ALGEBRAIC METHOD IN CALCULATIONS OF NANO-SCALED OBJECTS PROPERTIES

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Abstract – The quantum mechanical calculations by means of the algebraic formulation are considered for the nano-scaled objects. The one-dimensional chain of one-dimensional quantum oscillators is selected as a model object sufficient for a range of solid state applications. In the calculations, well known algebraic formulation entities are used, such as the one-dimensional Morse quantum oscillator and the U(2) Lie algebra. The relative importance of the surface effects in the nano-scaled object is represented by considering both the radiation mechanisms and the difference in the behaviour of the quantum oscillator subchains having different lengths. The automation method for dealing with the numerically undetermined coupling parameters is suggested.

I. INTRODUCTION

The algebraic method is considered to be the major methodology in quantum mechanical calculations, besides the (traditional) potential and empirical methodologies. It is rooted in the Heisenberg formulation, and its emergence is usually dated to the late 1970s [1]. The main idea of the method is to represent the energy spectrum of the object with the irreducible representation of the Lie algebra being isomorphic with the object states, and then to manipulate the algebra [2, 3].

The main benefits of the method are: (1) reduction of the volume of computations (the method doesn't require solving the Schroedinger's equation directly and the mathematical manipulations employed in method are considered comparatively "cheap"); (2) in-built provision for anharmonical effects (with the appropriate choice of potential function); (3) possibility to calculate wave functions and thus observables other than energies [1,2,4,5].

The problem of the appropriate algebra and representation choice and construction by now is considered solved, in general. There are some variants to consider here, mainly pertaining to the subsequent organisation of computation. The important implementation steps are: (1) to determine the number of dimensions *r* sufficient to describe the problem; (2) to determine the part of the spectrum requiring representation (bound, continuous, or both); (3) to select the potential function appropriate for the problem. The primary output of the method's aplication is the energy spectrum, so the principal areas benefitting from the method application are the molecular, nuclear and particle physics.

II. APPLICATION OF ALGEBRAIC METHOD

The application of the algebraic method to the real-world system (molecule, cluster etc.) usually starts with substitution of inter-atomic bonds with the quantum oscillators in one of the well-known potentials. The inherently anharmonic potential functions proposed by Morse and Poeschl-Teller are considered to be an especially good candidates for that. If the problem is limited to *r* dimensions ($r = 1,2,3$), the algebra U(r+1) for each bond is built. Next, Hamiltonian for the system is formed. The typical Hamiltonian for the system of *n* bonds (treated as a system of *n* coupled quantum oscillators) in algebraic formulation is [4,5]

$$H = \sum_{i}^{n} {}_{0\mathrm{i}} + \sum_{i}^{n} A_i C_i + \sum_{j}^{n} \sum_{i<j} A_{ij} C_{ij} + \sum_{j}^{n} \sum_{i<j} \lambda_{ij} M_{ij} \qquad (1)$$

where ${}_{0\alpha}$ are zero level energies of oscillators labelled α, C_α are Casimir (invariant) operators for the algebras corresponding to oscillators labelled α, $C_{\alpha\beta}$ are invariants describing anharmonicities involving oscillators labelled α and β, $M_{\alpha\beta}$ are Majorana operators describing oscillators (bonds) couplings. The coefficients A and λ depend on object's composition. These might be subsequently fitted to the experimental data. Then, the observables might be calculated etc.

The important point here is that the complete three-dimensional numerical treatment of systems even of relatively modest size ($10 - 10^2$ atoms), even in algebraic formulation, is still involving a very significant volume of computations.

III. Nanofilm and Its Related Model Object

It is well known that the size effects in the nano-objects are direction-related [6]. Nano-scaled objects (nano-objects) are classified, e.g., by the number of object's dimensions which lie in nano-size range (≈1—100 nm). One of the important types of the nano-objects is nanofilm — one-dimensional nano-object. Typically, such object would be placed either on a (massive) layer or between two (massive) layers. The energy (heat) flow in practically interesting setups of this kind is directed more or less along the axis of nano-dimension of the object. Considering the relation of lengths of layers and film along the film's nano-dimension axis, the object might be considered as being effected by plain wave with wavevector directed perpendicularly to the film's macro-plane ("side"). Furthering this assumption, the lateral energy flux in film might be considered negligible (non-existent) and so the problem might be reduced to the problem of longitudal energy flow in manifold of one-dimensional chains, and further, to the problem of energy flow in the one-dimensional chain of atoms.
The one-dimensional (linear) chain of quantum oscillators (harmonic or anharmonic), to which the one-dimensional chain of atoms is reduced, is the basic and well-researched example of the algebraic method application. The algebras involved for every bond are U(2) for the bound states-only problem.

IV. Scaling and Symbolic Computation

Not every nano-object would lend itself to the far-going simplification like discussed in Section III. Extending the calculation to two or three dimensions would generally require more complicated algebras — U(3) and U(4) per oscillator for bound states-only problems, — and the types of Lie algebras involved consist of $O(n^2)$ operators each. Considering more complex systems, like molecular crystals or nano-composites, would raise the complexity even more. Finally, the values of the series coefficients often are unknown. However, in many cases it's possible to reduce This suggests trying for solving in the symbolic form, which might already give a useful results. However, the sheer volume and complexity of such calculations even for systems of $10–10^2$ atoms necessitates using the software automation, specifically, a symbolic calculations software package. To this end, we primarily consider two open-source high-end mathematical software packages, MAXIMA and SAGE. As the method requires dealing principally with series and aggregates, even the middle-end packages (like MPFR, CLN, GMP etc.) might do, in certain circumstances.

V. Conclusion

We consider the application of algebraic method to the calculation of physical properties of nano-scaled objects. The method, while offering certain benefits, especially with regard to the volume of computations, requires careful application and would scale satisfactorily only in well-organised environment.

References

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