# RESONANT STATES IN THE PROPAGATION OF WAVES IN A PERIODIC , NON-LINEAR MEDIUM

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## A - CLASSICAL WAVES

Let us first consider a transparent linear medium where the refractive index is periodically modulated:

$$n^2 = k_0^2\left[1 + \varepsilon\, v\,(x)\right] \qquad \text{( in reduced units)}$$

where $v(x + l_0) = v(x)$ ( $l_0$ : modulation period). There exist unstable solutions of the wave equation in the gaps surrounding Bragg resonances. These resonances are defined by $\varphi = k_0\, a = n\, \pi$, $\varphi$ being the phase shift of the wave over $l_0$.

In the case considered in this first part, the modulation is harmonic ($v(x) = 2 \cos 2x$), and the gap associated with first Bragg resonance is defined by : $k_0^2 \in \left[k_-^2 , k_+^2\right]$, where $k_\pm^2 = 1 \pm \varepsilon$

Let us now add a non linearity (due to Kerr effect). Then : $n^2 = k_0{}^2 + 2\varepsilon \cos 2x + |\,\phi|^2$ $\phi$ being the wave amplitude. We first look for stationary (monochromatic) solutions of the wave equation $(\partial_x^2 - n^2 \partial_\tau^2)\, \phi = 0$, that is of the form $\phi = \phi(x)\, e^{i\tau}$ $(\tau = \omega_0\, t)$.

The problem is conveniently studied (3,4) with the help of the Poincaré map for variables $X_j = \phi\,(j\,\pi)$ , $Y_j = (d/dx)\, \phi\,(j\pi)$ (the modulation period $l_0$ is here equal to $\pi$).

It appears that the mapping

$$\begin{pmatrix} X_{j+1} \\ Y_{j+1} \end{pmatrix} = \begin{pmatrix} f(X_j, Y_j) \\ g(X_j, Y_j) \end{pmatrix}$$

is non integrable. The fondamental bifurcations of this dynamical system are the Arnold strong resonances : $\varphi = 2\pi/n$ $(n = 1,2,3,4)$, where $\varphi$ is the rotation number around the origin (which is also the wave phase shift over one period). We note that two of these values ($n = 1,2$) coïncide with Bragg resonances.

n = 1 resonance ($\varphi = 2\pi$ : 2nd Bragg order). We obtain the following bifurcation diagram :

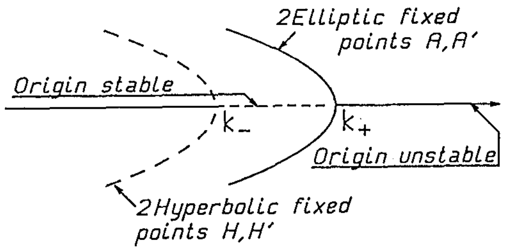


Fig.1 Bifurcation diagram for n=1 resonance

Neighborhood of $k_+$ : $k_0^2 = k_+^2 - \eta$. The origin is unstable inside the gap, and the phase portrait has the following form :

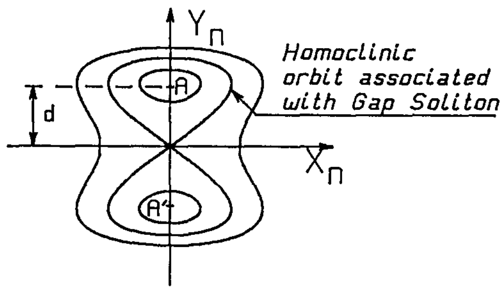


Fig.2 Phase portrait inside the gap

The two homoclinic orbits are associated with the celebrated gap solitons(1,2,3,4), which are immobile localized structures. The distance d of elliptic fixed points to the origin, which is a measure of the soliton amplitude, goes to zero when $\eta \to 0$. The non integrability of the mapping manifests itself by the stochastic behavior of the orbits near the origin. As a consequence, one-peak solitonic solutions are not allowed in large systems. Indeed the orbit points always escape from the origin after a finite number of iterations. Therefore the solutions are multi-peaks, with random inter-peak distances $l_i$, the average $l = \langle l_i \rangle$ diverging when $\eta \to 0$ like $\eta^{-\nu}$. The critical exponent is found to be $\nu \approx 1.4$.

When $\eta \to 0$ the rotation number around A or A' goes to zero and the mapping becomes integrable (or close to an integrable one). Then it can be shown that the soliton amplitude A obeys an ODE of the form :

$$\frac{d^2 A}{dy^2} - A + |A|^2 A = 0 \qquad (1)$$

y being a large-scale spatial variable. Eq. (1) admits a solution of the NLS type.

Neighborhood of $k_-$ : $k_0^2 = k_-^2 - \eta$ . The origin is now stable (we are outside the gap) and the phase portrait has the following form :

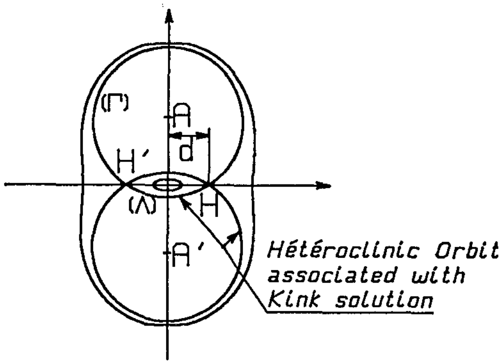


Fig.3 Phase portrait for $k_0^2 = k_-^2 - \eta$

It appears, in addition to elliptic points A, A'(which are now at finite distance from the origin), two hyperbolic points H, H' whose distance d to origin goes to zero as $\eta \to 0$. The finite amplitude orbit (Γ) is strongly chaotic. On the contrary the small orbit (Λ) is "nearly integrable" and is associated with a kink-like solution.

n = 2 resonance (1st Bragg order). The phenomena are exactly the same, except that the sign of wave function changes after each period. We therefore call "alternate" the solitons and kinks obtained in this case.

n = 4 resonance ($\varphi = \pi/2$). This resonance occurs exactly in the middle of the transparence band. The bifurcation of the mapping around the origin (which is elliptic) generates a set of 4 fixed elliptic points and 4 hyperbolic points, and the union of heteroclinic orbits is a set of two entangled ellipses.

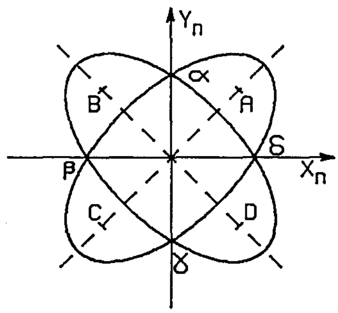


Fig 4 Phase portrait for n=4 . The "square structure".

We have called this configuration a " square".

<u>n = 3 resonance</u> ($\varphi = 2\pi/3$)

Here the bifurcation of the origin does not generates a strong resonance, because of the symmetry of the model (the non linearity is cubic). It would if some physical effect could break this symmetry, introducing a quadratic non linearity. In the present case this resonance can occur around an another elliptic fixed point of the mapping. We show on Fig.(5) this bifurcation around one of the fixed points of period-4 cycle considered above .

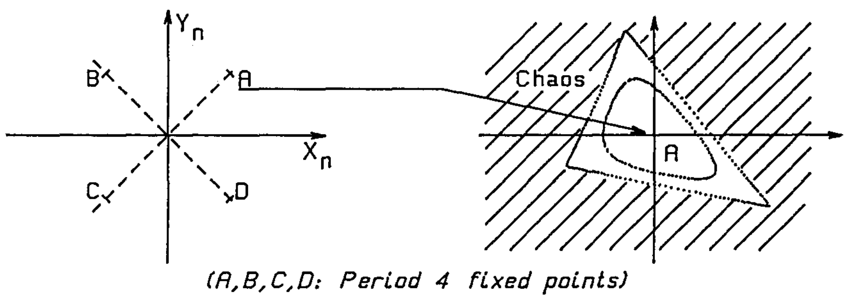


Fig 5 Resonance n=3. Phase portrait around a fixed point of the previous period-4 cycle.

The limit orbits form a curved triangle (we called "triangle" this new localized structure), and one observes that the orbits are strongly chaotic outside this triangle.

## Unstationnary regimes

Considering now the propagation of a narrow wave packet around frequency $\omega_0$, we have shown[5] that there exist solitonic solutions near the bifurcation points ($k_0^2 = k_+^2 - \eta$) which (for resonances n = 1, 2) take the form :

$\phi(x,t) \sim A \sin x \, e^{i\tau} + c.c.$

where A obeys the "slow" wave equation :

$$( i\,\partial_{\tau'} + \partial_y{}^2 )\, A - A + |A|^2 A = 0 \qquad (2)$$

where y, $\tau'$ are an appropriate large scale variables.

Eq. (2) is isomorphic to NLS equation through gauge transformation $A \rightarrow A\, e^{-i\tau'}$. Rather unexpectedly the gap solitons are of the NLS type (near the bifurcation point). Their amplitude a is small and they propagate at low velocity v. Quantities a, v and $\eta$ are related through the relation :

$$\alpha\, a^2 + \beta\, v^2 = \gamma\, \eta \qquad (3)$$

$\alpha, \beta, \gamma$ being numerical coefficients.

Concerning the square and triangle structures, a numerical study of the time-dependent problem have been made(6) showing that they are unstable, leading to chaotic regimes.

## B - RESONANT POLARONIC STATES ON A 1-D PERIODIC CHAIN(7)

We consider the interaction of a periodic chain of atoms with one unbounded electron. The atoms are considered as classical scatterers ( we neglect their quantum fluctuations in the limit of very large mass). The interaction potential of the electron with the $n^{th}$ atom at position $x_n$ is $- V ( x - x_n)$, and the elastic energy of the atomic chain is : $\frac{\kappa_o^2}{2} \sum_n (x_{n+1} - x_n)^2$.

The interaction couples the $x_n$'s and the electronic wave function $\phi$ ( x,t), and this coupling may be described by the Ehrenfest equations obeyed by the atoms variables. In the classical limit, and neglecting the inertia of the atoms, one obtains :

$$\kappa_0^2\, (u_n - u_{n-1}) = - \langle V'\,(x - x_n) \rangle \qquad (4)$$

where $u_n = x_{n+1} - x_n$ and $\langle\,\rangle$ means the quantum average with respect to $\phi$.

The functional dependence of the $x_n$'s on $\phi$ makes the Schrödinger equation

$$i\hbar\, \partial_t \phi = - \left\{ \frac{\hbar^2}{2m}\, \partial_x{}^2 + \sum_n V(x - x_n) \right\} \phi \qquad (5)$$

non linear. Solving Eqs.(4,5) amounts to study the propagation of the electronic wave on the nearly periodic atomic chain. The role of non linear Kerr effect in the previous problem is played here by the lattice deformation induced by the electron-lattice interaction.

In the simplest version of the model, V is taken $\delta$ - like :

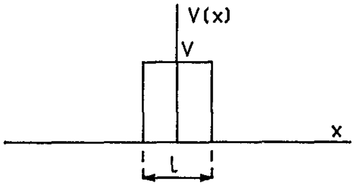


Fig 6 Shape of the interaction potential

with $V \rightarrow \infty$ and $l \rightarrow 0$ with $Vl \rightarrow \varepsilon$ finite. The Poincaré map connecting the fields over one period is for a stationary solution, ($\phi = \phi(x)\, e^{(i/\hbar)\, Et}$) :

$$\begin{pmatrix} X_{n+1} \\ Y_{n+1} \end{pmatrix} = \frac{1}{\cos\mu} \begin{pmatrix} \cos\theta_n & \sin(\theta_n - \mu) \\ -\sin(\theta_n + \mu) & \cos\theta_n \end{pmatrix} \begin{pmatrix} X_n \\ Y_n \end{pmatrix}$$

$$\theta_{n+1} = \theta_n - \lambda\,(X_{n+1} Y^*_{n+1} + \text{c.c.})$$

where $$E = \frac{\hbar^2 k^2}{2m}, \quad \theta_n = k\, u_n + \mu, \quad \text{tg}\, \mu = \frac{\varepsilon}{2k}$$

$$X_n = \phi_n, \quad Y_n = \frac{\cos\mu}{k} \frac{d\phi_n}{dx}, \quad \lambda = \frac{2k^3 \sin\mu}{\cos^2\mu}$$

This mapping is conservative in (X, Y, $\theta$) space, and it defines a non integrable dynamical system, whose qualitative properties are remarkably similar to those of the previous classical one. In particular it yields the same localized structures near the Arnold resonances, and these structures look like resonant polaronic states. However there is an additional constraint : the wave function must be normalized.

We shall briefly consider resonances $\theta = \pi/2$ and $\{\theta = 0, \pi\}$.

$\theta = \pi/2$ resonance. The two first equations of the mapping reduce to :

$$\begin{pmatrix} X_{n+1} \\ Y_{n+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} X_n \\ Y_n \end{pmatrix}$$

showing that $X_{n+1} Y_{n+1} = - X_n Y_n$. Therefore the $u_n$'s are of the form $(-1)^n \alpha$ ( $\alpha$ slow variable ).

Again the system becomes integrable near the bifurcation point (the mapping reducing to an integrable set of 3 ODE). And again the limit orbits produce the set of two entangled ellipses, as in the classical problem. It must be noted that these solutions cannot be normalized in an infinite system. Indeed we find that

$$X_n \sim \left[1 - \tanh^2(\nu n)\right]^{1/2}, \quad Y_n \sim \tanh(\nu n)\left[1 + \tan h^2(\nu n)\right]^{-1/2}$$

where $\nu \approx k\, l_o - (\pi/2)$. ($l_o$ : lattice period). The graphs of Xn and Yn are sketched on Fig.(7).

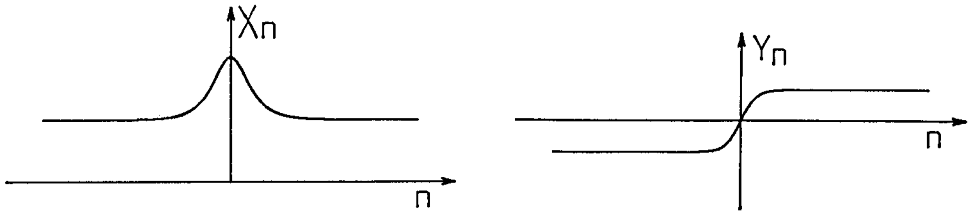


Fig 7 Graphs of Xn and Yn .

It is interesting to note that this resonant state corresponds to those found in acetylenic polymers. The Fermi wave number for these half filled band systems corresponds to $\theta_F = k_F l_0 = \pi/2$ and one finds a ground states resulting from Peierls condensation ( see Ref.(8) ). This state is doubly degenerate (states A,B) and their exists a "solitonic structure" connecting A and B along the chain. Our "square structure" has clearly the same form. And indeed we are treating here a one electron version of the polymer problem, the electron wave number being equal to $k_F$.

<u>Resonances $\theta = 0, \pi$</u>

$\theta = \pi$ yields an "alternate soliton"

$\theta = 0$ yields an "non alternate soliton"

Let us consider the case $\theta = \pi$.

Putting $(\xi_n, \eta_n) = (-1)^n (X_n, Y_n)$, we obtain for $\theta = \pi$

$$\begin{pmatrix} \xi_{n+1} \\ \eta_{n+1} \end{pmatrix} = \frac{1}{\cos\mu} \begin{pmatrix} 1 & 0 \\ 2\sin\mu & 1 \end{pmatrix} \begin{pmatrix} \xi_n \\ \eta_n \end{pmatrix}$$

and the eigen values $s_{\alpha,\beta}$ of the linearized map around $\theta = \pi$, obey equation :

$$s^2 + 2\frac{\cos\theta}{\cos\mu} s + 1 = 0$$

This permits to define a gap, or forbidden band by $k_0 l \in [\pi - \mu, \pi + \mu]$.

The mapping becomes integrable near the bifurcation point giving a solitonic solution, and we are also able to treat the unstationary problem. We then obtain propagative solitons obeying equation

$$\left(\frac{2\,im}{\hbar}\partial_t + \partial_x{}^2\right)\eta - 2\,\mathrm{tg}\,\mu\left[\delta - \frac{\lambda}{2\sin\mu}|\eta|^2\right]\eta = 0 \qquad (6)$$

when $\delta = k\, l_0 - (\pi + \mu)$.

Eq. (6) has solitonic solutions of the form :

$$\eta \sim a\,\mathrm{sech}\,[a\,(x - wt)]\, e^{(i\pi \frac{w}{w_0}(x - wt))}$$

where $w_0 = \hbar\,\pi / l_0$ and :

$$a^2 + \left(\frac{\pi w}{w_0}\right)^2 = 2\,\delta\,\mathrm{tg}\,\mu \qquad (7)$$

Finally we normalize $\phi$, which implies : $a = \frac{\pi^3}{2}\,\mathrm{tg}\,\mu\,\left(\frac{m w_0^2}{M c_s^2}\right)$

(M atomic mass, $c_S$ phonon velocity at k = 0).

Then the energy of the soliton can be written, with the help of relation (7) as :

$$E_s = E_0 + \frac{1}{2} m^* w^2 \text{ , with } m^* = -\frac{2\pi^2}{\varepsilon\, l_0}\, m_e \quad (m_e \text{ electron mass}).$$

It is worth remarking that the theory can be extended to the case of potential peaks with finite width and amplitude. Then $m^*$ may be of the same order of magnitude as $m_e$.

In the case of the $\theta = 0$ resonance, all goes along similar lines. The only differences are that the soliton is of the non alternate type, and $m^* \approx m_e$.

## References


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