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LETTER TO THE EDITOR

Resonant tunnelling through a nonlinear electrified chain

Ernesto Cota†, Jorge V José‡ and Guillermo Monsivais§

† Laboratorio de Ensenada, Instituto de Fisica, Universidad Nacional de México, Apdo Postal 2681, Ensenada BC, Mexico

‡ Physics Department, Northeastern University, Boston, MA 02115, USA

§ Instituto de Fisica, Universidad Nacional de México, Apdo Postal 20-364, 01000 Mexico DF

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Abstract. A study of electronic scattering from a nonlinear Schrödinger equation in a one-dimensional periodic chain in the presence of an applied electric field is presented. The scattering properties are measured as a function of the strength of the nonlinear cubic term, α. The stability, shapes and lifetimes of the *Stark ladder resonances*, present in the linear system, are studied as a function of α. It is found that these quantities are significantly modified by the nonlinearities, much more so for $\alpha > 0$ than for $\alpha < 0$.

The *resonant tunnelling* of an electronic wave through a series of potential barriers is a basic phenomenon in quantum mechanics (QM). This resonant tunnelling is essential in the understanding of transport properties in artificially fabricated superlattices, cf [1]. The transmission properties of the scattered electronic waves depend crucially on the linear superposition principle, of fundamental importance in QM. Recently, the transmission problem has been studied in the case where the underlying equation is nonlinear [2–5]. Delyon *et al* studied the band structure of the NLSE, in the tight-binding approximation, in one dimension [2]. Their work has been extended and clarified by various authors [3–5]. Using the elements of the theory of dynamical systems, as applied to the resulting nonlinear maps, these studies have mostly been directed at understanding the band structure and wavefunction properties of the model. The fundamental question of how the standard QM resonances get modified by the nonlinearities was not considered. To study this question we study the effects of nonlinearities on the nature and structure of the Stark ladder resonances (SLR), as a function of the nonlinearity parameter α. The nonlinearity considered in this letter is that of the nonlinear Schrödinger equation (NLSE). This type of nonlinearity has been studied extensively as a prototype in nonlinear studies. The model arises in many fields of physics. In electronic systems it would correspond to a Hartree type of density self-interaction; in superconductors to the Ginzburg–Landau equation; in superfluids to the Gross–Pitaievsky equation and in studies of nonlinear optics. The SLR have been studied extensively, theoretically [6–8], and evidence of their existence has been found recently experimentally in semiconductor superlattices [9] via the photoinjection of electron–hole pairs. The SLR, for particular parameter values, are characterized by being isolated and well approximated by Lorentzian lineshapes. As a function of the energy E they are separated by a distance $\Delta E = NFa$, where N is an integer, a the lattice spacing, $F = e\mathscr{E}$ with e the charge, and $\mathscr{E}$ the externally applied electric field. The resonances have a width at half maximum, Γ, that changes as function of F like $\Gamma = A\,\mathrm{e}^{-B/F}$, with B and A constants dependent on the form of the potential [6, 7]. This essential singularity in Γ appears because of Zener tunnelling between bands which is crucial in order to provide a full understanding of the SLR in the linear case. We describe below the modifications to the SLR produced by the self-interactions which lead to the nonlinear problem. Since most of the quantities calculated here are evaluated outside of the nonlinear region we can make use of the standard probes from scattering theory to ascertain the modifications introduced by the nonlinearities. The model studied in this letter is defined by the NLSE

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\sum_{n=0}^{N}(\delta(x-n)(\beta+\alpha|\Psi(x)|^2))-Fx\right]\Psi(x)=E\Psi(x). \tag{1}$$

Here $\Psi(x)$ is the single particle wavefunction at x, and we are taking atomic units with $\hbar^2/2m = 1$, with n an integer and a the lattice spacing fixed to one henceforth. The periodic δ-function potential of strength β, corresponds to the standard Kronig–Penney model. The nonlinear interaction is of δ-function type and with strength α. This means that the electron propagates freely between lattice sites and interacts only at $x = n$. The advantage of this choice is that one can solve the continuous NLSE exactly between lattice sites and it thus allows for a thorough analysis of the problem. We do not expect that this assumption will change the general nature of the results. This form for the nonlinear term has been considered previously by Grabowsky and Hawrylak in the zero-field case [5]. Their justification for this model invokes having a superlattice with periodic, very thin, inclusions of a nonlinear material that can produce the localized form of the nonlinearity. Note that the nature of the solutions to the nonlinear continuous equation is qualitatively different if the k-space is bounded (the tight-binding approximation) than if it is unbounded (including all the bands). Here we consider the continuous NLSE which entails including all the bands in the analysis of the model.

The problem studied here assumes a region $0<x<L$ where $\alpha, \beta \neq 0$, and $\alpha, \beta = 0$ for $x \leqslant 0$ and $x \geqslant L$. The transmission problem considers an incident wave at $x = L$ with $\Psi(x) = r_0\,\mathrm{e}^{-\mathrm{i}k_L(x-L)} + r_1\,\mathrm{e}^{\mathrm{i}k_L(x-L)}$, for $x \geqslant L$, and a transmitted wave $\Psi(x) = t\,\mathrm{e}^{-\mathrm{i}k_{-1}x}$ for $x \leqslant 0$, where $k_L = \sqrt{E+FL}$, and $k_{-1} = \sqrt{E}$ are the wavevectors at $x = L$ and $x = -1$, respectively. The energy E is measured from the top of the electric field ramp. The usual treatment of a scattering problem consists of finding the reflected and transmitted amplitudes, r_1 and t, in terms of the incident amplitude r_0 and E. Since the superposition principle is no longer valid in the nonlinear case, t is not uniquely defined by r_0. What has been done by previous authors [2–5] is to invert the problem by fixing the output t and then calculating the input r_0. In this case the problem is uniquely defined. The transmission and reflection coefficients are then given by $T = (k_{-1}/k_L)|t/r_0|^2$, and $R = |r_1/r_0|^2$, respectively. Current conservation remains valid so that $T + R = 1$. In order to calculate T as a function of E we solve the NLSE in terms of its exact Poincaré map between lattice sites, following a technique similar to that used in the linear case [7]. The effect of the electric field is approximated by a step potential which has been shown to be a good representation of the linear electric field potential. The wavefunctions between lattice sites are then plane waves of the form $\Psi_n = A_n\,\mathrm{e}^{\mathrm{i}k_n x} + B_n\,\mathrm{e}^{-\mathrm{i}k_n x}$, where the nth momentum in the nth cell, $n < x < (n+1)$, is given by $k_n = \sqrt{E+Fn}$. Using the continuity conditions for the wavefunction and its derivative at each lattice site we obtain the nonlinear map,

$$\Psi_{n+1}=\left(\cos(k_n)+\frac{k_{n-1}\sin(k_n)}{k_n\sin(k_{n-1})}\cos(k_{n-1})+(\beta+\alpha|\Psi_n|^2)\frac{\sin(k_n)}{k_n}\right)\Psi_n - \left(\frac{k_{n-1}\sin(k_n)}{k_n\sin(k_{n-1})}\right)\Psi_{n-1}. \tag{2}$$

Fixing the output to $|t|^2=1$ we vary α, noting that what matters is the product of $|t|^2$ and α. The input is then obtained from the equation,

$$r_0=t\frac{(\Psi_{L+1}-e^{-ik_L L}\Psi_{L+2})}{(e^{2ik_L L}-1)}. \tag{3}$$

In figure 1 we show the transmission coefficient as well as its contour plot as a function of E and α, for α within the range $\alpha\in[-0.2, 0.2]$, and $E\in[118, 122]$. We have chosen this region of energy so that a small number of SLR in the $\alpha=0$ case are well defined. We note a clear difference between the $\alpha>0$ and $\alpha<0$ regions. When $\alpha<0$, Γ increases so that for values of $\alpha\leqslant-0.4$, not shown in the figure, the nonlinear Stark ladder resonances (NSLR) overlap to an extent that they are no longer well defined. In contrast, for $\alpha>0$ the NSLR remain clearly separated with Γ decreasing as α increases while at the same time the lineshape is no longer Lorentzian. We can still identify $1/\Gamma$ with a transit time across the nonlinear region, as is usual in the linear case; thus for $\alpha>0$ the transit time increases while for $\alpha<0$ it decreases. The contour plot in figure 1 shows that for $\alpha<0$ the separation between the maxima in T is still well approximated by the Wannier or SLR condition, while for $\alpha>0$, even for relatively small values of α, this is no longer true. A qualitative understanding of the physics contained in figure 1 comes from considering the competition between the different terms in equations (1) and (2). When $\alpha=0$ the appearance of the SLR is due to the localizing effect of the electric field. To understand what goes on in this case one can use the Zener tilted

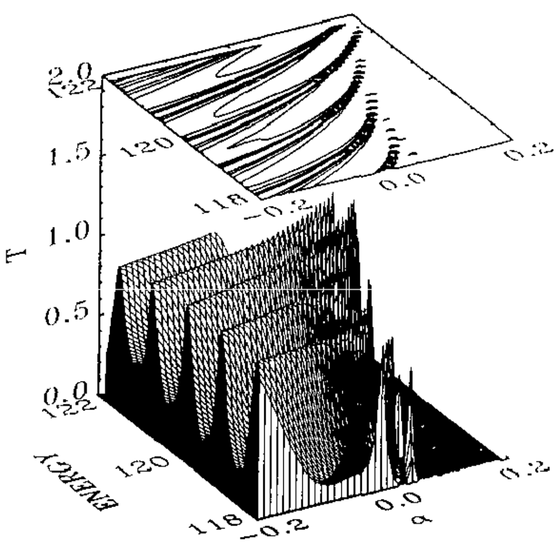

Figure 1. Transmission coefficient T as a function of energy and α for $L=100$, $F=0.8$. The contour plot corresponds to the projection of T onto the E versus α plane.

band picture and semiclassical quantization considerations. In equation (2) ($\alpha = 0$) we have a complex map in terms of which the SLR can be understood as a family of quasiperiodic orbits with frequencies given by the Wannier conditions. When $\alpha \neq 0$, the map is nonlinear with an unbounded phase space, and the nonlinearity also has a localizing effect on the solutions. The sign of α is crucial since the effective quartic potential in Ψ, given in equation (1), has different stability properties if $\alpha > 0$ than if $\alpha < 0$. For $\alpha > 0$ there are quasiperiodic as well as chaotically diverging orbits [4]. For $\alpha \geqslant \alpha_c(E, F)$, the orbits are chaotic with divergent r_0, so that T becomes extremely small (in our calculations we set the lower bound of $T \leqslant 10^{-10}$), so that all the Ψ solutions will be localized by the nonlinearity. By contrast for $\alpha < 0$ the Ψ solutions become more extended as α decreases in value. We note that the map $(\Psi_{n+1}, \Psi_n) = M(\Psi_n, \Psi_{n-1})$ in this case is much more complicated than in the $F = 0$ case [4] since the matrix M is an explicit function of n, thus making the stability analysis of the map more complex.

We now describe the NSLR in terms of their lineshapes and phaseshift properties. In figure 2 we show results for T and $d\theta_r/dE$ as a function of E for three cases, (a) $\alpha = 0$, (b) $\alpha = 0.06$ and (c) $\alpha = -0.15$. Here θ_r is defined from $r_1(E) = |r_1|\,e^{i\theta_r}$. The calculations of $d\theta_r/dE$ were carried out by iterating simultaneously two Poincaré maps, one for Ψ_n and the other for $d\Psi_n/dE$, obtained from taking the E derivative of equation (2). Because we evaluate $d\theta_r/dE$ in the region where the equations are linear we can assume that it is directly related to the transit time as in the linear case. Figure 2(a) shows well defined SLR with the expected behaviour for $d\theta_r/dE$, in accordance with linear scattering theory. As also seen in figure 1 for $\alpha > 0$, although less clearly, figure 2(b) shows lineshapes of isolated resonances clearly of non-Lorentzian forms. In the energy range considered we note that the two SLR for $\alpha = 0$ have become almost four. As seen in the contour plot this is so because the separation distance between NSLR decreases as α increases. We note that the zero values in T in figure 2(b) are purely generated by the nonlinearity. Since the NSLR are still isolated, one can approximate the nth NSLR by an energy-dependent complex pole of the analytic

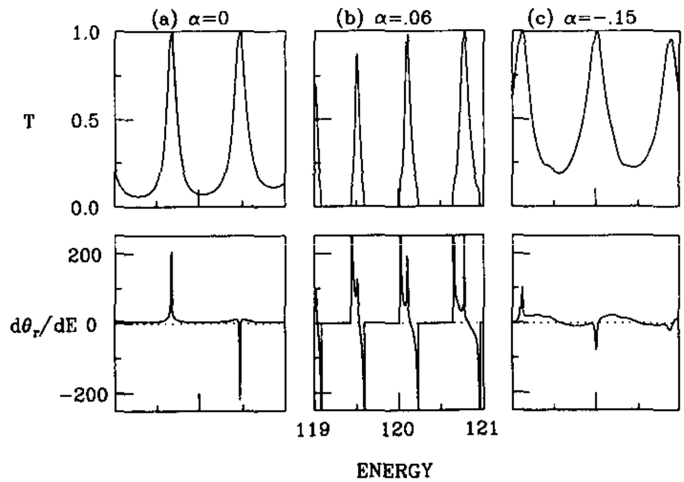

Figure 2. Transmission coefficient T and phaseshift derivative $d\theta_r/dE$ for three cases: (a) $\alpha = 0.0$, (b) $\alpha = 0.06$ and (c) $\alpha = -0.15$. The energy scale shown in (b) from 119–121 is the same in (a) and (c).

continuation of the resolvent operator to the non-physical sheet, as discussed in [8]. The pole has real and imaginary components, $\varepsilon(E)$ and $\Gamma_n(E)$ respectively. These quantities can be calculated in principle by perturbation theory. We observe from our calculations that close to a NSLR, for α small and positive, some of the resonances do not have the usual quadratic maximum but instead it is linear. This difference may have important consequences in the analysis of the resonant lineshapes. Furthermore, in contrast to the linear case we note extra peaks in figure 2(*b*) that appear in the wings of the lineshapes. This result shows that, as may have been expected, the connection between resonant states as detected by the maxima of T, and maxima in the derivatives of θ_r, known as Levinson's theorem in the linear case, does not hold in the nonlinear one. In figure 2(*c*) three NSLR for $\alpha = -0.15$ are shown. The lineshapes of these resonances look like standard resonances with a background larger than in figure 2(*a*). One could then assume that the properties of these resonances should be similar to those given in 2(*a*). That this is not so is evident from the result for $\mathrm{d}\theta_r/\mathrm{d}E$ which shows small peaks at positions where T has maxima. However, we have increased the number of points in the energy mesh and have found that those peaks are as small as shown and do not represent real resonances of the type shown in figure 2(*a*). A clear conclusion from the results presented in the figures is that the nonlinearities do modify singificantly the behaviour of the SLR and that the changes are strongly dependent on the sign of α.

The discussion of the results presented above has been qualitative. We now give a series of comparative quantitative results between the linear and nonlinear cases. In table 1 we list the results for the average energy separations of the maxima of T for different values of α as well as their half widths at half maximum, $\langle\Gamma\rangle_\alpha$, where the bracket represents an average taken with respect to a given set of NSLR, within a given energy interval and for a given value of α. As in the linear case, and for the parameters considered, we find that we can fit the results to the form $\langle\Gamma\rangle_\alpha = A_\alpha\,\mathrm{e}^{-B_\alpha/F}$. As shown in table 1 B_α decreases as α (<0) decreases while it increases as $\alpha>0$ increases. In the table we show results for $\langle\Delta E\rangle_\alpha$ to check the effect of nonlinearity on the Wannier condition. It is seen that varying α does change the linear condition $\langle\Delta E\rangle = NF$ somewhat for the parameter values considered. Note that as $\alpha(>0)$ first increases $\langle\Delta E\rangle_\alpha$ increases while for larger α it decreases singificantly as seen in the contour plot. For $\alpha<0$ the tendency is also to reduce $\langle\Delta E\rangle_\alpha$ as $\alpha<0$ decreases. A study of

Table 1. Results for the resonance averages of $\langle\Gamma\rangle_\alpha = A_\alpha\,\mathrm{e}^{-B_\alpha/F}$ and $\langle\Delta E\rangle_\alpha$, for α positive and negative. Here $L=100$, $\beta=2$ and $F=0.8$.

			$\alpha<0$		
α	0.0	−0.01	−0.02	−0.03	−0.04
A	0.470	0.4701	0.364	0.380	0.321
B	2.054	2.026	1.899	1.888	1.808
$\langle\Delta E\rangle_\alpha$	0.7986	0.7968	0.7959	0.7938	0.7924
			$\alpha>0$		
α	0.0	0.01	0.02	0.03	0.04
A	0.470	0.503	0.556	0.656	0.764
B	2.054	2.115	2.195	2.319	2.455
$\langle\Delta E\rangle_\alpha$	0.7986	0.8017	0.8036	0.8074	0.8134

the L dependence of the results mentioned above was also carried out. We found that within the interval $100 \leqslant L \leqslant 140$, the essential features of the results remain unchanged.

In conclusion, we have presented a study of the effects of nonlinearities on the stability of quantum mechanical resonances. We have taken as an example the SLR within the context of the NLSE with strength α. We found that the nonlinearities, or interactions, modify the nature of the SLR significantly, much more so for $\alpha > 0$ than for $\alpha < 0$. The transit times through the nonlinear medium were discussed and found to increase for $\alpha > 0$ and decrease for $\alpha < 0$. Of importance is that the lineshape of the resonances is no longer Lorentzian, more so for $\alpha > 0$ than in the $\alpha < 0$ case. A detailed discussion and further extensions of the results presented here will be reported elsewhere [10].

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