Contribution to the theory of plane domain walls in a ferromagnet

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Plane domain walls in a ferromagnet with exchange anisotropy are investigated. The one-dimensional discrete problem of minimization of the classical energy functional is solved rigorously. A linear combination of spin complexes, which corresponds to a classical domain wall, is found.

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INTRODUCTION

The thickness of plane domain walls in strongly anisotropic ferromagnets is comparable with the lattice constant, and in this case the continual approximation, usually employed in classical theory, turns out to be quite crude.[1] It follows from general configurations that allowance for the discrete character of the lattice should lead primarily to a finite domain-wall energy density in ferromagnets with large anisotropy (the continual theory gives an unlimited growth of the energy density in this limit). Discrete computer calculation points also to other peculiarities that vanish on going to the continuous description. Thus, a numerical investigation was carried out in Ref. 2 of the dependence of the energy on the position of the wall relative to the crystal lattice. To elucidate such peculiarities, it is of interest to solve exactly the domain wall problem in a realistic model of the ferromagnet. It will be shown below that this problem can be completely solved in a uniaxial ferromagnet at any value of the exchange-anisotropy constant. Since we are interested also in the quantum aspects of the problem, we write for the indicated model the Hamiltonian

$$H=-\frac{1}{2}J\sum_{m,\delta}\left[\frac{1}{g}(S_m^xS_{m+\delta}^x+S_m^yS_{m+\delta}^y)+S_m^zS_{m+\delta}^z\right]. \qquad (1)$$

Here $J>0$ and $g\geqslant 1$ is the exchange-anisotropy constant. S_m^α is the operator of the α-th spin component in the m-th site, and δ is the vector joining the nearest neighbors.

The model (1) is well known in magnetism theory and a number of magnets described by it are also known.[3] In a particular case it is possible to obtain from (1) the isotropic Heisenberg model ($g=1$), the Ising model ($g\to\infty$), and also the XY model ($g\to 0$). The model (1) is one of the two simplest models of a uniaxial ferromagnet (the other, customarily employed in the classical theory of domain walls, is the model with single-ion anisotropy,[1] which excludes, however, the spin $s=1/2$ in the quantum treatment). We note also that the problem of the domain wall in the Ising model is solved trivially, and this facilitates the analysis of the solution at $g<\infty$.

In the quantum case one uses in the theory of the spectrum of the system (1) the fact that the z-th projection of the total spin is a conserved quantity and that the stationary states can classified in terms of the eigenvalue n of the operator S^z. The spectrum of the one-dimensional system (1) was investigated completely at $s=1/2$ in a number of studies. In particular, for an anisotropic chain, explicit expressions were obtained for the energy[1)] and for the wave functions of the bound state of n magnons in the case of periodic boundary conditions,[4] as well as in the case of a semibounded chain.[5] These states are of interest also as a possible quantum analog of solitons of the Landau-Lifshitz equation.[6] In such an interpretation a domain wall corresponds to an extremely heavy complex.[6] Indeed, the mean value of $S_m{}^z$ in this state is not uniformly distributed along the chain and is described in the case of a semibounded system by a certain domain wall. We shall study this distribution and ascertain how accurately the quantum results for the energy and for $S_m{}^z$ agree with the corresponding classical results. As for the third characteristic of the wall, namely the mean value of $S_m{}^x$, the answer is quite simple: in a spin complex, just as in any system with fixed n, we have $S_m{}^x\equiv 0$, whereas in a classical wall the distribution of $S_m{}^x$ is not uniform. It becomes clear thus that by confining ourselves to consideration of a state with definite n we cannot achieve full agreement of the quantum and classical results. On the other hand, Pokrovskiĭ and Khokhlachev[7] have constructed for an infinite chain a stationary state in which the energies and the mean values of $S_m{}^z$ and $S_m{}^x$ are described by a solution of the equation of the classical theory, i.e., if the classical problem had been solved, it is possible to construct a corresponding stationary state of the quantum system. From the considerations given above it follows that this state is not the limit of the stationary state of a semibounded chain.

Analysis of this quite not ordinary situation has shown that actually there exists an entire class of states (a linear combination of spin complexes of a semibounded chain) in which the distribution of the mean $S_m{}^z$ is described by domain walls. These states (except for one—a spin complex) are stationary only in the limit $N_0\to\infty$, where N_0 is the average number of the bound magnons. The spin complex is stationary at all N_0. Among the indicated states there exists one corresponding to a classical wall. We shall find its explicit form. This state turns out to be a Gaussian combination of spin complexes. An exact connection of the complexes with the classical domain wall has thus been established within the framework of the model (1). We shall show that this state coincides with the one that can be obtained from the results of Ref. 7 and from the solution of the classical problem (4). We have observed in the present study also an analogy between the investigated domain wall and a Fermi step in an ideal gas. It is curious that a classical wall corresponds to a Fermi step of a gas within the framework of a grand canonni-

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cal ensemble, while the wall of a spin complex corresponds to a Fermi step of a gas within the framework of a canonical ensemble.

Having an explicit expression for the domain-wall energy, we shall discuss at the end of the paper its contribution to the low-temperature thermodynamics of a one-dimensional magnet.

1. CLASSICAL TREATMENT

As is customary in classical theory,[1] we replace in (1) the spin operators by classical vectors of length s:

$$S_m^z=s\cos\theta_m,\quad S_m^x=s\sin\theta_m\cos\varphi_m,\quad S_m^y=s\sin\theta_m\sin\varphi_m.$$

For the energy functional of the considered model we obtain in this case the expression

$$E\{\theta,\varphi\}=\frac{1}{2}Js^2\sum_{m,\delta}\left[1-\frac{1}{g}\sin\theta_m\sin\theta_{m+\delta}\cos(\varphi_m-\varphi_{m+\delta})-\cos\theta_m\cos\theta_{m+\delta}\right]. \quad (2)$$

In a study of plane domain walls it suffices to consider the case φ_m = const. The θ_m distribution that minimizes $E\{\theta\}$ should satisfy the equation $\delta E/\delta\theta_m = 0$, which takes for the model (2) the form

$$g\sin\theta_m\sum_\delta\cos\theta_{m+\delta}=\cos\theta_m\sum_\delta\sin\theta_{m+\delta}. \quad (3)$$

We consider first the one-dimensional case: $\delta = \pm 1$. To solve the nonlinear difference equation we change to a new variable f_m, where $\tanh f_m = \cos\theta_m$. From (3) we obtain after simple transformations an equation for f_m:

$$g\,\mathrm{sh}\,[(f_{m+1}+f_{m-1})/2]=\mathrm{sh}\,f_m\,\mathrm{ch}\,[(f_{m+1}-f_{m-1})/2].$$

This equation is valid if we stipulate for any m satisfaction of

$$f_{m+1}+f_{m-1}=2f_m,\quad f_{m+1}-f_{m-1}=2\sigma,\quad \sigma=\ln[g+(g^2-1)^{1/2}].$$

The solution of such equation has the simple form $f_m = (m + m_0)\sigma$, where m_0 is an arbitrary constant. With the aid of the solution obtained for f_m we can calculate the energy E_{DW}. We write the final result in the form

$$S_m^z=s\,\mathrm{th}\,(m+m_0)\sigma,\quad S_m^x=s[\mathrm{ch}\,(m+m_0)\sigma]^{-1},$$
$$E_{\mathrm{DW}}=2s^2J\,\mathrm{th}\,\sigma. \quad (4)$$

The solution (4) describes a domain wall in the one-dimensional case ($S_m^z\to\pm s$ as $m\to\pm\infty$). In the Ising model ($\sigma\to\infty$) we have $E_{\mathrm{DW}} = 2Js^2 < \infty$; this result can be obtained also by direct calculation. In the limit of weak exchange anisotropy ($g\approx 1 + 2\eta^2$ or $\sigma = 2\eta\ll 1$) the energy functional takes the form

$$E=\frac{1}{2}Js^2\int d\xi[\theta'^2-4\eta^2\cos^2\theta],$$

Eq. (3) goes over into the equation

$$\theta''-2\eta^2\sin 2\theta=0,$$

whose solution is well known[1]:

$$\cos\theta=\mathrm{th}\,(2\eta\xi),\quad E=4Js^2\eta.$$

The last expressions can be obtained at $\sigma = 2\eta\ll 1$ also from the general result (4).

We proceed to consider plane domain walls in multidimensional ferromagnets. For the sake of argument we confine ourselves to cubic structure, where each lattice site is defined by the Cartesian coordinates m_i of the radius-vector $\mathbf{m}$. We study first a plane wall with the normal along a diagonal of the cube (wall A). In this case $\theta_{\mathbf{m}}$ depends only on the scalar

$$\xi=\sum_{i=1}^d m_i,$$

where d is the dimensionality of the crystal. From (3) it is easy to derive the following equation for θ_ξ:

$$g\sin\theta_\xi(\cos\theta_{\xi+1}+\cos\theta_{\xi-1})=\cos\theta_\xi(\sin\theta_{\xi+1}+\sin\theta_{\xi-1}).$$

This equation coincides with the one we solved in the one-dimensional case, so that the problem of the type-A wall reduces to the one-dimensional problem solved above. The distribution of the spin density along the chosen chain of the crystal is given by expressions (4). For the wall energy density we easily obtain the result

$$E^{(A)}=2Js^2d^{1/2}a^{1-d}\,\mathrm{th}\,\sigma. \quad (5)$$

Here a is the lattice constant. The factor $d^{1/2}$, as follows from the calculations, takes into account the presence of neighboring chains and the increase of the area of the wall A compared with the area of the wall B in multidimensional crystals. We define the wall B as the one with the normal (1, 0, 0). The distribution of $\theta_{\mathbf{m}}$ in this wall is subject to the condition

$$\theta_{m_1m_2m_3}=\theta_{m_1m_2\pm1m_3}=\theta_{m_1m_2m_3\pm1}.$$

The equation for θ_{m_1} then takes the form

$$g\sin\theta_{m_1}(\cos\theta_{m_1+1}+\cos\theta_{m_1-1})$$
$$=\cos\theta_{m_1}(\sin\theta_{m_1+1}+\sin\theta_{m_1-1})-(g-1)(d-1)\sin 2\theta_{m_1}.$$

It is easy to grasp that the problem of a wall in a one-dimensional ferromagnet with exchange and single-ion anisotropy (with a definite ratio of the two anisotropy constants) reduces to the same equation. The indicated problem cannot be solved in the general case. In the continual approximation the equation becomes simpler, and for the energy of the wall B we obtain the expression

$$E^{(B)}=4Js^2\eta a^{1-d}d^{1/2},$$

which coincides, as it should in this limit, with the energy $E^{(A)}$. The energy $E^{(B)}$ can be easily calculated by a direct method also in the Ising model:

$$E^{(B)}=2Js^2a^{1-d},$$

in this limit

$$E^{(A)}=2Js^2d^{1/2}a^{1-d}>E^{(B)}.$$

In the Ising model, taking into account the different number of irregular bonds, it is easy to understand the difference between the energy densities of the two walls. From the continuity of the solution with respect to the parameter σ one should expect the inequality $E^{(A)} > E^{(B)}$ to be preserved in a certain range of anisotropy values, and possibly goes over into an equality only in the weak-anisotropy region. Thus, in the model considered, the energy of a plane wall depends on the position of the wall relative to the crystal lattice. There are no grounds for assuming that the considered energy difference exists only in cubic structure, but an answer to this question can be obtained only by a special investigation of other lattices.

2. ONE-DIMENSIONAL CASE—QUANTUM TREATMENT

We investigate first a wall describing the distribution $S_m{}^z$ in a heavy complex localized near the boundary of a semibounded chain. We obtained in another paper[5] explicit expressions for the energy and wave function of a bound state of n magnons. These expressions can be conveniently written in the form

$$|\psi_n\rangle=A_n\sum_{\{m_i\}}B_{m_1m_2\ldots m_n}S_{m_1}^-S_{m_2}^-\ldots S_{m_n}^-|0\rangle,$$

$$B_{m_1\ldots m_n}=\prod_{i=1}^{n}v_i^{m_i},\quad v_i=\operatorname{ch}(i-1)\sigma/\operatorname{ch}i\sigma,\quad \varepsilon_n={}^1/{}_2J\operatorname{th}\sigma\operatorname{th}n\sigma. \tag{6}$$

Here A_n is a normalization constant, and

$$\sum_{\{m_i\}}\ldots\equiv\sum_{1\leqslant m_1<m_2<\ldots<m_n}\ldots$$

As $n\to\infty$, the energy of the complex, as can be seen from (6), tends to a value $(1/2)J\tanh\sigma$, which coincides[2)] with the energy (2) of a classical domain wall at $s=1/2$. We need in addition to calculate $\langle\psi_n|S_m{}^z|\psi_n\rangle$ at larger n. Calculation of mean values of this type in a bound multiparticle state is a cumbersome problem that has so far been solved completely only for the case of a one-dimensional problem with a δ-function attraction.[9] The methods used in Ref. 9 for calculation and the results there cannot be used in our case so that the calculation of the average $S_m{}^z$ is a problem in itself. We write down first the easily derived relation

$$\langle\psi_m|S_m{}^z|\psi_n\rangle={}^1/{}_2-\rho_n(m),$$

where

$$\rho_n(m)=A_n{}^2\sum_{\nu=1}^{n}\sum_{\{m_i\}}\delta(m-m_\nu)|B_{m_1\ldots m_n}|^2,$$

$$A_n{}^{-2}=\sum_{\{m_i\}}|B_{m_1\ldots m_n}|^2=\prod_{i=1}^{n}\frac{v_i^2}{1-v_i^2}. \tag{7}$$

A simple analysis of the expression for $\rho_n(m)$ shows that at large n we have $\rho_n(m)\approx1$ in the region $m\ll n$ and $\rho_n(m)\approx0$ at $m\gg n$. We are interested in the behavior of $\rho_n(m)$ in the region $n\sim m$. Denoting $n-m$ by ζ, we can obtain, after prolonged calculations, for $n\sigma\gg1$ and $m\sigma\gg1$:

$$\rho(\zeta)=\sum_{j=0}^{\infty}(-1)^j\exp[j\sigma(2\zeta-1-j)]. \tag{8}$$

Expression (8) satisfies the relation $\rho(\zeta)=1-\rho(1-\zeta)$, and this symmetry is due in final analysis to the invariance of the states of the chain to the substitution $S_m{}^z\to-S_m{}^z$. It follows from the foregoing relation that $\rho(\zeta)>1/2$ at $\zeta\leqslant0$ $(m\leqslant n)$ and $\rho(\zeta)<1/2$ at $\zeta>0$ $(m>n)$. In the Ising model we obtain from (8) a real step: $\rho(\zeta)=1$ $(\zeta\leqslant0)$ and $\rho(\zeta)=0$ $(\zeta>0)$. This state is also called a spin cluster.

The classical expression for $\tilde{\rho}(\zeta)=\frac{1}{2}-S_\zeta{}^z$ can be obtained from (4) by replacing m with ζ:

$$\tilde{\rho}(\zeta)=[\exp(2\sigma(\zeta-m_0))+1]^{-1}. \tag{9}$$

Comparison of the series (8) with expression (9) shows that it is impossible to define the constant m_0 in (9) so as to satisfy $\rho(\zeta)=\tilde{\rho}(\zeta)$. The two expressions can be shown to coincide only in the region of weak anisotropy. Consequently, the energy of the heavy complex coincides with the energy of a classical wall at any value of the anisotropy, but $\langle\psi_n|S_m{}^z|\psi_n\rangle$ coincides with the classical distribution of the z-projection of the spin only for weak anisotropy. The substantial difference between the results for $S_m{}^x$ was already discussed in the Introduction.

We consider next a linear combination of spin complexes

$$|\Phi_{N_0}\rangle=\sum_n C_n^{(N_0)}|\psi_n\rangle,$$

where the distribution of $C_n^{(N_0)}$ has a maximum near the site N_0 and has a width Δn. In the general case this is a nonstationary state. Under the condition $\Delta n\ll N_0$ and at times $t\ll(\hbar/J)e^{N_0\sigma}$, it can be verified with the aid of the explicit expressions (6) that $|\Phi_{N_0}\rangle$ is stationary, i.e.,

$$e^{-iHt/\hbar}|\Phi_{N_0}\rangle=e^{-iE_{DW}t/\hbar}|\Phi_{N_0}\rangle.$$

In the limit as $N_0\to\infty$ the state $|\Phi_{N_0}\rangle$ can be regarded as stationary at all times, and this fact is in essence a manifestation of the asymptotic degeneracy of the level $\varepsilon=E_{DW}$ of an infinite crystal. It is easy also to verify that $\langle\Phi_{N_0}|S_m{}^z|\Phi_{N_0}\rangle$ is described by a domain wall whose type is determined by the coefficients $C_n^{(N_0)}$. Since $|\Phi_{N_0}\rangle$ is a linear combination of states with different n, in the general case $S_m{}^x$ is also different from zero. There are thus many states of the domain-wall type, and they are strictly stationary only in the limit as $N_0\to\infty$.

To find the state $|\Phi_{N_0}\rangle$, in which the mean energy values $S_m{}^z$ and $S_m{}^x$ would coincide with the classical results, we note that the classical expression (9) for $\tilde{\rho}(\zeta)$ recalls in form the Fermi-Dirac distribution function for an ideal gas with an equidistant spectrum (the level spacing at the proper units is equal to the lattice constant, m_0 plays the role of the chemical potential, and the anisotropy constant the role of the reciprocal temperature). It turns out that the analogy with statistical mechanics of an ideal gas can be traced also in the quantum case. Indeed, at large n Eq. (6) leads to a simple expression for the probability given by the amplitude $B_{m_1\ldots m_n}$:

$$|B_{m_1\ldots m_n}|^2=a_0\exp\left(-2\sigma\sum_i m_i\right),$$

where the constant a_0 does not depend on the indices m_i. This equality expresses the fact that at large n the flipped spins with small numbers n are rigidly anchored to the neighboring sites, and the coupling of spins with large i is determined by a parameter that does not depend on the number: $v_i = e^{-\sigma}$. The expression derived for $|B_{m_1 \ldots m_n}|^2$ shows that the problems of calculating $\rho_n(m)$ and A_n^{-2} coincide respectively in the quantum-mechanical problem with the problems of finding the occupation numbers $p_n(m)$ and of the partition function Z_n of an ideal Fermi gas with equidistant spectrum and with fixed particle number n. The connection is established in this case by the relations

$$2\sigma=\beta=T^{-1}, \quad A_n^{-2}=a_0 Z_n, \quad \rho_n(m)=p_n(m).$$

Using these equations we can obtain from (7) and (8) the partition function and the occupation numbers of the indicated system within the framework of a canonical ensemble. We proceed now to consider an ideal gas within the framework of a grand canonical ensemble. Although an ideal Fermi gas with equidistant spectrum (with finite level spacing) is not quite a pithy model of statistical physics ($E_0 \sim N^2$), analysis has shown that when calculating the occupation numbers one can proceed in accord with certain rules. Choosing a suitable condition for $\Sigma_m\, p(m)$, we obtain the chemical potential $\mu = N_0 + \alpha$ and

$$p(m)=[\exp((m-\mu)\beta)+1]^{-1},$$

where α is an arbitrary constant $|\alpha| \leqslant 1/2$. The difference between the $p(m)$ obtained here and the result (8) within the framework of the canonical ensemble must be attributed to peculiarities of the considered ideal-gas model.

The constructions of the grand canonical ensemble can by analogy be transferred to the quantum-mechanical problem of interest to us. The state whose normalization constant A is connected with the partition function takes in this case the form

$$|\Phi_{m_0}\rangle=A\sum_{k=-\infty}^{\infty}\exp\left\{-\frac{\sigma}{2}\left[k+\left(\frac{1}{2}-\alpha\right)\right]^2\right\}$$
$$\times|\psi_{N_0+k}\rangle, \quad m_0=N_0+\alpha, \quad |\alpha|\leqslant\frac{1}{2}. \qquad (10)$$

The state $|\Phi_{m_0}\rangle$ is so constructed that

$$\langle\Phi_{m_0}|S_m^z|\Phi_{m_0}\rangle={}^1/_2\,\mathrm{th}\,(m-m_0)\sigma,$$

i.e., the mean value of S_m^z is described by a classical expression. This equality can be proved also by direct calculation, using (8). The width of the Gaussian distribution in (10) is $\Delta k \sim \sigma^{-1/2}$, and in the Ising model (10) reduces to a cluster of N_0 flipped spins. The calculation of the mean value of S_m^z in the state (10) entails no difficulties in principle, and we present the final expression

$$\langle\Phi_{m_0}|S_m^x|\Phi_{m_0}\rangle=\tilde{\rho}(m)\exp(m-m_0)\sigma$$
$$=[2\,\mathrm{ch}\,(m-m_0)\sigma]^{-1}.$$

This result coincides with the classical result (4). It is easy to verify that $\langle\Phi_{m_0}|S_m^y|\Phi_{m_0}\rangle = 0$, and consequently in this state the mean values of S_m^α satisfy at any m the classical condition

$$\sum_{\alpha=x,y,z}(S_m^\alpha)^2=\frac{1}{4}.$$

The energy of the state (10) at large N_0 also coincides with $E_{\rm DW}$, so that the obtained state is a complete analog of a classical domain wall. It appears that state $B_{m_1 \ldots m_n}$ is singled out for some more profound region, e.g., the uncertainty principle. A detailed investigation of this question is outside the scope of the present discussion. We note only that the interpretation offered here of a classical wall as a linear combination of spin complexes is reminiscent of the interpretation of the classical spin wave as a linear combination of stationary states of a Hamiltonian (this combination is known as a coherent state[10]).

We show next how to obtain the explicit form of the state (10) from the results of Ref. 7 and the solution of the classical problem (4). In the case $s = 1/2$ the state considered in Ref. 7 can be written in the form

$$|\tilde{\Phi}\rangle=\prod_m\begin{pmatrix}\cos(\theta_m/2)\\ \sin(\theta_m/2)\end{pmatrix},$$

where θ_m is a solution of the classical-theory equation (3). Writing

$$|\tilde{\Phi}\rangle=\sum_n C_n^{(m_0)}\,|\psi_n\rangle,$$

using the solution (4) and the asymptotic expressions for the amplitudes $B_{m_1 \ldots m_n}$ from (6), we succeed after prolonged calculations in finding a Gaussian distribution for $C_n^{(m_0)}$.

In conclusion, we dwell briefly on the contribution of a domain wall to the low-temperature thermodynamics of a one-dimensional magnet. Although our quantum treatment applied only to the case $s = 1/2$, there are grounds (favored, in particular, by the results of Ref. 7) for assuming that the picture qualitatively described here is valid also at $s > 2$. In other words, we assume that at any s the spectrum of an open chain contains a degenerate (in first approximation) level of order N with energy $E_{\rm DW}$, and the states of this level can be chosen both in the form of spin complexes (fixed n) and in the form of linear combinations of the type (10) or of domain walls. In the case when all other excitations of the system (1) (magnons, volume complexes) lie higher, the considered level of the wall determines completely the low-temperature dynamics. In particular, the specific heat takes the form

$$c \propto \exp(-E_{\rm DW}/T).$$

This case is realized for a spin $s = 1/2$ at $g > 5/3$, when the magnon energy is $\varepsilon_{\rm M} = 1 - g^{-1}\cos k$. At $g < 5/3$ the magnon energy $\varepsilon_{\rm M} < E_{\rm DW}$ and $c \propto \exp(-\varepsilon_{\rm M}/T)$ down to very small values of the anisotropy, when the volume spin complexes assume a substantial role. Such a crossover type behavior was found earlier in Ref. 11 in a solution of the Yang-Gaudin integral equations. We emphasize here the direct connection between the indicated behavior and the presence of low-lying domain walls in the chain of spins $s = 1/2$. At $s > 2$ we have $\varepsilon_{\rm M} < E_{\rm DW}$ and consequently there is no region of the constant g where the wall could dominate in the low-temperature region. It appears that the magnons in these chains lie lower than all the spin complexes (this can be proved in the Ising model, and in the general case there is a known solution, which confirms the foregoing, only for two-magnon complexes), and they determine the low-temperature thermodynamics of an anisotropic chain.

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1)Complexes with different n have different energies.

2)For a complex in a chain with periodic boundary conditions, $\varepsilon_n \rightarrow J \tanh \sigma = 2E_{DW}$. This relation was obtained earlier for the weak-anisotropy region in Refs. 6 and 8.

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