TRIDIAGONAL PHYSICS

Part I: 20 min.

- Introduction
- Formulation
- Applications & Examples
- Perspectives

Part II: 15 min., Dr. Abdelmonem

- The J-matrix method
- Resonance search

Introduction

Tridiagonal Physics is the Physics obtained from the analysis of the matrix representation of relevant operators (e.g., the Hamiltonian) in a basis in which it is tridiagonal.

- Systematic program started in 2000
- Multi-disciplinary program
- Dhahran group + national/international membership, collaboration, and support
- Rich agenda: long list of significant problems

Formulation

- Consider H :

  diagonal rep. $H\phi_n = E_n\phi_n$

  too restrictive: discrete spectrum, small set of potentials

- Relax constraint: $H\phi_n \sim \phi_n + \phi_{n-1} + \phi_{n+1}$

$$H = \begin{pmatrix} a_0 & b_0 & & & & & \\ b_0 & a_1 & b_1 & & 0 & & \\ & b_1 & a_2 & b_2 & & & \\ & & b_2 & \times & \times & & \\ & & & \times & \times & \times & \\ & 0 & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix}$$

$$|\psi\rangle = \sum_n f_n |\phi_n\rangle$$

$$H|\psi\rangle = x|\psi\rangle \qquad (1) \longrightarrow$$

$$x f_n = a_n f_n + b_{n-1} f_{n-1} + b_n f_{n+1} \qquad (2)$$

$$x f_0 = a_0 f_0 + b_0 f_1 \qquad \langle\phi_n|\phi_m\rangle = \delta_{nm}$$

$$|\psi\rangle \Leftrightarrow \{f_n\} \qquad (1) \Leftrightarrow (2)$$

Spectrum $\{x\}$ includes discrete as well as continuous and larger class of potentials

$$x f_n(x) = a_n f_n(x) + b_{n-1} f_{n-1}(x) + b_n f_{n+1}(x) \qquad \int_{x_-}^{x_+} \rho(x) f_n(x) f_m(x) dx = \delta_{nm}$$

Normalization: $f_0 = 1 \longrightarrow f_n$ polynomial in x of degree n

Examples of such orthogonal polynomials:

- Hermite: $\frac{1}{\sqrt{2^n n!}} H_n(x), \quad x \in [-\infty, +\infty], \quad a_n = 0, b_n = \sqrt{\frac{n+1}{2}}$
- Cheybechev: $T_n(x), \quad x \in [-1, +1], \quad a_n = 0, b_n = \frac{1}{2}$
- Laguerre: $\sqrt{\frac{\Gamma(n+1)\Gamma(\nu+1)}{\Gamma(n+\nu+1)}} L_n^\nu(x), \quad x \in [0, +\infty], \quad a_n = 2n + \nu + 1, b_n = -\sqrt{(n+1)(n+\nu+1)}$

- **Associated tools**: Lanczos algorithm, Gauss quadratures, continued fractions, Pade approximations, ..etc.
- **In the literature**: Toda lattices, tight-binding models, recursion methods, 1D chain models, ..etc.

Applications & Examples

The J-matrix method

- Algebraic method of quantum scattering (1974, 1975)
- Atomic, molecular, nuclear, chemical
- Accuracy and convergence
- Multi-channel (rigorous formulation, 1997)
- Relativistic extension (2000)
- Book, Springer (2007)
- Active Groups: Russia, Saudi Arabia, North Europe, Australia, China, Brazil.

- **Dr. M. S. Abdelmonem (Part II)**

Discrete & Continuous Spectrum

(*all energies*)

$$H\phi_n = E_n\phi_n$$

$$E\,\phi_n = a_n\phi_n + b_{n-1}\phi_{n-1} + b_n\phi_{n+1}$$

- **Larger class of solvable potentials**:

  Ann. Phys. **317**, 152 (2005)

- **Example**: analytic solution for a new noncentral potential

$$V(r,\theta) = \alpha\,\frac{\cos\theta}{r^2}$$

J. Phys. A **38**, 3409 (2005)

Spectral Density

Resolvent operator: $G_{nm}(z) = \left(H - z\right)^{-1}_{nm}$

Project density: $\rho_n(x) = \frac{1}{2\pi \mathrm{i}}\left[G_{nn}(x + \mathrm{i}\,0) - G_{nn}(x - \mathrm{i}\,0)\right]$

H finite $\rightarrow$ G_{nn} non-analytic: interleaved poles & zeros

Three approximation methods:

- Analytic continuation
- Dispersion correction
- Stieltjes imaging

Phys. Rev. A **62**, 052103 (2005)

$$H = \begin{pmatrix} a_0 & b_0 & & & & & \\ b_0 & a_1 & b_1 & & 0 & & \\ & b_1 & a_2 & b_2 & & & \\ & & b_2 & \times & \times & & \\ & & & \times & \times & \times & \\ & 0 & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix}$$

$\lim_{n\to\infty}\left\{a_n, b_n\right\} = \left\{a_m, b_m\right\}_{m=1}^{K}$ $\longrightarrow$ K-band density with K–1 energy gaps

- **Impurity** at site k: $a_k \to a_k + \mu$ and/or $b_k \to \gamma b_k$

Density deformation: new density in terms of original one and deformation parameters μ and γ.

Phys. Lett. A (2007), in production

- Density associated with **nonlinear bifurcating map** that exhibit period doubling cascade:

  No. bands = half of the number of fixed points of the map (orbits period or bifurcation branches)

  J. Phys. A **39**, 6851 (2006)

Deformation of orthogonal polynomials

$$a_k \to a'_k \qquad b_k \to b'_k \neq 0 \quad \text{for a given integer } k$$

$$\rho(x) \to \rho'(x) \qquad P_n(x) \to P'_n(x)$$

$$\int_{x_-}^{x_+} \rho'(x) P'_n(x) P'_m(x)\, dx = \delta_{nm}$$

J. Phys. A **35**, 9071 (2002)

Study of resonance in the complex charge plane

Complex E-plane: for a given angular momentum and charge: bound states & resonances, complex scaling

Complex ℓ-plane: for a given E and Z: Regge poles ($\mathrm{Re}\,\ell = 0,1,..$), Regge trajectories (vary E)

Complex *Z*-plane: $$H - E = H_0 + V + \frac{Z}{r} - E$$

$$r\left(E - H_0 - \overset{\ell}{V}\right)\left|\psi\right\rangle = Z\left|\psi\right\rangle$$

Tridiagonal rep. $\longrightarrow$ straight-forward application of complex scaling

Scattering for a given E & ℓ but for all Z

Regge-like poles $(\mathrm{Re}\,Z = 0, \pm 1, \pm 2, ..)$

Regge-like trajectories (vary E)

J. Phys. A **37**, 5863 (2004)

Evaluation of new integrals involving orthogonal polynomials

$$\int_0^\infty x^\nu e^{-x/2} J_\nu(\mu x)\, L_n^{2\nu}(x)\, dx =$$

$$2^\nu \Gamma\left(\nu + \tfrac{1}{2}\right) \frac{1}{\sqrt{\pi\mu}} (\sin\theta)^{\nu+\frac{1}{2}} C_n^{\nu+\frac{1}{2}}(\cos\theta)$$

Where μ and ν are real parameters such $\mu \geq 0$, $\nu > -\frac{1}{2}$.

$\cos\theta = \frac{\mu^2 - 1/4}{\mu^2 + 1/4}$ and $C_n^\lambda(x)$ is the Gegenbauer polynomial.

Appl. Math. Lett. **20**, 38 (2007)

Perspectives

Group's work plan:

- Accurate evaluation of bound states & resonances
- Solutions of the Dirac equation with non-central potential for all energies
- J-matrix inspired quadrature & matrix tridiagonalization method
- Spectral decomposition of the Coulomb wave function
- ...etc.

Emails: bahlouli@kfupm.edu.sa

msmonem@kfupm.edu.sa

haidari@mailaps.org

الحمد لله

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السلام عليكم ورحمة الله وبركاته

Thank you