Breathers in Quantum Lattices

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Abstract

This project has been a collaboration with the group of Professor Eilbeck, at the Department of Mathematics of the Heriot–Watt University, at Edinburgh (U.K.). We have studied conditions of existence and properties of breathers in some anharmonic quantum lattices. This kind of problems evolves the determination of the spectrum of large sparse matrices, and supercomputers seem to be the natural tool to be used in this framework.

Dr. Palmero is Professor at the Department of Applied Physics I in the Computer Science Engineering School of the University of Seville (Spain). He has been working in some different areas of Nonlinear Physics, and his current research interests are in the study of problems related to localization of energy by nonlinearity in classical and quantum lattices (discrete breathers). He has been working in different national and international projects and it is author of a big number of specialized publications in this area.

Prof. Palmero began to work in 1998 at the research group Non Linear Physics of the University of Seville. He has been working in phenomena of localization of energy by nonlinearity in two–dimensional systems, as crystals, in problems related to the connection of some families of discrete breathers to Anderson modes. Also, he has been working in DNA models, in the interplay between geometry and nonlinearity, and in the interaction of moving breathers with impurities. Last years he has been working, in collaboration with Prof. Eilbeck at Edinburgh, in the field of quantum breathers, in non–translational invariant one–dimensional systems and in translational–invariant two–dimensional systems.

The phenomenon of localization of energy by nonlinearity in *classical* lattices has been much studied in last years and it is possible to say that, at present, it is relatively well understood. On the other hand, the understanding of the quantum equivalence of discrete breathers is very limited. There exist some theoretical results and some experimental observations of these states in different quantum systems, but the amount of results related to this area is not large. It is interesting also to mention of the study of quantum modes on small lattices can be very important to some applications in areas as quantum dots and quantum computing developments, and Bose–Einstein condensates in periodical optics traps.

The main problem in the framework of quantum breather problems is the determination of the matrix representation of the Hamiltonian operator and its spectrum, at least partially. In a lattice of f lattice points which conserves the number of quanta n (bosons or fermions), the problem involves the determination, by means of symbolics mathematics programs, of a p × p matrix where $p = (n+f-1)!/n!(f-1)!$ in boson case or $f!/n!(f-n)!$ in one–fermion type case. As second step, a total or partial numerical spectrum must be calculated, a hard problem when n and/or f becomes large. In some cases, where some symmetries exist, the matrix can be further diagonalized into smaller blocks but, in general, it is not possible and it is in this kind of problems where supercomputers and parallel computing can play a very important role. In figure a typical spectrum is shown.

Figure 1: Eigenvalues of the energy $E(k)$ as function of the momentum k for a QDNLS one–dimensional bosons system. $f = 125$ and $n = 2$.

In our work we focus in lattices described by the by the the quantum version of the discrete nonlinear Schrödinger equation containing bosons, also known as the bosonic Hubbard model. This is a particularly simple model for a lattice of coupled anharmonic oscillators, which has been used to describe the dynamics of a great variety of systems. Many of this results can be easily extended to other systems, i.e., periodic lattices containing fermions, described by an attractive fermionic Hubbard model with two kinds of particles with opposite spins, a model of interest in connection with the theory of high-T_c superconductivity, and it can be used to describe bound states of electron and holes in some nanostructures as nanorings.

As first step, I have optimized some symbolic mathematics programs to generate a Fortran subroutine which allows to calculate the numerical values of the Hamiltonian matrix of the system as function of a set of control parameters. I have used the commercial version of the program Maple, version 8.0, running in a standard PC. This programs, in some hours or few days of CPU, allows to obtain the matrix representation of the operator Hamiltonian for translational and non–translational invariant systems, for one or two–dimensional systems, with a number of sites and a number of quanta high enough to obtain physical relevant results. In general we have obtained a large hermitian sparse matrix, which lower triangular part we have stored in COO (coordinate) format or CSC (compressed sparse column) format. As an example, for a one–dimensional nontranslational invariant system with $f = 7$ and $n = 9$ bosons, with first–neighbor interaction, the metrics of the matrix is 5005×5005 and the number of nonzero elements 47047. Nevertheless, a very interesting future development could be the adaptation of this programs to some parallel versions of Maple-like software.

Mainly, we are interested in the largest algebraic eigenvalues and its eigenvectors. Thus, in order to find out the partial spectrum of this matrix we have written up a parallel fortran program which, reading some input files, where control parameters and some input parameters are stored, calculates the partial spectrum (eigenvectors and eigenvalues) of the system. We have used the parallel version of numerical library ARPACK (PARPACK), which use Arnoldi an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method (IRAM) and MPI. We have been working in a 52 processor Sun Fire E15k, located at the EPCC in Edinburgh, using form one to 48 processor. Perhaps the main characteristics of this program is that is standard, easily portable to other parallel machines, and general, in the sense that if we have to analyze a different system, we have to change the algebraic manipulation programs, not the Fortran routine.

At this stage of the research, we are analyzing some different systems as a one–dimensional non-translational invariant bosons system with impurities and a two–dimensional systems with two different fermions in order to determine the energy levels of bound states corresponding to two electrons and a hole (orto–trion and para–trion). We hope to obtain relevant results soon.

Some of the most relevant works published by Prof Palmero in last five years in the area of discrete breathers are:

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2. J Cuevas, F Palmero, JFR Archilla and F Romero Romero. Moving breathers in a bent DNA-related model Physics Letters A 299:221-225(2002)

3. B Sánchez-Rey, JFR Archilla, F Palmero and FR Romero. Breathers in a system with helicity and dipole interaction. Physical Review E 66:017601-017604 (2002). Selected by Virtual Journal of Biological Physics Research 4(1), July 1 (2002)

4. J Cuevas, F Palmero, JFR Archilla and FR Romero. Moving discrete breathers in a Klein–Gordon chain with an impurity. Journal of Physics A: Mathematical and General. 35:10519-10530(2002)

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6. J Cuevas, F Palmero, JFR Archilla and FR Romero. Interaction of moving localized oscillations with a local inhomogeneity in nonlinear Hamiltonian Klein-Gordon lattices. Theoretical and Mathematical Physics, 137(1): 1406-1411(2003)

7. D Hennig, E Starikov, JFR Archilla and F Palmero. Charge transport in poly(dG)-poly(dC) and poly(dA)-poly(dT) DNA polymers. Journal of Biological Physics. 30(3):227-238(2004)

8. F Palmero, JFR Archilla, D Hennig and FR Romero. Effect of base-pair inhomogeneities on charge transport along the DNA molecule, mediated by twist and radial polarons. New. J. Phys. 6:13.1-13.16(2004)

9. JC Eilbeck and F Palmero. Quantum breathers in an attractive fermionic Hubbard model. Nonlinear Waves: Classical and Quantum Aspects, (eds. F. Kh. Abdullaev and V. V. Konotop), Kluwer: Amsterdam, 399-412(2004)

10. JC Eilbeck and F Palmero. Trapping in quantum chains. Phys. Lett. A, 331(3-4):201-208(2004)

11. FR Romero, JFR Archilla, F Palmero, B Sánchez-Rey, A Alvarez, J Cuevas and JM Romero. Classical and quantum nonlinear localized excitations in discrete systems. Invited review chapter, to appear in Recent Research Developments in Physics, Transworld Research Network, India (2005)

12. F Palmero, J Dorignac, JC Eilbeck, RA Römer. Aharonov-Bohm effect for an exciton in a finite width nano-ring. Phys. Rev. B, to appear August (2005)