%$ of the exact value. The bilinear-biquadratic Hamiltonian

$$H = \sum_n [\mathbf{S}_n \cdot \mathbf{S}_{n+1} + \alpha (\mathbf{S}_n \cdot \mathbf{S}_{n+2})^2] \quad (14)$$

has been studied extensively,^{11,8,5,12} for various values of α , and it is instructive to compare the nearest-neighbor correlation for a few values of α available $C_{\{\alpha=-1\}}(1) = -0.425$, $C_{\{\alpha=+1/3\}}(1) = -0.444$. The two cases $\alpha = -1$ and $\frac{1}{3}$ correspond to a "gapless" and a "gapped" system.^{8,5,13} The estimate from our wave function thus appears to have the closest variational energy to the exact and yet the long-distance nature of the correlations seems quite different.

We will use a different representation to study the wave function, Eq. (10), that is very elegant and useful for understanding the structure in the wave function. We re-

TABLE I. $(-1)^r \langle S_0^z S_r^z \rangle$ as a function of r for different chain lengths studied by us. The last row is an estimate based on an extrapolation to infinite L .

	$C(r)(-1)^r$								
	1	2	3	4	5	6	7	8	9
4	0.4938	0.3209							
6	0.4694	0.2739	0.2757						
8	0.4613	0.2598	0.2360	0.2083					
10	0.4576	0.2536	0.2208	0.1860	0.1893				
12	0.4556	0.2504	0.2132	0.1755	0.1702	0.1595			
14	0.4544	0.2485	0.2088	0.1696	0.1602	0.1464	0.1487		
16	0.4536	0.2472	0.2060	0.1659	0.1542	0.1388	0.1371	0.1316	
18	0.4531	0.2463	0.2042	0.1634	0.1503	0.1339	0.1300	0.1228	0.1244
∞	0.451	0.243	0.196	0.153	0.134	0.115	0.103		

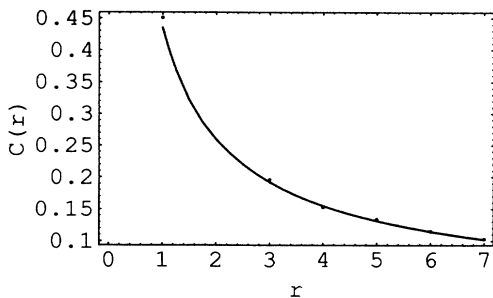


FIG. 2. The extrapolated infinite L correlations plotted against $0.435/r^{0.744}$. The curve was obtained by a log-log fit.

mind the reader of the Weyl representation of angular momentum. Consider a spin- S Hilbert space: we can represent¹⁴ the manifold of $2S + 1$ states as polynomials in z of degree $\leq (2S)$, and write the three spin operators as

$$S^- = \partial/\partial z, \quad S^z = S - z \frac{\partial}{\partial z}, \quad S^+ = 2Sz - z^2 \frac{\partial}{\partial z}. \quad (15)$$

The “wave functions” are thus proportional to $1, z, z^2, \dots, z^{2S}$, with 1 representing the states $|S, S\rangle$ and $z^{2S} \sim |S, -S\rangle$. In detail 1, x_n are $|\frac{1}{2} + \frac{1}{2}\rangle$, $|\frac{1}{2} - \frac{1}{2}\rangle$, and 1,

$$\Psi_c = \sum_{1 \leq r_1 < r_2 < \dots < r_{L/2} \leq L} e^{i\pi \sum_j r_j} \prod_{i < j} [[r_i - r_j]]^2 x_{r_1} x_{r_2} \dots x_{r_{L/2}}.$$

The effect of the Hund operator can be trivially written down in view (16) as

$$\Psi_{GH} = \left\{ \sum_{1 \leq r_1 < \dots < r_{L/2} \leq L} \exp \left[i\pi \sum_j r_j \right] \prod_{i < j} [[r_i - r_j]]^2 t_{r_1} \dots t_{r_{L/2}} \right\}^2. \quad (17)$$

The above form of the wave function is very compact and useful. It is also worth noting that the case of more than two copies of the Fermi gas with a similar projection onto the maximum local spin sector can be readily worked out in the Weyl basis: the conclusion is that the general spin- S wave function in this class is obtained by raising Eq. (17) to a power $2S$. In this basis, spin S enters as parameter and may be interpreted as the inverse temperature variable in an effective one-dimensional classical spin system. Let us note^{3,4} that Eq. (8) is known to be the exact ground state of the long-ranged Heisenberg model

$$H = \sum J_r \mathbf{S}_i \cdot \mathbf{S}_{i+r}, \quad (18)$$

where $J_r = J_0/\sin^2(r\pi/L)$. The spin-exchange operator becomes a differential operator in the x 's under the above substitutions. We have considered the possibility of finding an operator for which Ψ_{GH} is the exact ground state. We confined attention to operators of the form

$$H = \sum J_r \mathbf{S}_i \cdot \mathbf{S}_{i+r} + \sum K_r (\mathbf{S}_i \cdot \mathbf{S}_{i+r})^2 \quad (19)$$

$\sqrt{2}t_n, t_n^2$ are $|1, 1\rangle, |1, 0\rangle, |1, -1\rangle$. We will denote by x_n^α and y_n^α the wave function for the “c-” and “d-” like spin- $\frac{1}{2}$ systems, and by t_n^α the states of the spin-1 system, i.e., $S_n^\dagger(c) \rightarrow \partial/\partial x_n, S_n^\dagger(d) \rightarrow \partial/\partial y_n, S_n^\dagger \rightarrow \partial/\partial t_n$. We first set out the effect of the Hund symmetrization operator on a system consisting of two copies of $S = \frac{1}{2}$. The projection operator maps states $x_n^\alpha y_n^\beta$ to states t_n^γ as follows: $P_H 1 \rightarrow 1, P_H x_n \rightarrow (1/\sqrt{2})\sqrt{2}t_n = t_n, P_H y_n \rightarrow (1/\sqrt{2})\sqrt{2}t_n, P_H x_n y_n \rightarrow t_n^2$. Thus, the two inconvenient factors of $\sqrt{2}$ cancel out and, under P_H , the role of symmetrization is remarkably simple. We can thus consider two arbitrary states of the two spin- $\frac{1}{2}$ chains and at once write down the Weyl wave function for the symmetrized spin-1 chain as follows:

$$P_H \{ G(x_1 \dots x_{L/2}) F(y_1, \dots, y_{L/2}) \} \rightarrow G(t_1, \dots, t_{L/2}) F(t_1, \dots, t_{L/2}). \quad (16)$$

Since G and F are at most of degree one in each variable, the rhs is at most of degree 2 in t_n , which is, of course, consistent with its being a spin-1 wave function.

Let us first write the wave function, Eq. (8), $P_G(c)|\Psi_c\rangle$ in the above notation:

with arbitrary J_r and K_r and asked if Ψ_{GH} is an eigenfunction. The form above is by no means the most general spin operator, but is inspired by the form of Eq. (18). There is always, of course, a trivial set of $\{J_r, K_r\}$, namely, $\forall K_r = 0, \forall J_r = J_0$, which becomes the total spin operator (apart from trivial constants). The method consisted of operating on Ψ_{GS} with Eq. (19) for a fixed L , and to require the orthogonal state vector to vanish. The orthogonality condition gives an overdetermined set of linear equations with $\{J_r\}$ and $\{K_r\}$ as L independent parameters. For $L = 4$ and 6, we have found, respectively, 2 and 1 sets of constants which are presented below, whereas for $L = 8$, there is no set of constants other than the trivial one, implying that no systematic Hamiltonian exists for this wave function in the class of Eq. (19). We give below the nonzero constants and the eigenvalue.

$L = 4$:

$$J_1 = 7, \quad K_1 = -2, \quad \lambda = -64,$$

$$J_1 = 1, \quad K_2 = -1, \quad \lambda = -8.$$

$L = 6$:

$$J_1 = 1989 ,$$

$$J_2 = -779 ,$$

$$K_1 = -360 ,$$

$$K_2 = -1688 ,$$

$$K_3 = 1071 ,$$

$$\lambda = -30924 .$$

For $L = 8$ no constants exist. We spare our readers the details of the messy algebraic proof of this result.

The Gutzwiller-Hund wave function for the $S=1$ linear chain introduced in this paper is tantalizing in several respects. We have seen that the correlation functions appear to decay algebraically. The rate of decay exponent estimated by us essentially coincides with the

value 0.75 known for the wave function of Refs. 8 and 13, namely, the gapless spin-1 chain with $\alpha = -1$. This exponent is the same as that of the $k=2$ Wess-Zumino theory, as noted in Ref. 15. The variational energy for the nearest-neighbor model is also fairly close, although the $s = \frac{1}{2}$ case has a much closer coincidence. On the analytical front, the absence of a Hamiltonian in the class of Eq. (19) is somewhat disappointing, but it seems to be worthwhile to continue the search for this elusive operator in a wider class of Hamiltonians. Further, it seems possible to us that the wave function introduced here stands in the same relation to the spin-1 chain of Ref. 8, as does the spin- $\frac{1}{2}$ Gutzwiller state to the Bethe wave function, in terms of the absence of logarithmic corrections in the correlation functions.

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