HARMONIC OSCILLATORS AND RESONANCE SERIES GENERATED BY A PERIODIC UNSTABLE CLASSICAL ORBIT

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Abstract

The presence of an unstable periodic classical orbit allows one to introduce the decay time as a purely classical magnitude: inverse of the Lyapunov index which characterizes the orbit instability. The Uncertainty Relation gives the corresponding resonance width which is proportional to the Planck constant. The more elaborate analysis is based on the parabolic equation method where the problem is effectively reduced to the multidimensional harmonic oscillator with the time-dependent frequency. The resonances form series in the complex energy plane which is equidistant in the direction perpendicular to the real axis. The applications of the general approach to various problems in atomic physics are briefly exposed.

1 Introduction

The quantum quasistationary states may be subdivided into three types (although these types are not absolutely independent): (*i*) the shape resonances which decay by penetration through some potential barrier; (*ii*) the Feshbach resonances, i.e. the quasibound states of the particle in the field of the excited core, for instance, the doubly excited states of the helium atom; (*iii*) the resonances related with the unstable periodic classical orbits. The latter type of resonances is probably the less known one. The peculiarities of the density of states, corresponding to the periodic orbit (or cycle), were analyzed by Gutzwiller [1] and by Balian and Bloch [2]. The role of such orbits is a subject of intensive discussion in the current literature.

The connection between the stable periodic classical orbit and the quantum mechanical eigenvalues is obvious from the physical point of view: such trajectories are similar to the effective channels in space along which the wavefunction is concentrated. The pioneer study of the problem by Gutzwiller [1] suffers a number of deficiencies. For instance, the Gutzwiller theory does not give true value for the total amount of quantum numbers labeling the state (in this case it should be equal to the dimensionality of the configurational space). This deficiencies were discussed by Miller [3]. However it seems that the most appropriate method to treat the problem is the parabolic equation approach developed initially in the theory of radio wave propagation (see e.g. the monograph by Babich and Buldyrev [4] and the discussion below in Sec.2). This method provides adequate basis for the description of the eigenfunctions which are localized at the vicinity of the periodic stable orbit.

The case of the unstable periodic classical orbit was not the subject of such a detailed study. In particular Voros [5] showed that the expansion of the density of states over the closed orbits due

to Gutzwiller [1] is not convergent and thus has not rigorous mathematical meaning. We do not discuss the problem on such a rigorous level and do not analyze the density of states expansion. Instead of it we consider only the relatively narrow resonances which can be well manifested in the physical observables. The resonances of this type are shown below to be related with the short-period long-living unstable orbits.

The natural characteristics of the classical orbit lifetime is the inverse of the Lyapunov index which is commonly used to describe the orbit instability. Thus in this case the concept of lifetime is introduced exclusively within the framework of classical mechanics without an appeal to the quantum tunneling and the channels interaction as in the case of the resonance types (*i*) and (*ii*). Namely this circumstance allows us to single out the third type of resonances in the classification introduced above.

The unstable orbits were discussed by Heller [6] who demonstrated that in the vicinity of the orbits the wavefunctions are enhanced and the 'scars' are formed on them. The explanation is obvious: the classical system stays long in this region. We show that the individual unstable orbit is naturally related with the whole series of resonances and give the simplified description of the wavefunctions. The complex eigenenergies representing the series form an equidistant pattern in the direction of the imaginary energy axis. The basic ideas of the present approach were outlined by the authors some times ago [7]. Here they are developed further and elucidated. Some recent applications to the problems of atomic physics are discussed.

2 Parabolic Equation Method

We start our analysis with the trivial comment. In the classical mechanics the particle with the energy close to the top of the potential barrier stays near the top for a long time. In quantum mechanics one can associate with the barrier top the series of 'eigenstates' with the imaginary energies (see also [8]). Indeed, consider the one- or two-dimensional *parabolic barrier*. In the first case the particle coordinate is x, in the second case the cylindrical radial coordinate is denoted as ρ. The stationary Schrödinger equation (for the particle with unit mass) is written respectively as

$$\left(-\frac{\hbar}{2}\frac{d^2}{dx^2} - \frac{1}{2}\alpha^2 x^2\right)\psi = E^{(1)}\psi \tag{1}$$

and

$$\left(-\frac{\hbar}{2}\triangle_2^2 + \mu L_3 - \frac{1}{2}\alpha^2\rho^2\right)\psi = E^{(2)}\psi, \tag{2}$$

where $\triangle_2$ is the two-dimensional Laplace operator, L_3 is the corresponding angular momentum operator, α and μ are the potential parameters. The substitution of new variables $(x', \rho') = (x', \rho')\exp(-i\pi/4)$ transforms the equations (1), (2) into these for the harmonic oscillators. Respectively, the wave functions containing only the outgoing waves in the asymptotes are transformed into the oscillator eigenstates. Thus if the equations (1), (2) are considered with the outgoing wave boundary condition, then the imaginary 'eigenvalues' are obtained:

$$E^{(1)} = -i\alpha\hbar\left(n + \frac{1}{2}\right), \qquad E^{(2)} = \mu\hbar m - i\hbar\alpha\left(2n + \mid m \mid + 1\right). \tag{3}$$

It should be stressed that the corresponding 'eigenstates' form the natural basis set for the description of the time-evolution of the wave packet which is localized initially near the barrier top (e.g., for $\psi(x)\ |_{t=0}= \exp(-\beta x^2)/(1+\gamma x^2\ )$ with some positive parameters β and γ). The imaginary part of the energy generally describes the short-time evolution of the wave packet and is not necessarily related with the true ionization process, i.e. escape to infinitely large distances (this situation is described by the notion *Diabatic Quasistaionary State* (DQS) introduced by the authors, see Ref.[7]).

The method of parabolic equation allows one to apply these simple formulae to the more general problem. Its essence is summarized below.

Consider the vicinity of the unstable orbit. One can introduce the natural local reference system at this region related with the trajectory. Let the system origin move with the particle along the unstable periodic orbit. The transversal coordinate axes q_i ($i = 1, 2, 3, \ldots N-1$; N is the dimensionality of the system configurational space) are directed normally to the orbit. The longitudinal coordinate s is the distance along the orbit. Let q_i be chosen so that $q_i = 0$ on the orbit. Since our subsequent consideration is confined to the orbit vicinity this definition is quite sufficient to our purposes. In these variables the system Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial s^2} + H_{tr}(p_i, q_i, s), \tag{4}$$

where M is the effective mass (we treat here the transition to the new curvilinear coordinates in somewhat simplified manner what is unimportant for the subsequent discussion). The transversal motion Hamiltonian H_{tr} contains momenta p_i conjugate to the transversal coordinates q_i. It includes also the periodic parametric dependence on the coordinate s.

In the framework of the parabolic equation method the motion along the longitudinal coordinate s is treated semiclassically. This implies the following representation of the wave function:

$$\psi(q_1, q_2, \cdots q_{n-1}, s) = v_{E_0}^{-1/2} \exp\left(iS_{E_0}(t)/\hbar\right) \varphi\left(q_1, q_2, \cdots q_{n-1}, t\right). \tag{5}$$

Here S_{E_0} and v_{E_0} are respectively the action ($\int pdq$) and the velocity for the classical motion along the trajectory for the energy E_0 ($v_{E_0} = M^{-1}dS_{E_0}/ds$). The new 'time' variable t is directly related with the longitudinal coordinate s: $v_{E_0}dt = ds$. Substituting the wave function (5) into the Schrodinger equation $(H-E)\psi = 0$ one obtains (in the lowest order in the Planck constant $\hbar$) the following equation for the function φ:

$$i\hbar\frac{\partial\varphi}{\partial t} = \left(H_{tr}(p_i, q_i, t) - H_{tr}(0, 0, t) - E + E_0\right)\varphi. \tag{6}$$

The latter equation has the mathematical form of the *non-stationary* (*parabolic*) Schrodinger equation with the *mock* 'time' variable t directly related to the coordinate s. Note that our treatment starts with the *stationary* Schrodinger equation. Therefore the *true* time does not appear here.

The rigorous formulation of the method based on the asymptotic (semiclassical type) techniques implies that the Hamiltonian of the non-stationary problem should be replaced by its approximation quadratic in the coordinates q_i. These statements present the essence of the parabolic equation method introduced originally by Leontovich and Fock [9] (see also Ref.[10]).

3 Quantization Conditions

The important point for the further development is that the Hamiltonian H_{tr} is periodic in 'time' t since the orbit is periodic. The natural way to treat such a problem is to consider the *quasienergetic or Floquet states* (see e.g. the review Ref. [11]). The latter is introduced so that after the period T the corresponding wave function acquires the phase factor which contains the quasi energy ϵ:

$$\psi(t+T) = \exp(i\epsilon T)\psi(t). \tag{7}$$

Let now choose the function φ to be the quasi energy state. After the passage over the periodic orbit the total wave function ψ (5) should remain unchanged. This gives the following quantization condition:

$$E - E_0 - \epsilon + S_{E_0}(T)/T = 2\pi n\hbar/T, \tag{8}$$

where T is the period of the orbit, n is an integer. Note that the parabolic equation method assumes naturally the semiclassical condition for the motion over s-coordinate: $S_{E_0}/\hbar \geq 1$.

Since we assume here the quadratic approximation for the Hamiltonian H_{tr}, then the non-stationary Schrodinger equation (6) describes the $(N-1)$-dimensional oscillator with the parameters depending on the 'time' t.

The quasi energy spectrum for the time-periodic quadratic (in the coordinates and the conjugated momenta) system was discussed in the monograph by Malkin and Man'ko [12]. Their study is based on the mathematically rigorous analysis by Sugiura [13] and Williamson [14]. Here we give only the list of the statements which seems to be quite appealing.

(*i*) In the case of quadratic time-dependent Hamiltonian the classical Hamilton equations are linear and coincide with the quantum Heizenberg equations for the momentum and coordinate operators $\hat{p}$ and $\hat{q}$.

(*ii*) Let the general solution of the classical equations to be known:

$$(p(t),\ q(t)) = \Lambda(t)(p(0),\ q(0)), \tag{9}$$

where $\Lambda(t)$ is the evolution matrix acting on the array of the system coordinates q and canonically conjugated momenta p. Then the solution of the Heizenberg equations takes the form

$$(\hat{p}(t),\ \hat{q}(t)) = \Lambda(t)(\hat{p}(0),\ \hat{q}(0)) \tag{10}$$

with the same evolution matrix.

(*iii*) For an arbitrary fixed t_0 one can find the *time-independent* quadratic (in the coordinates and momenta) Hamiltonian $H_{eff}^{(t_0)}$ which generates the same result for the system evolution at the time t as the initial *time-dependent* Hamiltonian. This implies that the exact time-evolution operator can be presented as $\exp(iH_{eff}^{(t_0)}t_0)$.

(*iv*) The matrix $\Lambda(t)$ which describes the system evolution over its period is called the monodromy matrix. The spectrum of the corresponding operator $H_{eff}^{(T)}$ coincides with the quasi energy spectrum. We should emphasize here that this operator must be considered as a continuous limit $(t \to T)$ of the operator $H_{eff}^{(t)}$. For instance, in the one-dimensional case the phase point in principle can perform several 2π-rotations around the origin which do not influence the monodromy

matrix. However this rotations should be taken into account in the construction of the operator $H_{eff}^{(T)}$.

Thus the problem of finding the quasi energies is reduced to the analysis of the spectrum of the monodromy matrix (we assume further that its eigenvalues are non-degenerate). Moreover, the eigenvalues of the monodromy matrix are essentially the exponents of the eigenvalues of some quadratic Hamiltonian. The latter does not necessarily correspond to the real *oscillator* since the case of the *quadratic potential barrier* also can be realized. The spectrum of such a barrier was discussed above at the beginning of the Section 2. Taking all these possibilities into account one finds that the following basic types of the eigenvalues sets are feasible (the most general description is given by Williamson [14]):

$$\exp(i\omega T), \tag{11}$$

$$\exp(\pm\alpha T), \tag{12}$$

$$\exp(\pm i\mu T \pm \alpha T). \tag{13}$$

The first one corresponds to the real oscillator with the frequency ω in the normal mode of the Hamiltonian $H_{eff}^{(T)}$ whereas the second and the third cases are related respectively with the parabolic barriers (1) and (2). Note that in (13) four various eigenvalues are contained according to various choice of the signs.

The parameter α in (12) and (13) coincides with the Lyapunov index which characterizes the instability of the classical periodic orbit in the linear approximation for the equations of motion. Indeed, the Lyapunov index is defined by the relation $q_i(T)/q_i(0) = \exp(\alpha T)$. According to the statement (*ii*) it is related with the description of the quantum system.

The eigenstates of the time-evolution operator coincide with those of the operator $H_{eff}^{(T)}$. One has to bear in mind that in the multidimensional system the eigenstates of each type can appear several times. In order to distinguish them we introduce below the lower indexes. The diagonalization of $H_{eff}^{(T)}$ generates the subdivision of the transversal coordinate subspace into the direct sum of the subspaces each of which corresponds to some set of the eigenvalues discussed above. The natural coordinate basis in each subspace is given by the normal coordinates. Depending on the type of the eigenvalue (see above) the quadratic Hamiltonian $H_{eff}^{(T)}$ in each subspace is of the oscillatory type (with some frequency ω_{j_1}, $j_1 = 1, 2, ...N_1$) or corresponds to the quadratic barrier described by Eq. (1) or (2) with the related parameters α_{j_2} ($j_2 = 1, 2, ...N_2$) in the case (1) or the parameters α_{j_3} and μ_{j_3} ($j_3 = 1, 2, ...N_3$) in the case (2). The lower indexes enumerate the eigenvalues. The total amount of the eigenvalues is $N_1 + N_2 + N_3 = N - 1$.

Taking into account the relation (7) we obtain the quasi energy spectrum of the system:

$$\epsilon(\{n\},\{m\}) = \sum_{j_1} \hbar\omega_{j_1}\left(n_{j_2} + \frac{1}{2}\right) - i\sum_{j_2} \hbar\alpha_{j_2}\left(n_{j_2} + \frac{1}{2}\right) + \\ + \sum_{j_3} \hbar\left(\omega_{j_3} m_{j_3} - i\alpha_{j_3}\left(2n_{j_3} + \mid m_{j_3} \mid +1\right)\right) \tag{14}$$

with some integer n_j ($n_j > 0$), m_j. The summation is performed over all eigenvalues described above. The eigenfunctions φ are expressed readily as the products of the Hermit functions of the normal coordinates.

Let us summarize the meaning of the quantum numbers. The quantum number n quantizes the motion along the periodic orbit. The quantum numbers n_{j_1} quantize the stable vibrational modes of the transversal motion whereas n_{j_2} and n_{j_3} are theirs analogs in the case of unstable transversal modes. The quantum number m_{j_3} are the azimuthal quantum number for the rotations in the plane locally perpendicular to the cycle.

We should emphasize that the total amount of the quantum numbers (including n, see (8)) coincides with the dimensionality of the configuration space. However, since the resonance series lie along the imaginary axis in the complex energy plane, this series is manifested in the experimental observations as one peak. Thus some of the quantum numbers prove to be 'hidden' and the amount of the 'observable' quantum numbers is effectively reduced.

4 Discussion

The formulae (8) and (14) contain the essence of the present paper. They are quite transparent from the physical point of view. Let the orbit energy E_0 be chosen to satisfy the semiclassical quantization condition for the motion along the periodic orbit:

$$S_{E_0} = 2\pi n\hbar. \tag{15}$$

Then from (8) we obtain

$$E = E_0 + \epsilon. \tag{16}$$

Thus the quantization problem is separated: first, the motion over the unstable cycle should be quantized according to Eq.(15) and, second, the motion over the transversal coordinates is quantized giving the quasi energy spectrum (14). The analogous equations were discussed by Miller [3] in the case of stable orbit. They reflects effective separation of variables in the vicinity of the cycle: the quantum number n is large but the other quantum numbers are small being incorporated into the quasi energy spectrum.

These formulae are also in close relation to the Gutzwiller formula for the density of levels in the two-dimensional case:

$$\rho(E) = \frac{T}{2\pi}\mathrm{Im}\sum_{n=1}^{\infty}\frac{}{\sinh(n\alpha T/2)}\exp(inS/\hbar). \tag{17}$$

This sum can be rearranged similarly to the Miller [3] paper:

$$\rho(E) = \frac{T}{2\pi}\mathrm{Im}\sum_{n=1}^{\infty}\left[1-\exp(-n\alpha T)\right]^{-1}\exp\left[n(iS/\hbar-\alpha T/2)\right] = \tag{18}$$

$$= \frac{T}{2\pi}\mathrm{Im}\sum_{m=0}^{\infty}\left[1-\exp\left(iS/\hbar-m\alpha\right)\right]^{-1}\exp\left[n(iS/\hbar-3\alpha T/2)\right].$$

Thus the density of states has the poles at the complex energies given by the equations (8) and (14) (since $S_E = S_{E_0} + (\partial S/\partial E)(E-E_0)$, $\partial S/\partial E = T$). However the expression (17) is not applicable in the complex energy plane. Moreover the expansion of the states density over the

periodic trajectories does not converge [5]. Therefore the proper description of the individual resonance states given in the present paper is essential.

Our principle qualitative conclusion is as follows. Since the unstable closed classical orbit can be characterized by some 'decay time' (namely, the inverse of Lyapunov index), the Uncertainty Relation gives the related resonance width which is linear in the Planck constant $\hbar$ (in contradistinction to the shape resonances where the width is exponentially small). Moreover whole resonance series correspond to the individual orbit with the resonances lying in the complex energy plane equidistantly on the line parallel to the imaginary axis (see formula (14)).

The first point to be stressed is that the quadratic approximation demands localization of the wave function in the vicinity of the orbit whereas the resonance functions constructed above do not satisfy this requirement since they rise exponentially in the case of the quadratic potential barrier. This contradiction is removed if one notices that the complex transformation of the transversal coordinates $q = q' \exp(i\pi/8)$ makes the eigenfunctions decreasing. The close analogy is traced here with the method of the complex rotation of the coordinates. This method of the resonance states calculation proves to be very efficient in the analysis of quite complex atomic systems [15]. The physical meaning of this states follows from theirs role in the description of the initially prepared wave packet (see discussion in the Sec.2).

The formula (14) implies that the quantum numbers n_j are not too large in order to confine the major part of the probability to the applicability domain of the quadratic approximation for the Hamiltonian H_{tr}. Nevertheless it is worth to stress that the resonances of this type generate series in the complex energy plane (in the quadratic approximation the series are equidistant in the direction of the imaginary energy axis). This constitutes the principle difference between the resonances discussed in the present paper and the shape or Feshbach resonances. In particular, this difference is manifested in the shape of the resonance profiles in the physical observables such as the cross sections, transition probabilities etc.

In principle the situation is feasible when the quadratic approximation is not applicable even for the lowest values of n_i ($n_i = 0$). This problem is not important for the general construction of the present theory since in fact its small parameter is the Planck constant (or inverse particle mass). However it can limit applicability of the theory to the concrete systems. If the quadratic approximation is dropped, then the theory is reduced to the description of the quasi energy states of the periodic Hamiltonian with the more general (non-quadratic) dependence on the coordinates. The practical realozation of this approach (see the next Section) gives good results.

5 Some Applications to Atomic Physics

In this Section some recent applications to the atomic physics are briefly discussed. We emphasize some modifications of the general scheme which are necessary in the concrete applications. The states of the atom in the uniform electric field serve in the text books as a typical example of the shape resonances. These resonances have negative energy and decay by the penetration of the potential barrier. The resonances exist also for positive energies where they have different origin being related with the unstable periodic classical trajectory. The electron moves between the atomic nucleus and the turning point against the force exerted on it by the uniform field. The calculations [16], [17] within the present approach demonstrate an excellent agreement with the accurate numerical data both for the resonance positions and widths.

For the motion of the electron in the field of two Coulomb centers the unstable classical trajectory also represents an interval of line. The calculations of the resonances were carried in this case by Du *et al* [18].

In the cited examples the resonance width corresponds to the true ionization (transitions to the continuum). An alternative situation appears for the helium atom where Klar [19] have found classical unstable equilibrium configurations (in which the electron-electron and electron-nucleus separations do not vary with time but the system rotates as a whole). Within the present approach these configurations are related [20] with the Rydberg series of broad resonances (doubly excited states) which are interpreted as DQS. Their widths describe not the transitions to the continuum (autoionization) but the interaction of the diabatic configurations.

The equilibrium electron configurations in the helium atom give an example of the correlated motion of the electrons which is not described by the effective central field approximation conventional in the theory of atoms. The description of the electron correlations is one of the fundamental problems in atomic physics.

The other example of the correlated electron motion appears in the study to the two-electron continuum states which are the final states in the electron impact ionization ((e, 2e) process) or double photoionization ((γ, 2e) process) of the atom. In the near-threshold domain the theory of the process was developed by Wannier [21] (see also the review by Read [22]). The physical idea is that the electrons fly apart from the core (with the charge Z) being at equal distances from it, i.e. at the so called Wannier ridge $r_1 = r_2$ ($\vec{r}_1$, $\vec{r}_2$ are the electron vectors relative to the atomic nucleus). Otherwise one of the electrons is decelerated and is captured into the high lying Rydberg state. Hence sliding off the Wannier ridge leads to the population of the one-electron continuum. For the double escape process this part of the flux is lost. In the framework of the present approach this is described in terms of the effective width and the whole double escape process is presented [23] as the system survival on the Wannier ridge.

Due to the Coulomb electron-electron repulsion the emission of the electrons in the opposite direction has the highest probability, i.e. $\theta_{12} \approx \pi$, where θ_{12} is the angle between $\vec{r}_1, \vec{r}_2$).

It is convenient to use collective hyperspherical coordinates: hyperradius $R = (r_1^2 + r_2^2)^{1/2}$ and hyperangle $\alpha_h = \tan(r_1/r_2)$. The Wannier treatment presumes two basic assumptions:

(*i*) The vicinity of the Wannier saddle configuration $\vec{r}_1 = -\vec{r}_2$ (i.e. $\alpha_h = \frac{1}{4}\pi$), $\theta_{12} = \pi$ is considered with the quadratic approximation in the variables $(\alpha_h - \frac{1}{2}\pi)$ and $(\pi - \theta_{12})$.

(*ii*) The motion over the hyperradius R is treated semiclassically.

The hyperradius R plays the role of the longitudinal coordinate s of the Sections 2, and $(\alpha_h - \frac{1}{4}\pi)$ and $(\pi - \theta_{12})$ are the transversal coordinates q_i. In the original Wannier theory [21], [22] the processes in the small-R region (inner zone, $R < R_0$) are not considered. They are replaced by some boundary condition on the border R_0 and the system evolution in the outer zone to the free electron motion regime ($R \to \infty$) is considered. Thus in contradistinction to the previous examples we do not have the *periodic* classical trajectory in this case. The basic trajectory corresponds to the double electron escape and terminates at $R \to \infty$.

The analysis of the *total* double escape cross sections within the present approach was carried out in Ref. [23]. Some special treatment is required to account for the electrons deceleration (as R increases) due to the Coulomb attraction to the residual core. This effect becomes crucial when the energy excess E above the double ionization threshold is small. The postadiabatic scheme was developed which allowed us to reproduce not only the Wannier power threshold law but also the

deviations from it for small but finite E.

In addition to the total double escape cross section the final electron distributions over the angles and energies is of great interest as a direct manifestation of the electron correlations. In a good approximation the angular coordinate θ_{12} is separated from the hyperangle α_h. Then the general scheme of the Sections 2 and 3 shows that the angular dependent wave function obeys [24], [25] the non-stationary Schrodinger equation for the harmonic oscillator with the time-dependent frequency (it is worth reiterating that the mock time is simply related with the longitudinal coordinate R). The final ($R \to \infty$) angular distributions depend crucially on the boundary (or initial) condition imposed on the border of the reaction zone. Although this point is completely obvious in the present formulation via the non-stationary harmonic oscillator (see also Ref. [26]), it was missed by the previous authors [27] who claimed that the Gaussian angular correlation pattern universally appear.

In the present approach the problem of the angular correlations is formulated in terms of the wave packet propagation from R_0 to $R \to \infty$. Some general features of the propagation can be established in the harmonic approximation for the problem under consideration [24], [25]. The more accurate scheme of the calculations drops the harmonic approximation. It incorporates the exact Coulomb interaction between the electrons and also the effective centrifugal potential which appears for the double continuum states with the non-zero orbital momentum L. The quantitative agreement with the experimental data is achieved along this way and a number of new qualitative features of the double escape process are revealed [28] - [30].

Acknowledgments

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