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1990 J. Phys.: Condens. Matter 2 3497

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Energy minimisation and generalised self-consistency conditions in the recursion method

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Received 21 August 1989

Abstract. A problem arises in electronic structure calculations involving some generalised self-consistency condition. Examples are the self-consistency of the potential or the magnetic moment, the latter being discussed here in detail. The problem reduces to ensuring that when one requires analytic consistency between different quantities the numerical method used must preserve the analytic relation to arbitrary precision. Specifically we deal with the recursion method coupled with Gaussian quadrature for the calculation of the integrated density of states and show that the conventional prescription for the evaluation of the total energy fails to satisfy the analytic condition that its minimum correspond to the self-consistent solution. We illustrate the magnitude of the effect and a way to overcome it using examples from a model density of states and a real calculation.

1. Introduction

In almost all electronic structure calculations the crucial quantity which we want to calculate is the total ground state energy subject to a generalised self-consistency condition. For example this can involve the potential seen by an electron, the Hellmann-Feynman force on a displaced atom or, in our case, the local magnetic moment in the calculation of the ferromagnetic ground state of iron. A particular problem arises in electronic structure calculations which use the recursion method (Haydock 1980) coupled with Gaussian quadrature (Nex 1978) for the analysis of the resulting continued fraction, but analogous difficulties exist in other contexts. In this short communication we will illustrate how a commonly used computational prescription for the calculation of the total energy fails to satisfy the analytic condition that its minimum correspond to the self-consistent solution and how this problem can be cured. We compare the new prescription with the standard method for absolute accuracy and then use it briefly in the context of longitudinal fluctuations in ferromagnetic iron to show the extent to which this problem can affect a calculation.

This work re-emphasises the following general consideration. If one requires an *analytic* relationship between quantities calculated in different ways, e.g., total energies and forces, then it is crucial that this analyticity be preserved in the numerical formulation to arbitrary precision. What is important is the correlation of errors, not their absolute magnitude.

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The object of the calculations is to obtain the total energy of the system subject to some given constraints as a function of a specified input parameter. This could be the displacement of an atom or the exchange splitting Δ between the up and down spin electrons in the calculation of the magnetic moment per atom. We will examine the latter case in detail below but first want to discuss the more general aspects of the problem. It is known from analytic theory that the self-consistency condition yields a minimum, U_{\min} , of the total energy U . However it can easily happen, for a variety of reasons, that *computationally* the minimum U_{\min} does not correspond to the energy U_{sc} when the self-consistency condition is satisfied. This is unsatisfactory because it raises the issue of which energy to take and can lead to other inconsistencies. Whereas this may not be a problem if one just wants a single energy, it becomes disastrous when small energy differences, such as those in our study of longitudinal fluctuations, are sought.

Incidentally, one normally *does* want to use the self-consistency condition to find the minimum rather than obtaining it directly from a minimisation of the total energy since the former contains far more information. Suppose we are modelling some physical effect by setting up a periodic system with a supercell containing L atoms. Then from one iteration of the electronic structure calculation we obtain L pieces of information, namely the deviations from self-consistency on each site. For example these could be the Hellmann–Feynman forces which tell us how to adjust the displacements of each atom to move the whole configuration towards self-consistency. This is vastly more efficient than working only with the energy and doing L separate calculations on different configurations to obtain the same information. Thus the use of the self-consistency condition is essential, and with it a formulation of the total energy whose minimum is truly identical computationally with the self-consistency condition.

A discrepancy between U_{\min} and U_{sc} can arise from a number of reasons. Here we will be particularly concerned with the problem of using Gaussian quadrature to calculate integrals over the local densities of states obtained from the recursion method. The problem reduces to calculating the integrals involved in the total energy expression and those involved in the self-consistency condition using algorithms which ensure that the errors in all the computed quantities are correlated. We describe below how the standard procedure for the calculation of the total energy fails to preserve the analytic relation between self-consistency and energy minimisation and how this problem can be avoided by recasting the total energy expression so that it becomes a function of a single integrated quantity. In this way no discrepancy can arise.

The problem and its solution are best explained using an example. We consider a very simple model for a ferromagnetic system so that the crucial issue which we want to address is not obscured by the description of the details and approximations used in a realistic Hamiltonian. Define $n_{\sigma}(E)$ as the local density of states (DOS) for electrons of spin σ and split the up and down bands by an amount Δ so that

$$n_{\uparrow}(E) = n(E + \Delta/2) \quad (1.1a)$$

$$n_{\downarrow}(E) = n(E - \Delta/2). \quad (1.1b)$$

The system is filled up to the Fermi energy E_{F} so that the total number of electrons is given by

$$N = N_{\uparrow}(E_{\text{F}}) + N_{\downarrow}(E_{\text{F}}) = \int_{-\infty}^{E_{\text{F}}} (n_{\uparrow}(E) + n_{\downarrow}(E)) dE. \quad (1.2)$$

Splitting the bands results in the formation of a magnetic moment

$$m = N_{\uparrow}(E_{\text{F}}) - N_{\downarrow}(E_{\text{F}}) \quad (1.3)$$

which is related to Δ by the self-consistency condition

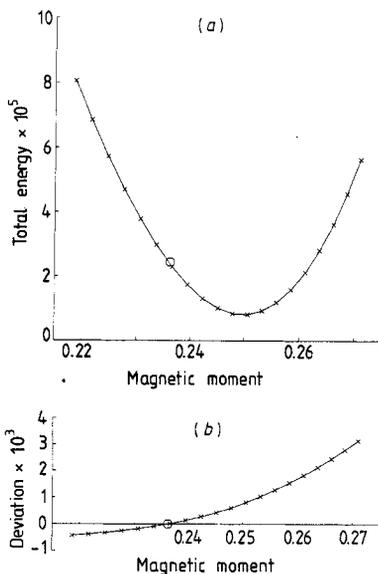


Figure 1. (a) Total energy and (b) deviations from self-consistency for the ferromagnetic state as a function of magnetic moment evaluated using the conventional quadrature procedure. 10 levels used in the quadrature obtained from two split semi-elliptical densities of states. The circle shows the position of the quadrature self-consistent moment.

$$\Delta = Im. \tag{1.4}$$

For a given value of I , the Stoner exchange interaction, the self-consistency condition yields the ferromagnetic ground state whose total energy is given by

$$U = U_{\text{band}} + \frac{1}{4}Im^2 \tag{1.5}$$

where

$$U_{\text{band}} = \int_{-\infty}^{E_F} E(n_{\uparrow}(E) + n_{\downarrow}(E)) dE. \tag{1.6}$$

As we shall show in more detail in § 2 (see figure 1), evaluating U_{band} using equation (1.6) within the quadrature approach results in a discrepancy between the actual minimum of the total energy curve, U_{min} , and the energy of the self-consistent solution, U_{sc} , specified by equation (1.4).

This problem can be avoided by integrating U_{band} by parts which results in

$$U_{\text{band}} = E_F(N_{\uparrow}(E_F) + N_{\downarrow}(E_F)) - \int_{-\infty}^{E_F} (N_{\uparrow}(E) + N_{\downarrow}(E)) dE. \tag{1.7}$$

In this way both the total energy and the self-consistency condition are expressed completely in terms of the same quantities, $N_{\sigma}(E)$. Let us for the moment regard $N_{\sigma}(E)$ not as the true integrated DOS but as some computationally defined quantity including arbitrary errors. It is easy to show by differentiating (1.5) with (1.7) that the energy minimum corresponds exactly to the self-consistency condition (1.4), irrespective of how large the errors in $N_{\sigma}(E)$ may be. In this way the numerical formulation preserves the analytic relation between total energy and self-consistency to arbitrary precision and does not rely on the convergence of the integrated DOS at all. We conclude that any discrepancies between the energy minimum and the self-consistency condition can be avoided by computing all the quantities involved by analytically related algorithms.

The simple case we have sketched above and the detailed numerical results on which we report below, all concern ferromagnetic systems. However our results and conclusions have a more general relevance. The evaluation of the band energy is the central component of most calculations carried out with the recursion method. For example it is crucial in the determination of the relative stability of different crystal structures (see Kelly 1980, p 363). It is also involved in the calculation of phonon spectra (Finnis *et al* 1987) and in defect relaxations where preserving the analytic relations between the total energy of a configuration and the forces on the atoms is important. This problem is very similar to the one we are discussing.

Analogous difficulties can also be found in other contexts arising from different reasons. For example when considering the equilibrium configuration of a set of atoms j , the minimum of the total energy corresponds to the 'self-consistency' condition $F_j = 0$ where F_j is any residual Hellmann–Feynman force experienced by atom j . In certain types of calculation the total energy is evaluated from the electronic structure expressed in terms of localised orbitals on the atoms, so that one moves the orbitals with the atoms during the relaxation. In such cases one has to employ approximate formulae for the Hellmann–Feynman forces which correspond precisely to a differentiation of the total energy expressed in terms of those orbitals (Sutton *et al* 1988). We have nothing to add to the discussion of this well-known problem, but merely point out that our difficulty is of a similar nature.

Having outlined the nature of our problem and its solution, we now turn to a more detailed consideration. We shall discuss what causes the problems with equation (1.6) within the quadrature approach and how these can be solved by using equation (1.7) or by the alternative approach based on terminators. We then describe the best numerical implementation of the new method and examine its absolute accuracy by comparing its results with an exactly soluble model. Lastly, in § 3, we briefly illustrate the extent to which this problem can affect a real electronic structure calculation using as an example the energies of longitudinal fluctuations in iron.

2. Numerical results and their interpretation

The recursion method has enjoyed popularity in tackling a wide range of problems from the determination of the relative stability of transition metal alloy structures to the relating of the electronic and topological structure in amorphous semiconductors. Its ability in dealing with systems of low symmetry lacking periodicity is its chief attraction. This is achieved by focusing on the local DOS, $n_0(E)$, projected on a starting state $|u_0\rangle$. This is related to the Green function $G_0(E)$ corresponding to $|u_0\rangle$ at an energy E which can be expressed as a continued fraction:

$$n_0(E) = -(1/\pi) \text{Im}(G_0(E)) \quad (2.1a)$$

$$n_0(E) = -(1/\pi) \text{Im}[[1/\{E - a_0 - b_1^2/[E - a_1 - b_2^2/(E - a_2 - \dots)]\}]]. \quad (2.1b)$$

The recursion coefficients a_n and b_n are given by

$$H|u_n\rangle = a_n|u_n\rangle + b_{n+1}|u_{n+1}\rangle + b_n|u_{n-1}\rangle \quad (2.2)$$

for the Hamiltonian H . Recursion calculations are almost invariably based on a tight-binding Hamiltonian and are usually carried out in two stages. First the coefficients are obtained by using the recursion relation (2.2) and for real systems only a relatively small

number of them can be calculated. The coefficients are then used to obtain the DOS and other derived quantities, most notably the integrated DOS.

The problem of the analysis of the coefficients has aroused considerable interest since the early days of the method as the two competing philosophies of Gaussian quadrature (Nex 1978, 1984) and analytic termination (Haydock *et al* 1972, Turchi *et al* 1982, Beer and Pettifor 1985, Luchini and Nex 1987) have emerged. Gaussian quadrature arose out of Nex's investigation of the bounds on the DOS (Nex 1978). He found that the integrated DOS has continuous upper and lower pointwise bounds which can be calculated from the recursion coefficients. The difference between the bounds narrows with increasing number of levels included in the quadrature. A differentiation of these bounds yields estimates for the DOS which, though not bounded themselves, are usually very reliable. On the other hand termination basically involves substituting a simple analytic expression for the part of the continued fraction which was not computed (the ellipsis of equation (2.1*b*)). This rather crude procedure is adequate for the simpler cases but gives large spurious oscillations in the DOS for even slight mismatches between the essential singularities of the computed coefficients and of the terminator. In this paper we are mostly interested in quadrature and refer the interested reader to Haydock and Nex (1984 and 1985) for a critical comparison of the two approaches.

Before discussing our numerical results we specify the mathematical formulation of our model in greater detail. To examine the total energy curve we need to compute the energy of a configuration away from the self-consistency condition. The energy of such a non-equilibrium configuration is given by

$$U = U_{\text{band}} + \frac{1}{4}Im^2 + \mathbf{h} \cdot \mathbf{m} \quad (2.3)$$

where the magnetic field \mathbf{h} is related to the exchange splitting Δ by

$$h = \frac{1}{2}(\Delta - Im). \quad (2.4)$$

Luchini *et al* (1990) discussed this in the framework of a Landau formulation where the deviation from equilibrium is represented by the field h . For the self-consistent moment (equation 1.4) this vanishes and the total energy is just the ground state energy (1.5). This field plays the rôle of the force in an elastic system where the analogue of the magnetic moment is the displacement.

Since the problem we are examining does not depend on the details of the Hamiltonian, for simplicity we first consider the case where all the recursion coefficients are constant. Thus our magnetic system consists of two semi-elliptical densities of states corresponding to the up and down electrons, whose centres are separated by an amount Δ . The full magnetic phase diagram of this system was discussed by Heine *et al* (1981).

Within the quadrature approach the integrated DOS is approximated by

$$\int_{-\infty}^{E_F} n(E) dE \approx \sum_{E_i < E_F} w_i(E_i(E_F)) + \alpha w(E_F) \quad (2.5)$$

where α is a constant, usually 0.5, the E_i are the poles of the continued fraction extended so that the last pole exactly coincides with E_F and the w_i are the Gaussian quadrature weights (Nex 1978, 1984). Conventionally the band energy (1.6) is computed using

$$\int_{-\infty}^{E_F} En(E) dE \approx \sum_{E_i < E_F} E_i(E_F)w_i(E_i(E_F)) + \alpha E_F w(E_F). \quad (2.6)$$

Figure 1 shows the plots of the total energy and the field as a function of magnetic

moment. The energy is computed using (2.3) with the conventional evaluation of the band energy given by (2.6). It is quite clear that the energy minimum does not correspond to the self-consistent solution which has zero magnetic field. Figure 1 was obtained using 10 levels of the continued fraction. Since the recursion coefficients are constants it is very simple and inexpensive to check that the effect decreases only very slowly with number of levels. It is not an artifact of the truncation though of course it would disappear if we could completely resolve all the eigenvalues of the system. This would never be achieved in a real calculation.

As we mentioned earlier the problem lies in the evaluation of the band energy. The correct procedure is to integrate the band energy by parts as in (1.7). In this way one is *only* using the integrated DOS coming from Gaussian quadrature in *all* the terms of the total energy. Explicitly

$$U = E_F(N_\uparrow(E_F) + N_\downarrow(E_F)) - \int_{-\infty}^{E_F} (N_\uparrow(E) + N_\downarrow(E)) dE + \frac{1}{2}I(N_\uparrow(E_F) - N_\downarrow(E_F))^2 + [\Delta - I(N_\uparrow(E_F) - N_\downarrow(E_F))](N_\uparrow(E_F) - N_\downarrow(E_F)). \quad (2.7)$$

In other words the total energy is now only a functional of the integrated DOS. Through the moment this same quantity is also involved in the definition of the self-consistency condition so that no inconsistency can arise. While the form of the band energy in equation (1.6) contains the *analytic* relation between the energy and $\Delta = Im$, the form in equation (1.7) explicitly preserves it to *arbitrary numerical accuracy*. The analytic relation is automatically contained in the numerical prescription and does not depend on the asymptotic convergence of the continued fraction coefficients.

There are other ways of looking at the prescription in equation (2.7). The simplest statement is probably to note that though Gaussian quadrature itself is a differentiable approximation, it does not claim to preserve relations between quantities analytically related by differentiation. Since the relation between the total energy and the field or force involves a derivative one should use some caution. Doing the integration by parts analytically in equation (2.7) automatically takes this into account.

Equation (2.7) also reminds us of the fact that the success of cluster calculations depends on the cancellation of large errors. For example it is well-known that the typical cluster sizes and numbers of levels used in real calculations lead to systematic errors much larger than the energy differences one is trying to compute. It is the *correlation* of errors in quantities calculated with a known setup that allows one to have an adequate energy resolution. The prescription in equation (2.7) extends this philosophy from the calculation to the processing of the recursion coefficients.

This viewpoint is useful when considering the issue of the alternative approach based on terminators. A terminator imposes the same set of errors on all continued fractions. So as long as one does not use a different terminator for different quantities there is no problem with preserving the analytic relation between them. Indeed terminators have been used successfully in phonon calculations (Finnis *et al* 1984) and defect relaxations (Ohta *et al* 1987, Paxton and Sutton 1988) where it is more important for the analytic relation between forces and energies to be preserved than for the DOS to be accurate.

Before discussing a computation with a real Hamiltonian we wish to examine the more numerical details of the implementation. In particular the evaluation of the integral of the integrated DOS in equation (2.7) is crucial and deserves some thought. Since Gaussian quadrature yields a pointwise continuous approximant to the integrated DOS it is tempting just to feed this to an integrating routine. Indeed this is sufficient for

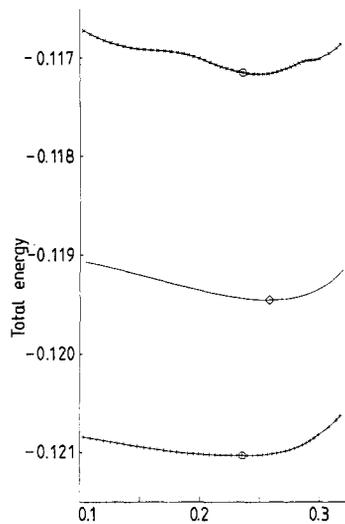


Figure 2. Total energies obtained from the conventional quadrature procedure (upper curve), the new quadrature procedure (lower curve) and the exact solution (middle curve). The quadrature self-consistent moment, indicated by the big circles, is different from the exact one. 10 levels were used in the quadrature and one can see that though the moment has not yet converged to its asymptotic value it does coincide with the minimum of the energy evaluated with the new procedure.

the simpler cases but rapidly becomes problematic for densities of states with many singularities or if accurate quantitative answers are required. Modern recursion calculations tend to use large numbers of levels leading to eigenvalues resolved to machine precision near the band edges so that the integrated DOS in that region looks like a series of step functions. Most standard integrating routines find these difficult to deal with.

In fact there is a more satisfactory approach which at the same time affords the ‘best’ way of computing the integral. Since we know that the quadrature integrated DOS must be smooth between the eigenvalues of the truncated continued fraction these can be found first. The integration can then be split up into segments delimited by them so that all the numerical integrals are taken over intervals where the integrated DOS is smooth and slowly varying. These can be tackled easily by a standard integrating routine to the desired accuracy. Moreover this approach is pleasing because it makes maximum use of all the information in the continued fraction.

This discussion raises the intriguing question of the absolute accuracy of the new method. In practice we have no way of estimating it but we can use the exactly soluble case of the two split semi-elliptical densities of states to give us a feeling for the orders of magnitude involved. Figure 2 shows the exact total energy together with the results from the usual evaluation of the band energy (equation (2.6)) and from the new method (equation (2.7)). It can be seen that the new method is better than the conventional prescription in terms of absolute accuracy though the effect is not very large. By itself it does not warrant the use of the new procedure which is much more expensive in computer time. Thus if we only require the estimate of the total energy of a particular configuration the conventional method is adequate. This really is what we expect since the greatest error is in the truncation of the continued fraction and this is the same for both the old and the new procedures. The increase in absolute accuracy comes from the fact that we have a greater correlation between the errors and so greater cancellations.

We note that over the wide scale of figure 2 the curve obtained from the conventional method, as well as not positioning the minimum correctly, picks up a substantial amount

of spurious structure leading to inaccuracies if energy differences between different configurations are sought. By contrast the results from the new procedure have precisely the same shape as the exact curve. Hence as well as preserving the identity of the self-consistent moment and the energy minimum, energy differences are also extremely reliable.

3. Results for a realistic Hamiltonian and conclusions

Finally we turn to a brief exposition of how badly the problem we have been discussing can affect a real electronic structure calculation. We study the itinerant electron magnetism of iron and use essentially the same physical picture and You and Heine (1982). Our model amounts to taking a non-magnetic band structure and imposing an exchange splitting Δ_j on each site j . We then solve for the electronic structure using the recursion method and calculate the local moments m_j and energies U_j projected on each site. By varying the magnitudes and directions of the exchange splitting a wide variety of configurations can be examined. This model has recently been elaborated and improved by Luchini and Heine (1989) who fully included the s and p electrons in the context of spiralling arrangements of spins. The much larger bandwidth of this model compared to previous d-band-only calculations forces one to use a correspondingly larger numbers of levels (≈ 90) to obtain the same energy resolution and thus the full accuracy of the 'best' method for performing the integration of the integrated DOS described above is required.

Here we simply want to examine the local energies for a longitudinal magnetisation fluctuation around the ferromagnetic ground state. Hence we consider a sinusoidal variation in magnetic moment superimposed on a ferromagnetic background and adjust all the Δ_j at atomic positions l_j until

$$m_j = m_{\text{FM}} + \delta m \sin(\mathbf{q} \cdot \mathbf{l}_j) \quad (3.1)$$

for a magnetisation wave of wavelength $\lambda = 2\pi/q$ with amplitude δm as shown in figure 3(a). Clearly the issue of the position of the energy minimum is crucial to this problem since we are perturbing around it.

Figure 3 shows the local energies for a long wavelength and small amplitude magnetisation wave evaluated with the conventional and with the new procedure. It is quite clear that the energy changes obtained with the conventional procedure are completely dominated by the lack of coincidence between the energy minimum and the self-consistent moment as shown in figure 1. A small *caveat* has to be made. Strictly speaking the value of the local energy i.e., the contribution of a particular site to the total energy, is physically meaningless. However in the long wavelength limit it must tend to its value for a uniform magnetisation. Hence in the spirit of the local environment approach (Heine 1980) in which these calculations are carried out we feel justified in interpreting figure 3 as follows.

To first order, since we are perturbing around the total energy minimum we would expect to see the local energy follow a 'sin²' profile. In the region of the wave where the moment is closest to the ferromagnetic value we would expect to observe the effects of the gradient term in the local energy and therefore the largest deviation from the sin² form. These considerations are borne out quite accurately by the energies calculated by the procedure of equation (2.7). However the plot computed using equation (2.6) shows quite clearly that the energies correspond to a perturbation

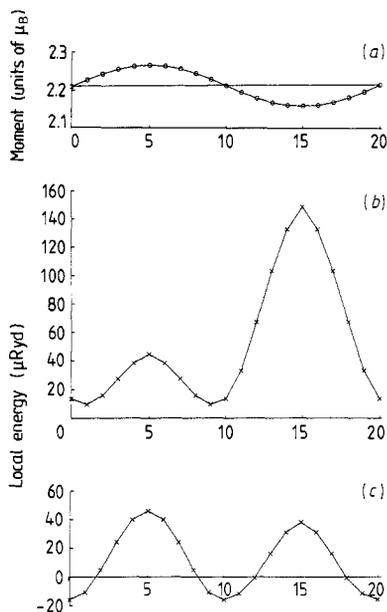


Figure 3. Longitudinal fluctuations around the ferromagnetic ground state for the spd model of iron. A fluctuation with amplitude $0.07 \mu_B$ and a wavelength of 20 sites is shown here. (a) Moment in μ_B along the magnetisation wave. (b) Local energy in μRyd along the wave evaluated using the conventional quadrature procedure relative to the energy of the ferromagnetic ground state. (c) Local energy in μRyd along the wave evaluated using the new quadrature procedure relative to the energy of the ferromagnetic ground state.

around a moment smaller than the effective energy minimum resolved by the procedure. That is they are consistent with figure 1. Clearly the total configuration energies which are the object of the calculation are very different in the two cases. Full details are given in Luchini *et al* (1990) where the spectrum of longitudinal fluctuations is calculated.

As a conclusion we simply want to focus the attention again on the general lesson which can be learnt from our investigation. This goes beyond the specific problems associated with Gaussian quadrature in the recursion method though we have seen how our discussion is in line with previous developments and puts various bits of recursion lore in a coherent picture. When one requires analytic relations between various computed quantities it is not sufficient for them to be accurate to the same number of significant figures. It is crucial that the numerical procedure used explicitly preserve the analytic relation at every step to arbitrary precision.

Acknowledgments

We acknowledge with pleasure many conversations with J H Samson and R Haydock and the help and guidance of V Heine in preparing the manuscript. One of us (MUL) wishes to acknowledge the financial support of the *Fondazione Angelo della Riccia*, Florence.

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