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Quantum belief propagation: An algorithm for thermal quantum systems

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We present an accurate numerical algorithm, called quantum belief propagation, for simulation of one-dimensional quantum systems at nonzero temperature. The algorithm exploits the fact that quantum effects are short-range in these systems at nonzero temperature, decaying on a length scale inversely proportional to the temperature. We compare to exact results on a spin-1/2 Heisenberg chain. Even a very modest calculation, requiring diagonalizing only ten-by-ten matrices, reproduces the peak susceptibility with a relative error of less than 10^{-5}, while more elaborate calculations further reduce the error.

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The fact that interactions are short-ranged in many physical systems is a major simplification in finding quantum ground states. The classic example of this is the density matrix renormalization group (DMRG),[1] which relies on the ability to approximate the ground state by a matrix product state. While it has long been believed that such an approximation is possible whenever there is a spectral gap, due to conformal field theory calculations[2] and decay of correlations,[3,4] only very recently has a general proof been given that such an approximation is possible whenever there is a local Hamiltonian and a gap.[5]

At nonzero temperature, the system is in a mixed state instead. Here, matrix product density operators[6] play the same role that matrix product states do in studying pure states, and a nonzero temperature plays a similar role when it comes to representing mixed states as matrix product density operators as does a gap for representing pure states as matrix product states. Indeed, it has been shown that good matrix product operator representations exist for quantum systems at any nonzero temperature.[7] In this paper we present quantum belief propagation (QBP), another method for finding matrix product density operators for thermal states, which avoids the problem of Trotter error in other methods.

Belief propagation[8] for classical systems (CBP) is essentially a Bethe-Peierls solution of a classical statistical mechanics model. CBP is exact on trees, and is often a very good approximation on lattices with few loops. At the end of this paper we will discuss application of the QBP equations to higher dimensional systems and trees, but for now we will focus discussion on belief propagation for one dimensional lattices. In this case, CBP become equivalent to a transfer matrix technique: one solves the problem on a chain of N sites to get a partition function that depends on the value of the spin on the Nth site. Then, one adds a coupling of the Nth spin to one additional spin, traces out the Nth spin, arriving at a partition function that depends on the value of the spin on the $N+1$st site. One proceeds in this way, iteratively solving longer and longer chains.

In a quantum system, we will proceed in a similar way. However, now the operator coupling the Nth spin to the $N+1$st spin need not commute with the rest of the Hamiltonian. This means that to study properties of the chain of $N+1$ spins, it is not sufficient simply to know the density matrix of the Nth spin in an N-site chain. However, our physical intuition tells us that at a nonzero temperature, quantum effects should be short range. Our main result in the next section realizes this intuition in the QBP equations, which involve two terms. One is a "classical" term that is local, coupling the Nth spin to the $N+1$st spin. The other is a "quantum" term, which is nonlocal, coupling the $N+1$st spin to several other spins; however, this quantum term is exponentially decaying on a length scale set by the inverse temperature. This will allow us to accurately describe statistical properties of the $N+1$st spin knowing only the reduced density matrix of spins $N, N-1, \ldots, N-l_0+1$, for some l_0, so that we keep track of a reduced density matrix for l_0 spins. We then iterate these equations by tracing out spin $N-l_0+1$ and then computing statistical properties of spin $N+2$, keeping always a reduced density matrix on the last l_0 spins on the chain.

Quantum belief propagation equations. The QBP equations describe how the partition function, $\exp(-\beta H)$, changes when H is changed by some perturbation A. We take A, H Hermitian throughout. We will apply this result to the following case: we have a nearest-neighbor Hamiltonian, with $h_{i,i+1}$ the term coupling spin i to spin $i+1$. We will take $H = h^{(N)} \equiv \Sigma_{i=1}^{N-1} h_{i,i+1}$, so that H is the Hamiltonian for the first N spins, and $A = h_{N,N+1}$. We define

$$H_s = H + sA. \tag{1}$$

Then, $H_1 = h^{(N)} + A = h^{(N+1)}$.

Although ultimately we want to compute $\exp(-\beta H_s)$ at $s=1$, we begin by computing the derivative $\partial_s \exp(-\beta H_s)$. Let $A_{ab}(s)$ denote matrix elements of A in a basis of eigenstates of H_s, with energies $E_a(s), E_b(s)$. Define the operator $A^{\omega,s}$ by its matrix elements: $(A^{\omega,s})_{ab} = A_{ab}(s)\delta(E_a(s) - E_b(s) - \omega)$. We will do most of the calculations in terms of $A^{\omega,s}$ rather than A for simplicity, although we will convert certain results back into results in terms of A itself using the integral

$$(\partial_s \exp(-\beta H_s)) = \int d\omega (\partial_\epsilon \exp[-\beta(H_s + \epsilon A^{\omega,s})]), \tag{2}$$

where all derivatives with respect to ϵ are taken at $\epsilon=0$ throughout.

One result for the derivative on the right-hand side of Eq. (2) (not the result we will use!) is $(\partial_\epsilon \exp[-\beta(H_s + \epsilon A^{\omega,s})]) = -\exp(-\beta H_s)\left(\frac{\exp(\beta\omega)-1}{\omega} A^{\omega,s}\right)$. One problem with this is that

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the operator norm $\|\frac{\exp(\beta\omega)-1}{\omega}A^{\omega,s}\|$ may be exponentially large. The QBP equations will improve on this, writing

$$\partial_s \exp(-\beta H_s) = \eta \exp(-\beta H_s) + \exp(-\beta H_s)\,\eta^{\dagger}.$$

where $\|\eta_s\| \leq (\beta/2)\|A\|$ Finally, η will be a local operator as discussed below.[11]

To find the QBP equations, we begin by studying a certain correlation function. Let B be an arbitrary operator. Then,

$$\begin{aligned}\partial_\epsilon \operatorname{tr}(\exp[-\beta(H_s+\epsilon A^{\omega,s})]B) &= -\int_0^\beta d\tau \operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}(-i\tau,H_s)B)\\ &= -\frac{\exp(\beta\omega)-1}{\omega}\operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B).\end{aligned} \tag{3}$$

Adding and subtracting $-(\beta/2)\operatorname{tr}(\{\exp(-\beta H_s),A^{\omega,s}\}B)$ to Eq. (3) gives

$$\begin{aligned}&\partial_\epsilon \operatorname{tr}(\exp[-\beta(H_s+\epsilon A^{\omega,s}))B\}\\ &\quad= -\frac{\beta}{2}\operatorname{tr}(\{\exp(-\beta H_s),A^{\omega,s}\}B) + \left(\frac{\beta}{2}(1+e^{\beta\omega}) - \frac{e^{\beta\omega}-1}{\omega}\right)\\ &\qquad\times \operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B),\end{aligned} \tag{4}$$

where we used

$$\operatorname{tr}(A^{\omega,s}\exp(-\beta H_s)B) = \exp(\beta\omega)\operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B).$$

We now focus on the correlation function $\operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B)$, following a procedure very similar to that in Ref. 9. In Ref. 9 the result was expressed in terms of anticommutators, as A,B were fermionic operators and hence anticommutated if they were separated in space, while here we will express the result in terms of commutators, since we intend to apply it to bosonic operators where the Lieb-Robinson bound is expressed as a bound on the commutator. Using $\operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B) = \frac{1}{1-\exp(\beta\omega)}\operatorname{tr}(\exp(-\beta H_s)[A^{\omega,s},B])$, we have

$$\begin{aligned}&\left(\frac{\beta}{2}(1+e^{\beta\omega}) - \frac{e^{\beta\omega}-1}{\omega}\right)\operatorname{tr}(\exp(-\beta H_s)A^{\omega,s}B)\\ &\quad= \beta F(\omega)\operatorname{tr}(\exp(-\beta H_s)[A^{\omega,s},B]),\end{aligned} \tag{5}$$

where

$$F(\omega) \equiv \frac{1}{2}\frac{1+e^{\beta\omega}}{1-e^{\beta\omega}} + \frac{1}{\beta\omega} = -\frac{\coth(\beta\omega/2)}{2} + \frac{1}{\beta\omega}. \tag{6}$$

Thus for any operator B, we have

$$\begin{aligned}\partial_\epsilon \operatorname{tr}(\exp[-\beta(H_s+\epsilon A^{\omega,s}))B\} = &-\tfrac{\beta}{2}\operatorname{tr}(\{\exp(-\beta H_s),A^{\omega,s}\}B)\\ &+\beta F(\omega)\operatorname{tr}(\exp(-\beta H_s)\\ &\times[A^{\omega,s},B]),\end{aligned}$$

and hence

$$\begin{aligned}\partial_\epsilon \exp[-\beta(H_s+\epsilon A^{\omega,s})] &= -\frac{\beta}{2}\{\exp(-\beta H_s),A^{\omega,s}\}\\ &\quad+F(\omega)[\exp(-\beta H_s),A^{\omega,s}]\\ &= \eta_s^{\omega}\exp(-\beta H_s) + \exp(-\beta H_s)(\eta_s^{\omega})^{\dagger},\end{aligned} \tag{7}$$

where

$$\eta_s^{\omega} = -\left(\frac{\beta}{2} + \beta F(\omega)\right)A^{\omega,s}. \tag{8}$$

We define

$$\eta_s = \int d\omega\,\eta_s^{\omega}. \tag{9}$$

Equations (2) and (7) are the QBP equations for $\partial_s \exp(-\beta H_s)$. The anticommutator in Eq. (7) is a "classical term." It is the only term present if $[A,H]=0$, in which case these equations reproduce the classical belief propagation equations. The commutator in Eq. (7) is a "quantum" term. It is odd in ω and vanishes at $\omega=0$. We now discuss locality properties of the quantum term, assuming that H is local in the sense of having a Lieb-Robinson bound.[10] We have[9]

$$\begin{aligned}\beta\int d\omega F(\omega)A^{\omega,s} &= \int d\omega\left(-\frac{\beta}{2}\coth(\beta\omega/2) + \frac{1}{\omega}\right)A^{\omega,s}\\ &= -\int d\omega \sum_{n\neq 0}(\omega - 2\pi n i/\beta)^{-1}A^{\omega,s}\\ &= i\sum_{n\geq 1}\int_{-\infty}^{\infty} dt\,\operatorname{sgn}(t)\exp(-2\pi nt/\beta)A(t,H_s),\end{aligned} \tag{10}$$

where the sum is over integer n and $A(t,H_s) = \exp(iH_s t)A\exp(-iH_s t)$. The integral over t is exponentially decaying for $t \gtrsim \beta$ and so, using a Lieb-Robinson bound, η is local.

Numerical implementation and results. In this section we discuss the numerical implementation of the QBP equations, and the results of their application to the antiferromagnetic spin-1/2 Heisenberg chain. The idea is to take the QBP equations, which depend on A and $H=h^{(N)}$, and instead set $H = \sum_{i=N-l_0+2}^{N-1} h_{i,i+1}$, for some constant $l_0 \geq 2$. Since η is local, this approximation is justified for small enough β; as β increases, l_0 must increase and the numerical effort is exponential in l_0, since one must diagonalize matrices of size 2^{l_0}.

Although translation invariance is *not* necessary, it is useful as we can then apply translations to $H = \sum_{i=N-l_0+2}^{N-1} H_{i,i+1}$ to make H equal to $h^{(l_0-1)}$, so for the Heisenberg chain with coupling constant $J=1$, $H = \sum_{i,1\leq i\leq l_0-2} \vec{S}_i \cdot \vec{S}_{i+1}$. We set $A = h_{l_0-1,l_0}$. We set T to be the operator which translates one site to the right. We define ρ to be a reduced density matrix for sites $1\cdots l_0$, so that ρ is a 2^{l_0} dimensional matrix. Define

$$O = \mathcal{S}' \exp\left(\int_0^1 \eta_{s'} ds' \right), \tag{11}$$

where the $\mathcal{S}'$ denotes that the integral is s' ordered.

The algorithm to compute the free energy per site of an infinite chain proceeds through the following four steps. (i) Initialize ρ to $\exp(-\beta H)$. (ii) Approximately compute the operator O as described below. (iii) Go through a series of n_{it} iterations of the following three steps: (a) Replace ρ with $O\rho O^{\dagger}$. (b) Trace out the first site, so that ρ is replaced with $\mathrm{tr}_1(\rho) \otimes \mathbb{1}_{l_0+1}$. Here, tr_1 denotes a partial trace over the first site, and $\mathbb{1}_{l_0+1}$ is the unit operator on the l_0+1th site. At this stage ρ is now a density operator on sites $2 \cdots l_0+1$. Translate by one site, so that ρ becomes a density operator on sites $1 \cdots l_0$ again. (c) Define $Z = \mathrm{tr}(\rho)$ and then replace ρ with $Z^{-1}\rho$.

After these iterations, we (iv) Output $\ln(Z)$ from the last step as the free energy. This procedure relies on a series of iterations of steps (a)–(c) to find the ρ which is the fixed point of the map,

$$\rho \to Z^{-1} T^{\dagger} (\mathrm{tr}_1(O\rho O^{\dagger}) \otimes \mathbb{1}_{l_0+1}) T. \tag{12}$$

The number of iterations required for convergence appears to increase roughly linearly with l_0 and β, but the computational effort grows only linearly in the number of iterations. The locality of the operators η, O justifies tracing out the first site in step (b). After n_{it} iterations, ρ is approximately proportional to the reduced density matrix $\mathrm{tr}_{1 \cdots n_{it}}(\exp(-\beta h^{(l_0-1+n_{it})}))$, where the partial trace is over sites $1 \cdots n_{it}$.

To compute correlation functions of operators such as $S_i^z S_{i+j}^z$ we follow the following procedure. We go through steps (i)–(iii) as above, with n_{it} iterations in step (iii). On the last of the n_{it} iterations, after step (a) we copy ρ to a new matrix ρ_{corr}. We then replace ρ_{corr} with $S_0^z \rho_{corr}$, thus inserting the first of the two operators. On steps (b) and (c) of the last iteration we replace of the map $\rho \to Z^{-1}\,\mathrm{tr}_1(\rho) \otimes \mathbb{1}$ and $\rho_{corr} \to Z^{-1}\,\mathrm{tr}_1(\rho_{corr}) \otimes \mathbb{1}$, where the same Z is used for both ρ and ρ_{corr}. When then proceed through j more iterations of steps (a)–(c), and on the last iteration after step (a) we replace $\rho_{corr}$with $S_0^z \rho_{corr}$, inserting the second of the two operators, before proceeding with steps (b) and (c). We then proceed through several more iterations in which at each step we map $\rho \to Z^{-1}\,\mathrm{tr}_1(O\rho O^{\dagger}) \otimes \mathbb{1}$, $\rho_{corr} \to Z^{-1}\,\mathrm{tr}_1(O\rho_{corr} O^{\dagger}) \otimes \mathbb{1}$ and finally output the ratio $\mathrm{tr}(\rho_{corr})/\mathrm{tr}(\rho)$.

To compute the matrix O, we approximate by dividing the integral over s' into n_{slice} different slices:

$$O \approx \exp\left(\frac{\eta_{s(n_{slice})}}{n_{slice}} \right) \cdots \exp\left(\frac{\eta_{s(2)}}{n_{slice}} \right) \exp\left(\frac{\eta_{s(1)}}{n_{slice}} \right), \tag{13}$$

where $s(m) = (m-1/2)/n_{slice}$. To compute the matrix exponential for each slice, $\exp(\eta_{s'})$ for $s' = (1/2)(1/n_{slice})$, $(3/2) \times (1/n_{slice})$, $(5/2)(1/n_{slice}), \cdots$ we used a Taylor series method, while to compute $\eta_{s'}$ itself we diagonalize $H_{s'}$ and transform A into a basis of eigenvector of $H_{s'}$. We use the fact that H and A conserve total S^z to speed up both this diagonalization and the multiplication $\rho \to O\rho O^{\dagger}$.

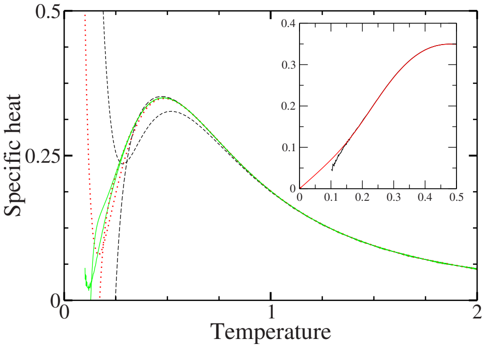

FIG. 1. (Color online) Specific heat against temperature for $l_0 = 3$ (dashed line), 5 (dotted line), 7 (solid line). Curves that go negative are from $-3\beta^2 \partial_\beta \langle S_i^z S_{i+1}^z \rangle$, while those that diverge positively are from $\beta^2 \partial_\beta^2 \ln(Z)$. Inset: $l_0 = 9$ and Bethe ansatz.

Since η_s is non-Hermitian, but $\|\eta_s\|$ is not too large, the Taylor series method is a good choice for computing the matrix exponential. Equation (13) approximates the s' dependence of $\eta_{s'}$ by taking its value halfway through the slice, which gives us first order accuracy in $\partial_{s'} \eta_{s'}$ for free. Further, $\eta_{s'}$ is in fact only very weakly dependent on s' and so a small n_{slice} suffices, as seen by the following test: set $l_0 = 3$. Then, after one iteration of steps (a) and (b) and before normalizing in step (c), the matrix ρ should be equal to the thermal density matrix for a three site chain. At $\beta = 1$, the largest eigenvalue should be equal to e. For a calculation with $n_{slice} = 1$, the largest eigenvalue was found to be 2.718 224; for $n_{slice} = 2$, we find 2.718 267, and for $n_{slice} = 3$ we find 2.718 275.

We have tested QBP by computing the susceptibility, $\beta \Sigma_j \langle S_i^z S_{i+j}^z \rangle$, at the susceptibility peak, using the known location[12] of the peak at $T_{max} = 1/\beta = 0.640\,851\,030\,85$. The exact result for the susceptibility is

$$\chi_{exact}(T_{max}) = 0.146\,926\,279 \cdots \tag{14}$$

while a calculation using $l_0 = 5$, $n_{it} = 20$, $n_{slice} = 20$, and correlations up to $j = 20$ gives

$$\chi_{QBP}(T_{max}) = 0.146\,927\,031 \cdots \tag{15}$$

for a relative error of $\approx 5 \times 10^{-6}$. The calculation took $\lesssim 0.08$ s on a 1.5 GHz PowerPC G4 processor, and using conservation of S^z the largest matrix diagonalized was ten by ten. A larger calculation, with $l_0 = 9$, $n_{slice} = 50$, $n_{it} = 30$ improves this to $\chi_{QBP}(T_{max}) = 0.146\,926\,251 \cdots$ for a relative error of $\approx 2 \times 10^{-7}$.

We calculated the specific heat C as a function of temperature in two ways: first, by calculating $\beta^2 \partial_\beta^2 \ln(Z)$ using $\ln(Z)$ from the algorithm, and, second, by calculating $-3\beta^2 \partial_\beta \langle S_i^z S_{i+1}^z \rangle$. The results are shown in Fig. 1, where to take derivatives we calculated $\ln(Z)$ and $\langle S_i^z S_{i+1}^z \rangle$ for $\beta = 0.1, 0.2, 0.3, \ldots, 10.0$. As l_0 gets larger, the curves remain accurate to lower temperature. The peak specific heat for $l_0 = 7$ was $0.349\,914 \cdots$ from the second derivative calculation and $0.349\,717 \cdots$ from the first derivative, both of which compare very well with the Bethe ansatz result of $0.349\,712 \cdots$.

The accuracy can be improved by going to larger l_0. Another improvement is to take $H=h^{(l_0-2)}+(1/2)h_{l_0-2,l_0-1}$ and $A=(1/2)(h_{l_0-2,l_0-1}+h_{l_0-1,l_0})$ instead of $H=h^{(l_0-1)}$ and $A=h_{l_0-1,l_0}$. We still have $H+A=T^{\dagger}HT+h_{0,1}$ in this case, but the slightly different form of the perturbation seems to work better. The figure inset shows a comparison of Bethe ansatz data to $l_0=9$ (where the largest matrix diagonalized is 126 dimensional).

Discussion. The implementation of the QBP equations here must be considered as preliminary. More work is needed to optimize the algorithm and, most importantly, to quantify the sources of error. Despite this, the method yields accurate results, giving qualitatively correct behavior even at $l_0=3$ where QBP can be implemented as a "pen-and-paper" technique.

In contrast to QBP, thermodynamic DMRG[13] computes low-lying eigenvalues for finite size chains up to size $N=30$; the results were accurate to quite low temperatures, but required an extrapolation to avoid finite size effects. In that work, chains of size up to $N=14$ were exactly diagonalized, so if we improve the linear algebra routines used in our implementation it should certainly be possible to do QBP with an $l_0\sim 14$. It may be possible to do QBP with $l_0\sim 30$ using DMRG techniques to avoid keeping *all* of the eigenstates of H and instead truncate to some smaller subset of eigenstates of H. Extrapolation of our results suggests that this should permit access to temperatures $T/J\sim 1/36$.

Transfer matrix DMRG[14] is related to QBP procedure in that both procedures look for the largest eigenvalue of a transfer matrix. In the case of transfer matrix DMRG, the transfer matrix comes from a Trotter approximation. In QBP, the transfer matrix is given by Eq. (12). Accurate results were obtained at much lower temperatures than here in Ref. 14, but significantly larger matrices were diagonalized in that study, and the higher temperature results for peak susceptibility and specific heat do not appear to be as accurate. It is likely that the higher accuracy of our method at high temperature comes from the lack of Trotter error: the error becomes exponentially small in l_0 once l_0 becomes of order $J\beta$. We now describe a procedure that combines some of the ideas of QBP and transfer matrix DMRG. Introduce M copies of the system, each with density matrix $\exp(-\beta h^{(N)}/M)$, so that the joint density matrix is $\exp(-\beta h^{(N)}/M)\otimes\cdots\otimes\exp(-\beta h^{(N)}/M)$. Let P_i be the operator that cyclically permutes the value of the spin on site i between the M different copies. Then,

$$\begin{aligned}&\mathrm{tr}(P_1P_2\cdots P_N\exp(-\beta h^{(N)}/M)\otimes\cdots\otimes\exp(-\beta h^{(N)}/M))\\&\quad=\mathrm{tr}\exp(-\beta h^{(N)}).\end{aligned}$$

Let ρ by a 2^{l_0M}. dimensional matrix. We will define a QBP procedure such that after n_{it} iterations, ρ is approximately proportional to the reduced density matrix

$$\begin{aligned}&\mathrm{tr}_{1\cdots n_{it}}(P_1\cdots P_{n_{it}}\exp(-\beta h^{(l_0-1+n_{it})}/M)\otimes\cdots\otimes\\&\quad\times\exp(-\beta h^{(l_0-1+n_{it})}/M)).\end{aligned}$$

Define O by Eq. (11), for $H=h^{(l_0-1)}$ at inverse temperature β/M, and map

$$\begin{aligned}\rho\rightarrow{}&Z^{-1}T^{\dagger}(\mathrm{tr}_1(P_1(O\otimes\cdots\otimes O)\rho(O^{\dagger}\otimes\cdots\otimes O^{\dagger}))\otimes\mathbb{1}_{l_0+1}\\&\otimes\cdots\otimes\mathbb{1}_{l_0+1})T.\end{aligned}\tag{16}$$

For $M=1$, this reduces to the QBP implementation described here, while for $l_0=2$, this becomes very similar to the transfer matrix used in transfer matrix DMRG. The question is whether for $M>1$, $l_0>2$ more accurate results can be obtained, possibly using DMRG to find the fixed point ρ of this transfer matrix.

QBP can be directly applied to finite size chains and to infinite or finite trees. The ability to compute real-space correlation functions and handle translationally noninvariant systems are advantages of this method, and in future this method will be applied to disordered systemswhere transfer matrix DMRG will have problems. Probably the most interesting question is the possible application of QBP to higher dimensional systems, by replacing the higher dimensional lattice with a Cayley tree or Husimi cactus with the correct local structure.

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