

Knot and Conformal Field Theory Approach in Molecular and Nuclear Physics

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It is shown that the eigenvalue of a quadratic Casimir operator of quantum universal enveloping (QUE) algebra of SU_2 explains successfully the observed rotational spectra of a molecule. A similar idea is applied to two nuclei. The problem of dissociation (binding) energy for the molecules (nuclei) is discussed shortly.

Witten¹⁾ has developed the theory of QUE algebra in a set of three papers. The theory is generally covariant and gauge invariant. He gave a q deformed Casimir operator of SU_2 quantum group as an example, with which we concern ourselves in this paper. Most of the tools²⁾ to prove the theoretical results are familiar with the high-energy physicists, except, perhaps, for the knot, braid and link theory³⁾ which is developed further in recent years, in connection with the exact solvability⁴⁾ of many models in solid state physics and statistical mechanics. We wish to show that, in spite of its historical origin, the result is quite useful to interpret the rotational spectra of molecules and nuclei.

In this paper we shall give some examples in both fields and wish to discuss shortly the dissociation (binding) energy for molecules (nuclei). From a practical point of view it is not necessary to understand the whole detail of the theory. We shall begin with the eigenvalue of the quadratic Casimir operator of QUE algebra for SU_2 and state the physical significance of it in relevance to the available information. It is given by

$$x(q, J) = \frac{1}{2} \frac{q + q^{-1}}{(q^{1/2} - q^{-1/2})^2} \frac{(q^J - q^{-J})(q^{J+1} - q^{-J-1})}{(q^{J+1/2} + q^{-J-1/2})^2}, \quad (1)$$

where J is the total angular momentum and q the deformation parameter of the algebra. Here $x(q, J)$ is symmetric under $q \rightarrow 1/q$ and becomes $J(J+1)$ in the limit $q \rightarrow 1$. The deviation of q from 1 is interpreted as a measure of the strength of the deformation of the representation space in angular momentum, or that of the eigenvalue of the observable in the same space in it.

If one looks at the expression (1), he sees that it gives a gradual shrinking with the increase of J for a fixed q different from 1. He may immediately realize that such a behavior is common in molecular⁵⁾ and nuclear⁶⁾ rotational spectra without making a detailed check.

Before entering into an application, it would be useful to add a few more remarks. The parameter q in the theory is related to the coupling constant k of the three

dimensional Chern-Simons theory through

$$q = e^{2\pi i / (k + c_2(G)/2)} \quad (2)$$

Here $c_2(G)$ is an eigenvalue of the quadratic Casimir of the relevant group G . In order to get a real q one is required to make an analytic continuation from a large integer k to an infinite complex number k with an appropriate ratio of its real and imaginary part. Such a continuation is certified by the famous Knizhnik and Zamolodchikov differential equation.⁷⁾ Except for the conformal field theory, the derivation of Eq. (1) is algebraic, provided that the expectation value of Wilson lines in Chern-Simons gauge theory with gauge group G in a path integral formulation are projected on a plane, which are adjusted to the similar projections of knots, links or braids. In Eq. (1) the nearest neighbor interactions were taken into account with the help of the vertex and the interactions around a face models, which is simplified by considering the adjoint representation of SU_2 group. In this sense, the validity of Eq. (1) should be tested experimentally.

The rotational level is expressed as

$$E(q, J) = Bx(q, J), \quad (3)$$

where B is an adjustable constant. We shall not concern its numerical value, since we are only interested in the relative frequency interval (level spacing) for the molecule (nucleus) in this paper. If one wishes he can get it from Eqs. (1) and (3) by

Table I. Rotational spectra of ${}^6\text{Li}^{19}\text{F}$ molecule.

| vibronic q. n. (v) calculated q PRCS | $J' \leftarrow J''$ | observed frequency (MHz) | calculated frequency (MHz) |
|--|---------------------|--------------------------------|----------------------------------|
| $v=0$ $q=1.003847$ PRCS= $2.11 \cdot 10^{-13}$ | 1-0 | 89740.465 (0.02) | 89740.488 |
| | 2-1 | 179470.35 (0.10) | 179470.39 |
| | 3-2 | 269179.18 (0.10) | 269179.14 |
| | 4-3 | 358856.19 (0.10) | 358856.13 |
| | 5-4 | 448491.07 (0.10) | 448490.82 |
| | 6-5 | 538072.65 (0.10) | input |
| $v=1$ $q=1.003855$ PRCS= $5.26 \cdot 10^{-14}$ | 1-0 | 88319.178 (0.02) | 88319.192 |
| | 2-1 | 176627.91 (0.10) | 176627.92 |
| | 3-2 | 264915.79 (0.10) | 264915.74 |
| | 4-3 | 353172.23 (0.10) | 353172.19 |
| | 5-4 | 441386.83 (0.10) | input |
| $v=2$ $q=1.003864$ PRCS= $2.37 \cdot 10^{-14}$ | 1-0 | 86921.199 (0.02) | 86921.198 |
| | 2-1 | 173832.04 (0.10) | 173832.05 |
| | 3-2 | 260722.24 (0.10) | 260722.23 |
| | 4-3 | 347581.39 (0.10) | input |
| $v=3$ $q=1.003905$ PRCS= $2.17 \cdot 10^{-11}$ | 1-0 | 85546.64 (0.02) | 85546.65 |
| | 2-1 | 171082.27 (0.10) | 171082.90 |
| | 3-2 | 256597.84 (0.10) | 256598.37 |
| | 4-3 | 342082.66 (0.10) | input |

making use of q determined in this paper for a particular energy band.

The result of an analysis on ${}^6\text{Li}{}^{19}\text{F}$ molecule⁸⁾ is tabulated in Table I. The value of q and a pseudo reduced chi-square (PRCS), which is defined by neglecting the weight arising from an error, are given for each vibronic state ν in the first column. The angular momenta relevant to the absorption spectra are shown in the second column. The third and the fourth column indicate the observed and the calculated frequency, respectively. We have chosen the ratios of relative frequencies in succession as inputs and tabulated the final results in terms of the frequency interval of the two highest ranking states of each band. One sees that our formula (1) reproduces the data in an extremely good accuracy. So far we cannot find out an exception of those good fittings, as far as the pure rotational frequencies of the molecules concern.^{9),10)} If one wants to talk about an interband transition, he has to take into account a slight difference between q values of the relevant bands.

At this stage, we are waiting a datum with a more significant numbers, where theory fails.

The similar study has been made for ${}^{130}\text{Ce}$ ¹¹⁾ and ${}^{174}\text{Hf}$ ¹²⁾ nucleus. The results are given in Tables II and III, where the final expression is shown in terms of the energy of the highest J state. Here the result is not as impressive as that for the molecule. However, we think that our approach is better than a yrast method,¹³⁾ which is semi-classical and in some sense an analogue of that in molecular spectroscopy. The

reason why we believe this, arises from the nature of Eq. (1). The functional form of it has a nice convergence property at high J and admits an extrapolation. If one expands it around $q=1$, he may find extra J dependences which are not contained in the current molecular physics and yrast approach. Of course, this point should be tested by a further analysis of data and a more extensive study. For the moment we leave a final conclusion for future.

There arise many interesting problems, if one once finds a good functional

Table II. Energy spectra of ${}^{138}\text{Ce}$ nucleus.

| J^π | observed energy (MeV) | calculated energy (MeV) $q=1.07495$ PRCS=0.0618 |
|---------|-----------------------|---|
| 16^+ | 4.558 | input |
| 14^+ | 3.864 | 4.022 |
| 12^+ | 3.314 | 3.397 |
| 10^+ | 2.811 | 2.701 |
| 8^+ | 2.054 | 1.970 |
| 6^+ | 1.324 | 1.259 |
| 4^+ | 0.7105 | 0.6438 |
| 2^+ | 0.2539 | 0.2025 |
| 0^+ | 0 | input |

Table III. Energy spectra of ${}^{172}\text{Hf}$ nucleus.

| J^π | observed energy (keV) | calculated energy (keV) $q=1.043276$ PRCS= $5.14 \cdot 10^{-5}$ | observed energy (keV) | calculated energy (keV) $q=1.047225$ PRCS= $4.60 \cdot 10^{-4}$ |
|---------|-----------------------|---|-----------------------|---|
| 8^+ | 1009.6 | input | | |
| 6^+ | 608.26 | 609.45 | 1307.4 | input |
| 4^+ | 297.38 | 297.76 | 1062.17 | 1063.37 |
| 2^+ | 90.985 | 90.820 | 900.24 | 900.10 |
| 0^+ | 0 | input | 828.13 | input |

form adapted to the rotational spectra of molecules, in addition to those discussed by Herzberg⁵⁾ in an introductory part of his book. In statistical physics, we usually estimate the partition function on the rotational part by replacing a sum over $J(J+1)$ dependence by a continuum. Is it possible to perform the similar integral by the functional form (1), exactly? In tables of dissociation energies for molecules, they are tabulated at most four significant numbers in units of eV.⁵⁾ Could we improve this situation under a new approach? The author supposes that a complete resolution of this problem may require to find out a functional form which explains the observed vibronic spectra with the same level as that for the rotational ones. We shall postpone this problem in the future.

The similar question remains in nuclear physics even if we succeed to explain the level structure. Franzini and Radicati¹⁴⁾ have shown that Wigner's supermultiplet theory¹⁵⁾ can be applied to the description of the binding energies of nuclei up to rather high mass numbers. They gave a mass dependent parameter of supermultiplet term, $b(A)$ in Fig. 2 of that paper, which can be expressed by a 9-th degree polynomial in A , according to them. If we introduce a single function, known as Rosin-Rammler distribution,¹⁶⁾ it can be reproduced approximately by $89.1 \exp(-1.62A^{0.203})$. This is a long-range effect in A space. The present author¹⁷⁾ had tried to analyze the binding energies of nuclei by making use of the so-called Weizsäcker-Bethe mass formula, by taking into account the pairing effect. He used a good sign factor, but he did not use a good A dependent coefficient function in that analysis, which was reflected to the estimate of the binding energies for hypernuclei in similar approach. If we use the Rosin-Rammler distribution, instead of A^{-1} and $A^{-4/3}$ dependences used there, we expect to have a better semi-empirical formula which applies to low- as well as high-mass regions.¹⁸⁾

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