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Vortex Solitons in Poly-Acetylene

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Abstract: ***Solitons in Poly-Acetylene have been both predicted theoretically and found experimentally. However as is shown in this paper Vortex Soliton solutions are also possible. One feature of the Vortex solutions is that a small change in the parameters (bond angles) induces a large change in the interaction potential. This induces extended discontinuities in the wave vector space of the system. A large block of states are even absent due to the presence of vortices. A depleted number of states is thus forced to accommodate the original number of spins and charges in the system. The only way this is possible that two spins pair up to form a spin less charged Vortex. As a result vortices may be with spin or without spin and also with or without charge. This phenomenon is confirmed via numerical simulations on Poly-Acetylene.***

Keywords: Poly-Acetylene, Nonlinear optical lattice, vortex Solitons, Sine-Gordon Equation, DNLS.

1. Introduction

Solitons in conducting polymers have been attracting considerable attention in recent years [21]. In these conducting polymers, Poly-acetylene is a particularly important example. Each carbon atom in a pure trans-polyacetylene contributes only a single $p\pi$ electron, and π band is only half full.

It was recognized that in addition to electron and hole excitations in such a dimerized chain a new type of excitation could exist: namely, a domain wall separating regions of different bonding structure. In view of the fact that the domain wall is a nonlinear shape preserving excitation which propagates freely, it has been called a soliton. To determine the shape of the soliton calculations were carried out by Su, Schrieffer and Heeger. The dynamics of the Solitons is given by the non linear Schrodinger equation. We note that the nonlinear Schrodinger equation also describes the dynamics in the non linear optical lattice. Hence we consider the dynamics of the nonlinear optical lattices in BEC. However we note that our results of spin charge separation are valid for both Bose Einstein condensates and Poly-acetylene.

Bose Einstein Condensation (BEC) has been both predicted and observed in harmonic oscillator potentials [11]. Nonlinear optical lattices have been known to simulate BEC [14]. It is therefore natural to assume a harmonic potential at each site of the nonlinear optical lattice. Further, Solitons have been predicted [9] and observed [6] in these lattices. We know from the seminal work of Krumhansl and Schrieffer [7] that a double well potential gives rise to domain wall Solitons. Since domain wall Solitons are indeed observed [15] in nonlinear optical lattices we suggest that a double well potential may model nonlinear optical lattices. Using the double well model for coupled nonlinear optical lattices we obtain Soliton solutions for one and higher dimensions. For the one dimensional lattice we find domain wall Solitons which induce lattice compression, which have been observed experimentally [2].

Recently in the seminal paper of H. Sakaguchi and B.A Malomed [5] the Lagrangian corresponding to the Gross –Pitaevskii equation was derived. The potential in the Lagrangian is the double well potential which has been treated in the classic paper of Krumhansl and Schrieffer [7]. As shown in [7] the double well potential admits Domain wall Solitons. Further we find light and dark Solitons in the coupled lattice (but not in the uncoupled lattice) which is again verified by recent experiments on coupled lattices [16, 10].

2. Model

Following Sakaguchi and Malomed [5] we use

$$iu_t = \frac{1}{2}(u_{xx} + u_{yy}) + (g_0 - cos(2x) - cos(2y))|u|^2 u \quad (1)$$

The discretized form of the above equation is

$$i\frac{du_{n,m}}{dt} = \Delta u_{n,m} - (g_0 - cos(2x) - cos(2y))|u_{n,m}|^2 u_{n,m} \quad (2)$$

where m, n are the lattice indices for the 2D optical lattices and the Laplacian $\Delta u_{n,m}$ is given by

$$\Delta u_{n,m} = (u_{n+1,m} + u_{n-1,m}) + u_{n,m+1} + u_{n,m-1} - 4u_{n,m} \quad (3)$$

This is the discretized form of the GPE. Note that this DNLS has been treated extensively by [1] . For the origin of the factor $(g_0 - \cos(2x))$ refer to [1]. As in [1] we define the norm

$$N = \sum_{n,m} |u_{n,m}|^2 \quad (4)$$

Further Lagrangian corresponding to (1) in the discrete form is

$$L = \sum_{n,m}[\quad u_{n,m+1}u_{n,m} + u_{n+1,m}u_{n,m} - u^2_{n,m} + (g_0 - \cos(2x))u^4_{n,m}] \quad (5)$$

To solve (2) we use

$$u_{n,m} = u^{(0)}_{n,m} e^{i\Lambda t} \quad (6)$$

Where $u^{(0)}_{n,m} = A\exp(-a|n| - b|m|)$ (7)

We wish to find under what condition of a and b we will find stable solution of (2)

Substituting (6),(7)in (2) we get

$$\Lambda A e^{-a|n|-b|m|} = A\begin{bmatrix} e^{-a|n+1|-b|m|} + e^{-a|n-1|-b|m|} + e^{-a|n|-b|m+1|} \\ +e^{-a|n|-b|m-1|} - 4e^{-a|n|-b|m|} \end{bmatrix} \quad (8)$$
$$-A^2 e^{-2(|n+1|-b|m|)} e^{-a|n|-b|m|}$$

Dividing by $Ae^{-a|n+1|-b|m|}$ one may obtain

$$\Lambda = \left[e^{-a} + e^{a} + e^{-b} + e^{b} - 4\right] - (g_0 - \cos(2x)) \quad (9)$$

However

$$N = \sum_{n,m} |u_{n,m}|^2 = \sum_{n,m} |u^{(0)}_{n,m}|^2 = A^2 \sum_{n,m} e^{-2a|n|} - 2b^{|m|} = \frac{A^2}{\operatorname{Tanh} a \operatorname{Tanh} b} \quad (10)$$

$$A^2 = N \operatorname{Tanh} a \operatorname{Tanh} b \quad (11)$$

We have

$$\sum_{n,m}[u_{n,m+1}u_{n,m} + u_{n+1,m}u_{n,m}] =$$
$$A^2 \sum_{n,m}\left[e^{-a|n|-2b|m+1|} e^{-a|n|-2b|m|} + e^{-a|n+1|-b|m|} e^{-a|n|-b|m|}\right]$$
$$= A^2 \sum_{n,m}\left[e^{-a|n|-b|m|} + e^{-a|n|-b|m|}\right]\left[e^{-b} + e^{-a}\right]$$
$$= \left[e^{-b} + e^{-a}\right] A^2 \sum_{n,m}\left[e^{-2a|n|-2b|m|}\right] \quad (12)$$

$$A^2 = N \operatorname{Tanh} a \operatorname{Tanh} b \quad (13)$$

Substituting (13) in (5) we obtain

$$\sum_{n,m}\left[e^{-2a|n|-2b|m|}\right] = \frac{1}{\operatorname{Tanh} a \operatorname{Tanh} b} \quad (14)$$

Hence

$$\sum_{n,m}\left[u_{n,m+1}, u_{n,m} + u_{n+1,m}u_{n,m}\right] = N\left[e^{-b} + e^{-a}\right] \quad (15)$$

Without loss generality considering all the neighboring points we may write

$$\sum_{n,m}\left[u_{n,m+1}, u_{n,m} + u_{n+1,m}u_{n,m}\right] = N\left[e^{b} + e^{-b} + e^{a} + e^{-a}\right]$$
$$= 2N(\operatorname{sech} b - \operatorname{sech} a) \quad (16)$$

$$\sum_{n,m} u^2{}_{n,m} \to N \quad (17)$$

$$\sum_{n,m}(g_0 - \cos(2x))u^4{}_{n,m} = (g_0 - \cos(2x))\sum_{n,m} u^4{}_{n,m}$$
$$= (g_0 - \cos(2x))\frac{N^2}{16}\frac{\operatorname{Cosh}(2a)\operatorname{Cosh}(2b)\operatorname{Sinh} a \operatorname{Sinh} b}{\operatorname{Cosh}^3(a)\operatorname{Cosh}^3(b)} \quad (18)$$

After the summation the Lagrangian becomes

$$L_{eff} = N(\operatorname{sech} b - \operatorname{sech} a) - N + (g_0 - \cos(2x))\frac{N^2}{16}\frac{\operatorname{Cosh}(2a)\operatorname{Cosh}(2b)\operatorname{Sinh} a \operatorname{Sinh} b}{\operatorname{Cosh}^3(a)\operatorname{Cosh}^3(b)} \quad (19)$$

For a stationary profile we must have

$$\frac{\partial L_{eff}}{\partial N} = \frac{\partial L_{eff}}{\partial a} = \frac{\partial L_{eff}}{\partial b} = 0 \quad (20)$$

$$\frac{\partial L_{eff}}{\partial N} = (\operatorname{sech} b - \operatorname{sech} a) - 1 + (g_0 - \cos(2x))\frac{N}{8}\frac{\operatorname{Cosh}(2a)\operatorname{Cosh}(2b)\operatorname{Sinh} a \operatorname{Sinh} b}{\operatorname{Cosh}^3(a)\operatorname{Cosh}^3(b)} = 0 \quad (21)$$

$$\frac{(g_0 - \cos(2x))\,N}{8} X = 1-(\operatorname{sech} b - \operatorname{sech} a) \;\; where \;\; X = \frac{\operatorname{Cosh}(2a)\operatorname{Cosh}(2b)\operatorname{Sinh} a \operatorname{Sinh} b}{\operatorname{Cosh}^3(a)\operatorname{Cosh}^3(b)} \quad (22)$$

$$N = \frac{8}{X\left(g_0 - \cos(2x)\right)}\left[1-(\operatorname{sech} b - \operatorname{sech} a)\right] \quad (23)$$

As $\left[1-(\operatorname{sech} b - \operatorname{sech} a)\right] \to 0 N \to 0 \quad g_0 \to \cos 2x \;\; N$ *attains* max *imum*

3. Vortex Solutions

For the 2D lattice

$$\frac{\partial^2 u^{(0)}_{n,m}}{\partial x^2} + \frac{\partial^2 u^{(0)}_{n,m}}{\partial y^2} - \left(g_0 - \cos(2x) - \cos(2y) + \Lambda\right) = 0 \quad (24)$$

The Laplacian in polar coordinates is given by

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \quad (25)$$

We rewrite (24) in polar coordinates where we have absorbed g_0, Λ in A_1, A_2

$$\frac{\partial^2 f}{\partial r^2} + \frac{\partial f}{r\partial r} + \frac{\partial^2 f}{\partial \theta^2} - A_1 \cos(\Omega_1 \theta) - A_2 \cos(\Omega_2 \theta) = 0 \quad (26)$$

Equation (25) is the double Sine-Gordon equation which admits vortex solutions [21]. We look for solutions of the form

$$f(r,\theta) = e^{im\theta} w(r) \quad (27)$$

where m is the vortex degree

We thus obtain for the radial equation

$$\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} - \frac{m^2}{r^2} = 0 \quad (28)$$

For large r there is very little change in w and we can neglect the double derivative term. We then have

$$\frac{1}{r}\frac{\partial w}{\partial r} - \frac{m^2}{r^2} = 0 \quad (29)$$

This may be written as

$$\frac{\partial w}{\partial r} = \frac{m}{r} \quad (30)$$

which has the solution

$$w = m\ln(r) \quad (31)$$

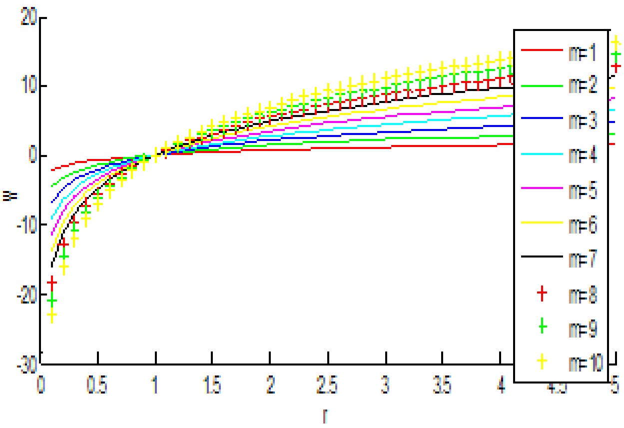

Figure 1

The vortex solution is given by

$$f(r,\theta) = e^{im\theta} m\ln(r) \quad (32)$$

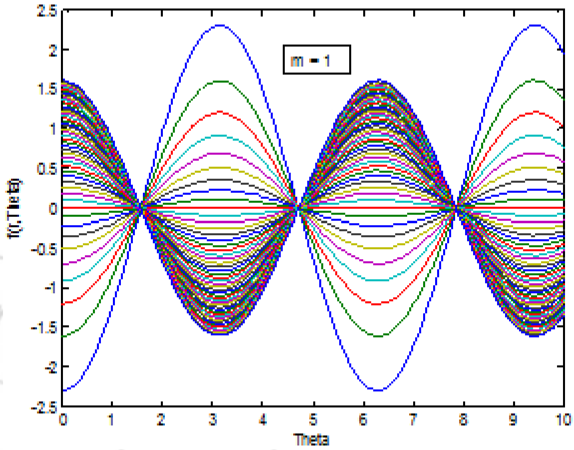

Figure 2

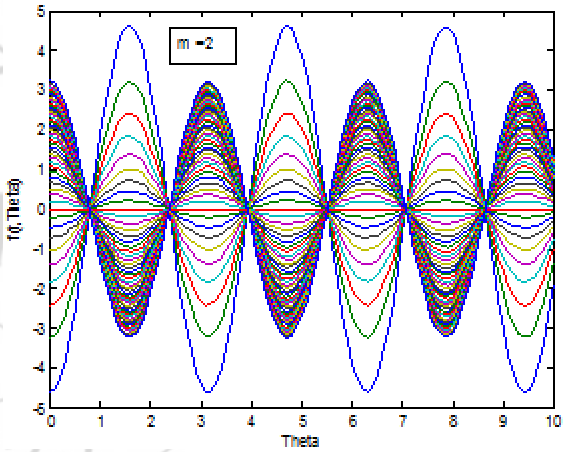

Figure 3

4. Energy Gaps in the Presence of Vortices

The characteristic feature of Vortex solutions is that the system undergoes very large changes in energy due to very small changes in external parameters. This feature induces energy gaps in the system. To understand this feature it is best to use the SSH Hamiltonian.

$$H_{SSH} = H_\pi + H_{\pi-ph} + H_{ph} \quad (33)$$

In this Hamiltonian H_π describes the electron electron interactions, H_{ph} describes the lattice and $H_{\pi-ph}$ describes the interactions between these two. An effective Hamiltonian used is the tight binding Su-Schrieffer-Heeger (SSH) Hamiltonian. This Hamiltonian

$$H_{\pi} = -t_0 \sum_{n,m,s} \left(c^{\dagger}_{n+1,m,s} c_{n,m,s} + c^{\dagger}_{n,m,s} c_{n+1,m,s} \right) + \left(c^{\dagger}_{n,m+1,s} c_{n,m,s} + c^{\dagger}_{n,m,s} c_{n,m+1,s} \right) \quad (34)$$

where α is the electron-phonon interaction constant and t_0 the hopping constant for an undimerized structure. $c^{\dagger}_{n+1,m,s}$ and $c^{\dagger}_{n,m,s}$ are the electron creation and annihilator operators on position n, m with spin s, respectively.

$$H_{\pi-ph} = \alpha \sum_{n,m,s} \left(u_{n+1,m} - u_{n,m}\right)\left(c^{\dagger}_{n+1,m,s} c_{n,m,s} + c^{\dagger}_{n,m,s} c_{n+1,m,s}\right) + \left(u_{n,m+1} - u_{n,m}\right)\left(c^{\dagger}_{n,m+1,s} c_{n,m,s} + c^{\dagger}_{n,m,s} c_{n,m+1,s}\right) \quad (35)$$

u_n is the deviation from the undimerized structure on site n,m

$$H_{ph} = \sum_{n} \frac{p_n^2}{2m} + \frac{1}{2}\left(u_{n,m+1} - u_{n,m}\right)^2 \quad (36)$$

To diagonalize the above Hamiltonian we use the Fourier transform of the creation (annihilation) operators:

$$c_{ks} = \frac{1}{\sqrt{N}} \sum_{n,s} e^{-ik(n+m)a} c_{nms} \quad (37)$$

k is the wave vector and ranging from 0 to $\pi / 2a$

Where N is the number of monomer units in the chain.

$$c_{ks-} = \frac{1}{\sqrt{N}} \sum_{n,s} e^{-ik(n+m)a} c_{nms} \quad (38)$$

$$c_{ks+} = \frac{-i}{\sqrt{N}} \sum_{n,s} (-1)^n e^{-ik(n+m)a} c_{nms} \quad (39)$$

The Hamiltonian can now be written as

$$H(u) = \sum_{k} \varepsilon_k \left(c^{\dagger}_{ks+} c_{ks+} - c^{\dagger}_{ks-} c_{ks-} \right) + \Delta_k \left(c^{\dagger}_{ks+} c_{ks-} + c^{\dagger}_{ks-} c_{ks+} \right) + 2Nku^2 \quad (40)$$

Where

$$\Delta_k = 4\alpha u \sin(ka)$$
$$\varepsilon_k = 2t_0 \cos(ka) \quad (41)$$

And Brillouin zone is defined by

$$-\frac{\pi}{2a} \le k \le \frac{\pi}{2a} \quad (42)$$

Finally the Hamiltonian can be diagonalized using the Bogoliubov transformation

$$a_{ks-} = \alpha_k c_{ks-} - \beta_k c_{ks+} \quad (43)$$

$$a_{ks+} = \beta_k c_{ks-} + \alpha_k c_{ks+} \quad (44)$$

The diagonal Hamiltonian is

$$H = E_k \left(n_{ks+} - n_{ks-)} \right) + 2Nku^2 \quad (45)$$

$$E_k = \left(\varepsilon_k^2 + \Delta_k^2 \right)^{1/2} \quad (46)$$

Here Δ_k is the band gap. Note that band gap is proportional to the coupling parameter α which plays the same role as ρ discussed earlier.

5. Charge and Spin States of Vortices

As pointed out in section 3 changes in the case of vortices changes of external parameters induce changes in the effective potential. This alters the number of states available in the system. The total number charges in the system is Q and the number of states is N. The following cases arise:

1. N =Q

In this case each state is assigned one charge

2. N<Q

In this case each state is assigned one charge and extra charges remain.

3. N>Q

Each state cannot be assigned a charge or spin. Hence vortices with or without spin and with or without charge are possible.

6. Conclusion

We have found vortex solutions in the case of 2D nonlinear optical lattices. In the presence of these vortices there is a large change in the internal parameters of the system caused by only a slight change of the external parameters. This behavior allows us to describe the system in terms of the SSH Hamiltonian which predicts that there will be an energy gap in the system and causes large blocks of states to be absent from the wave vector space. These results in vortices with or without spin or charge are possible.

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