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$\mathcal{L}^{\otimes N}$—Generalization of Partial Algebraization Method for Spectral Problems and Heisenberg Model[1]

SONG Zhi and SHEN Hong
Department of Physics, Nankai University, Tianjin 300071, China
SUN Chang-pu[2]
Theoretical Physics Division, Nankai Institute of Mathematics, Tianjin 300071, China
and
Physics Department, Northeast Normal University, Changchun 130024, China

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Abstract

In terms of the N-multiple direct product of Lie algebra the method of partial algebraization for quantal spectrum problems is generalized to deal with the cases of many-mode coupling. Using this generalized method to the antiferromagnetic Heisenberg model, we explicitly obtain some analytic and numeral results for the eigenstates and eigenvalues.

I. Introduction

As a new class of quantal problems, the quasi-exactly-solvable quantal problem (QESQP) has been discovered and solved by the so-called partial algebraization method of the spectrum (PAMP)[1–3]. At present, the discussions concerning this problem have ranged from the supersymmetry[4–5] to the conformal field theories[6].

Now we briefly describe the central ideas of the PAMP as follows. For the Hamiltonian $\hat{H}$ of a quantal system, if we can choose a proper basis for the Hilbert space such that $\hat{H}$ has a block structure in this basis, i.e.,

$$\hat{H} = \text{diag.}[\hat{h},\, \hat{h}']$$

where $\hat{h}$ is an $n \times n$ matrix with small n and $\hat{h}'$ an infinite dimensional matrix or an $m \times m$ finite dimensional matrix with large m, then we can diagonalize $\hat{h}$ without affecting $\hat{h}'$ and obtain a part of the spectra of $\hat{H}$. To this end we should try to express $\hat{H}$ as an element of the universal enveloping algebra $\mathcal{U}(\mathcal{L})$ of a Lie algebra $\mathcal{L}$ with generators T_i ($i = 1, 2, \ldots, M$), i.e.,

$$\hat{H} = H(T_1, T_2, \ldots, T_M) = H(\{T_i\})$$

where H is a holomorphic function. If we can do it, $\hat{H}$ is then the Hamiltonian of the QESQP and has a block structure on the basis for the spaces of all the irreducible representations of $\mathcal{L}$. Because a Hamiltonian $\hat{H}$ is usually expressed in terms of differential operators, i.e.,

$$\hat{H} = H\left(-i\hbar\frac{\partial}{\partial x}\cdots\right),$$

[1]The project supported by National Natural Science Foundation of China.

[2]Mailing address: Theoretical Physics Division, Nankai Institute of Mathematics, Tianjin 300071,China.

the PAMP depends on an inhomogeneous differential realization of a Lie algebra. The general formulas of this realization[6] was given based on the boson realization method[7].

In this article, the PAMP is generalized to the cases with multiple product of a Lie algebra as dynamic Lie algebra of the system. The antiferromagnetic Heisenberg model is studied as an example and some analytic and numeral results about eigenstates and eigenvalues are obtained in explicit forms. Some information about ground states given from the calculation is expected to be useful for the practical problems in the condensed matter physics, such as high-T_c superconductivity.

II. $\mathcal{L}^{\otimes N}$—Generalization of the PAMP

Let

$$\{E_{\alpha_i},\, H_k | i = 1,\, 2,\, \ldots,\, M - L;\; k = 1,\, 2,\, \ldots,\, L\}$$

be a Cartan-Weyl basis for an L-rank simple Lie algebra $\mathcal{L}$ and $V^{[\Lambda_s]}$ be the carrier space of an irreducible representation $\Gamma^{[\Lambda_s]}$ with the basis $|\Lambda_s,\, M_s\rangle$ that satisfies

$$\begin{cases} E_\alpha |\Lambda_s,\, \Lambda_s\rangle = 0 \qquad \text{for a positive root,} \\ H_k |\Lambda_s,\, M_s\rangle = M_s^k |\Lambda_s,\, M_s\rangle\,, \\ E_{\pm\alpha} |\Lambda_s,\, M_s\rangle = \Gamma^{(s)}_{M_s+\alpha,\, M_s} |\Lambda_s,\, M_s + \alpha\rangle\,, \end{cases} \tag{1}$$

where

$$\Lambda_s = (\Lambda_s^1,\, \Lambda_s^2 \cdots \Lambda_s^L)$$

is the highest weight and

$$M_s = (M_s^1,\, M_s^2,\, \cdots,\, M_s^L)$$

is a weight of the representation. The n-multiple product of this Lie algebra $\mathcal{L}$ is

$$\mathcal{L}^{\otimes N} \equiv \mathcal{L} \otimes \mathcal{L} \otimes \cdots \otimes \mathcal{L} \qquad (N \text{ times})$$

with the generators

$$\begin{cases} E_\alpha(i) = \underset{1}{I} \otimes \underset{2}{I} \otimes \cdots \otimes \underset{i-1}{I} \otimes \underset{i}{E_\alpha} \otimes \underset{i+1}{I} \otimes \cdots \otimes \underset{N}{I}\,; \\ H_k(i) = \underset{1}{I} \otimes \underset{2}{I} \otimes \cdots \otimes \underset{i-1}{I} \otimes \underset{i}{H_k} \otimes \underset{i+1}{I} \otimes \cdots \otimes \underset{N}{I}\,. \end{cases} \tag{2}$$

For some practical problems in physics, the Hamiltonian is an element of the universal enveloping algebra $\mathcal{U}(\mathcal{L}^{\otimes N})$ of $\mathcal{L}^{\otimes N}$, i.e.

$$\begin{aligned} \hat{H}(N) &= \hat{H}(E_{\alpha(i)},\, H_k(i)) \\ &= \sum A^{a,b,\cdots,c}_{i,j,\cdots,t} \hat{X}^{m(a,i)}_{a(i)} \cdot \hat{X}^{m(b,j)}_{b(j)} \cdots \hat{X}^{m(c,t)}_{c(t)}\,, \end{aligned} \tag{3}$$

where for $d = a,\, b,\, \ldots,\, c$ and $l = i,\, j,\, \ldots,\, t$,

$$\hat{X}_d(l) \in \{E_\alpha(i),\, H_k(i) | i = 1,\, 2,\, \ldots,\, N;\; \alpha = 1,\, 2,\, \ldots,\, M - L;\; k = 1,\, 2,\, \ldots,\, L\}$$

and $m(d, l) = 1, 2, \ldots$. From the irreducible representations $\Gamma^{[\Lambda_s]}$ $(s = 1, 2, \ldots, N)$ on the spaces $V^{[\Lambda_s]}$, we construct an irreducible representation $\Gamma^{[\Lambda]}$ of $\mathcal{L}^{\otimes N}$ as

$$\Gamma^{[\Lambda]} \equiv \Gamma^{[\Lambda_1, \Lambda_2, \cdots \Lambda_N]} = \Gamma^{[\Lambda_1]} \otimes \Gamma^{[\Lambda_2]} \otimes \cdots \otimes \Gamma^{[\Lambda_N]}$$

on the product space

$$V^{[\Lambda]} \equiv V^{[\Lambda_1, \Lambda_2, \cdots \Lambda_N]}$$

with the basis

$$|\Lambda, \tilde{M}\rangle^N \equiv |\Lambda_1, M_1\rangle \otimes |\Lambda_2, M_2\rangle \otimes \cdots \otimes |\Lambda_N, M_N\rangle \,. \tag{4}$$

The Hilbert space of the problem is the total space

$$V = \sum_{\Lambda}\!{}^{\oplus} d_\Lambda V^{[\Lambda]}$$

where d_Λ denotes the degeneracy. Because the representation $\Gamma^{[\Lambda]}$ is also a representation for the universal enveloping algebra $\mathcal{U}(\mathcal{L}^{\otimes N})$ and $\hat{H}(N) \in \mathcal{U}(\mathcal{L}^{\otimes N})$,

$${}^N\langle \Lambda, \tilde{M}|\hat{H}(N)|\Lambda', \tilde{M}'\rangle^N = \delta_{\Lambda\Lambda'}\, {}^N\langle \Lambda, \tilde{M}|\hat{H}(N)|\Lambda, \tilde{M}'\rangle^N \,, \tag{5}$$

i.e., the Hamiltonian $\hat{H}(N)$ has a block structure

$$\hat{H}(N) = \sum_{\Lambda}\!{}^{\oplus} \hat{h}(\Lambda)$$

with

$$\hat{h}(\Lambda) = ({}^N\langle \Lambda, \tilde{M}|\hat{H}(N)|\Lambda, \tilde{M}'\rangle^N)$$

on the above basis. Therefore, we can diagonalize each one of the blocks $\hat{h}(\Lambda)$ without touching the others.

Especially, when $\hat{H}(N)$ takes the form

$$\hat{H}(N) = \hat{H}(\cdots \vec{E}_\alpha \cdot \hat{E}_{-\alpha} \cdots H_k \cdots) \,, \tag{6}$$

each block $\hat{h}(\Lambda)$ is also reduced into a smaller block structure

$$\begin{aligned} \hat{h}(\Lambda) &= \sum_{\Sigma}\!{}^{\oplus} \hat{h}^{[\Sigma]}_{(\Lambda)} \,, \\ \hat{h}^{[\Sigma]}_{(\Lambda)} &= \Big({}^N\langle \Lambda, \tilde{M}|\hat{H}(N)|\Lambda, \tilde{M}'\rangle^N \,\Big|\, \sum_{i=1}^{N} M_i = \sum_{i=1}^{N} \tilde{M}_i = \Sigma\Big) \,. \end{aligned} \tag{7}$$

Here, we have considered a fact that the sum

$$\Sigma = M_1 + M_2 + \cdots + M_N$$

of the weights is invariant under the action of $E_\alpha(i) \cdot E_{-\alpha}(j)$ and then

$$V^{[\Lambda]}_{(\Sigma)} = \{|\Lambda, \tilde{M}\rangle^N \,|\, \sum_{i=1}^{N} M_i = \Sigma)\}$$

is an invariant subspace of $V^{[\Lambda]}$. On these smaller $\hat{H}(N)$-invariant subspaces we can diagonalize $\hat{h}^{[\Sigma]}_{(\Lambda)}$ rather easily and thereby obtain a part of the spectra of $\hat{H}$.

III. An $SU(2)^{\otimes N}$ Case: Antiferromagnetic Heisenberg Model

The following discussion will focus on the case of $\mathcal{L}$=SU(2), which is just the antiferromagnetic Heisenberg model

$$\hat{H} = J\sum_{\langle i,j\rangle} \hat{\vec{S}}(i)\cdot\hat{\vec{S}}(j)\,, \qquad (j>0)\,, \tag{8}$$

where S_x, S_y and S_z are the generators of SU(2). In the case of 1–D chain, equation (8) can be rewritten as the form (6)

$$\hat{H} = \frac{1}{2}J\sum_{i=1}^{N}[\hat{S}^{+}_{(i)}\hat{S}^{-}_{(i+1)} + \hat{S}^{+}_{(i+1)}\vec{S}^{-}_{(i)} + 2S^{z}_{(i)}S^{z}_{(i+1)}] \tag{9}$$

in terms of

$$\hat{S}^{\pm} = \hat{S}_x \pm i\hat{S}_y\,.$$

We denote by $|j\,m\rangle$ the angular state of single particle and then we get a basis

$$\prod_{k=1}^{N}\!{}^{\otimes}|j_k,\,m_k\rangle = |j_1,\,m_1\rangle\otimes|j_2,\,m_2\rangle\otimes\cdots\otimes|j_N m_N\rangle$$

for the Hilbert space. According to the above general discussion, we observe that the subspaces

$$V^{[M]}_{(j_1,j_2,\cdots,j_N)}:\Big\{\prod_{k=1}^{N}\!{}^{\otimes}|j_k,\,m_k\rangle\;\Big|\;\sum_{k=1}^{N}m_k = M\Big\}$$

are $\hat{H}$-invariant. In usual Heisenberg model, the particles located on different sites have the same spin s, and then we only consider the cases of $j_1 = j_2 = \cdots = j_N = s$ and define

$$V^{[M]}_{(s)} = V^{[M]}_{(s,s,\cdots,s)}:\Big\{\prod_{k=1}^{N}\!{}^{\otimes}|\,m_k\rangle \equiv \prod_{k=1}^{N}\!{}^{\otimes}|s,\,m_k\rangle\;\Big|\;\sum_{k=1}^{N}m_k = M\Big\}\,.$$

For the two cases with $s = 1/2$ and $s = 1$ respectively, we obtain the dimensions of the $\hat{H}$-invariant subspace

$$\dim(V^{[M]}_{(1/2)}) = \frac{N!}{((N/2)+M)!((N/2)-M)!}\,, \tag{10a}$$

$$\dim(V^{[M]}_{(1)}) = \sum_{k=0}^{[N-|M|-\varepsilon(N,M)]/2}\frac{N!}{\Delta}\,, \tag{10b}$$

where

$$\varepsilon(N,\,M) = \frac{1}{2}[1-(-1)^{N+M}]\,,$$

$$\Delta = \Big(\frac{1}{2}[M+N-2k-\varepsilon(N,\,M)]\Big)!\Big(\frac{1}{2}[N-M-2k-\varepsilon(N,\,M)]\Big)!(2k+\varepsilon(N,\,M))!\,.$$

Now, on each $\hat{H}$-invariant subspace $V_{(s)}^{[m]}$, we can diagonalized $\hat{H}$ for given N, M and S. On the spaces $V_{(1/2)}^{[M]}$ and $V_{(1)}^{[M]}$, we respectively obtain the analytic eigenstates

$$|\phi_{(1/2)I}^{NM}\rangle = \frac{1}{\sqrt{\dim(V_{(1/2)}^{[M]})}} \cdot \sum_{m_1+m_2+\cdots+m_N=M} \left\{ \bigotimes_{k=1}^{N} |m_k\rangle \right\}, \tag{11a}$$

$$|\phi_{(1)I}^{NM}\rangle = \frac{1}{\sqrt{\Omega}} \sum_{k=0}^{[N-|M|-\epsilon(N,M)]/2} (\sqrt{2})^{2k+\epsilon(N,M)} \sum_{\substack{\Sigma m_i=M, \\ \Sigma|m_i|=N-2k-\epsilon(M\,N)}} \left\{ \bigotimes_{l=1}^{N} |m_l\rangle \right\}, \tag{11b}$$

and the corresponding eigenvalues

$$\begin{aligned} E\left(\frac{1}{2}\right)_1^{NM} &= +\frac{1}{4}QJ\,, \\ E(1)_1^{NM} &= +QJ\,, \end{aligned} \tag{12}$$

where Q is the number of nearest neighbor and

$$\Omega = \sum_{k=1}^{[N-|M|-\epsilon(N,M)]/2} 2^{2k+\epsilon(N,M)} \frac{N!}{\Delta}\,. \tag{13}$$

In fact, considering that

$$|\phi_{(1/2)I}^{NM}\rangle = \frac{1}{\sqrt{\dim(V_{(1/2)}^{[M]})}} \Bigg\{ \sum_{m_1+\cdots+m_{i-1}+m_{i+2}+\cdots+m_N=M-1} |m_1\rangle \otimes \cdots \otimes |m_{i-1}\rangle$$

$$\otimes(|\uparrow\rangle_i \otimes |\uparrow\rangle_{i+1}) \otimes |m_{i+2}\rangle \otimes \cdots \otimes |m_N\rangle$$

$$+ \sum_{m_1+\cdots+m_{i-1}+m_{i+2}+\cdots+m_N=M} |m_1\rangle \otimes \cdots \otimes |m_{i-1}\rangle$$

$$\otimes(|\uparrow\rangle_i \otimes |\downarrow\rangle_{i+1} + |\downarrow\rangle_i \otimes |\uparrow\rangle_{i+1}) \otimes |m_{i+2}\rangle \otimes \cdots \otimes |m_N\rangle + \sum_{m_1+\cdots+m_{i-1}+m_{i+2}+\cdots+m_N=M+1} |m_1\rangle$$

$$\otimes \cdots \otimes |m_i\rangle \otimes (|\downarrow\rangle_i \otimes |\downarrow\rangle_{i+1}) \otimes |m_{i+2}\rangle \otimes \cdots \otimes |m_N\rangle \Bigg\},$$

and $\vec{S}(i) \cdot \vec{S}(i+1)$ has three degenerate eigenstates

$$|\uparrow\rangle_i \otimes |\uparrow\rangle_{i+1} = \left| \left(\frac{1}{2}, \frac{1}{2}\right) 1,\, 1 \right\rangle,$$

$$|\downarrow\rangle_i \otimes |\downarrow\rangle_{i+1} = \left| \left(\frac{1}{2}, \frac{1}{2}\right) 1,\, -1 \right\rangle,$$

$$|\uparrow\rangle_i \otimes |\downarrow\rangle_{i+1} + |\downarrow\rangle_i \otimes |\uparrow\rangle_{i+1} = \sqrt{2} \left| \left(\frac{1}{2}, \frac{1}{2}\right) 1,\, -1 \right\rangle$$

with the same eigenvalue 1/4, it is easy to verify that $|\phi_{(1)I}^{NM}\rangle$ is an eigenstate with the eigenvalue $E_{(1/2)I}^{NM}$. The above conclusion for $|\phi_{(1/2)I}^{NM}\rangle$ is also proved in a similar way. Here, we have denoted $|1/2,\, 1/2\rangle$ and $|1/2,\, -1/2\rangle$ by $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively.

For the calculation of the eigenstates $|\phi_{(s)k}^{NM}\rangle$ and corresponding eigenvalue $E_{(s)k}^{NM}$ of the Hamiltonian $\hat{H}$ of the antiferromagnetic Heisenberg model, some numeral results are obtained and listed as follows.

On the basis $\{|\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle, |\downarrow\downarrow\uparrow\uparrow\rangle\}$ for the space

$$V_{(1/2)}^{[M=0]}(N=4)$$

we have the eigenstates

$$\phi_1 = \begin{bmatrix} -\frac{1}{4}\sqrt{2}\left(1-\frac{\sqrt{3}}{3}\right) \\ \frac{1}{4}\sqrt{2}\left(1+\frac{\sqrt{3}}{3}\right) \\ -\frac{\sqrt{6}}{6} \\ -\frac{\sqrt{6}}{6} \\ \frac{1}{4}\sqrt{2}\left(1+\frac{\sqrt{3}}{3}\right) \\ -\frac{1}{4}\sqrt{2}\left(1-\frac{\sqrt{3}}{3}\right) \end{bmatrix}, \quad \phi_2 = \begin{bmatrix} \frac{1}{2}\sqrt{1-\frac{\sqrt{2}}{2}} \\ -\frac{1}{2}\sqrt{1+\frac{\sqrt{2}}{2}} \\ 0 \\ 0 \\ \frac{1}{2}\sqrt{1+\frac{\sqrt{2}}{2}} \\ -\frac{1}{2}\sqrt{1-\frac{\sqrt{2}}{2}} \end{bmatrix}, \quad \phi_3 = \begin{bmatrix} 0 \\ 0 \\ \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \\ 0 \\ 0 \end{bmatrix},$$

$$\phi_4 = \begin{bmatrix} \frac{1}{4}\sqrt{2}\left(1+\frac{\sqrt{3}}{3}\right) \\ -\frac{1}{4}\sqrt{2}\left(1-\frac{\sqrt{3}}{3}\right) \\ -\frac{\sqrt{6}}{6} \\ -\frac{\sqrt{6}}{6} \\ -\frac{1}{4}\sqrt{2}\left(1-\frac{\sqrt{3}}{3}\right) \\ \frac{1}{4}\sqrt{2}\left(1+\frac{\sqrt{3}}{3}\right) \end{bmatrix}, \quad \phi_5 = \begin{bmatrix} -\frac{1}{2}\sqrt{1+\frac{\sqrt{2}}{2}} \\ -\frac{1}{2}\sqrt{1-\frac{\sqrt{2}}{2}} \\ 0 \\ 0 \\ \frac{1}{2}\sqrt{1-\frac{\sqrt{2}}{2}} \\ \frac{1}{2}\sqrt{1+\frac{\sqrt{2}}{2}} \end{bmatrix}, \quad \phi_6 = \begin{bmatrix} \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} \end{bmatrix}, \tag{14}$$

and the corresponding eigenvalues

$$\left.\begin{aligned} E_1 &= -\frac{1}{4}(3+2\sqrt{3})J\,, \\ E_2 &= -\frac{1}{4}(1+2\sqrt{2})J\,, \\ E_3 &= -\frac{1}{4}J\,, \\ E_4 &= \frac{1}{4}(3-2\sqrt{3})J\,, \\ E_5 &= \frac{1}{4}(1-2\sqrt{2})J\,, \\ E_6 &= \frac{3}{4}J\,. \end{aligned}\right\} \tag{15}$$

On the 20-dimensional space $V_{(1/2)}^{[M=0]}$ ($N = 6$), 70-dimensional space $V_{(1/2)}^{[M=0]}$ ($N = 8$) and 19-dimensional space $V_{(1)}^{[M=0]}$ ($N = 4$), we use computer to obtain all the eigenstates and eigenvalues. Because of the lack of space in this paper, we only give the energy levels of the ground states as

$$\left.\begin{aligned} E_g^{06}\left(\frac{1}{2}\right) &= -2.4937\ J\,, \\ E_g^{08}\left(\frac{1}{2}\right) &= -3.3750\ J\,, \\ E_g^{04}(1) &= -4.6458\ J\,. \end{aligned}\right\} \tag{16}$$

IV. Discussion

It follows from Eq. (16) that the energies of ground states of each site are

$$\left.\begin{aligned} \mathcal{E}_1 &= \frac{1}{4}E^{04}\left(\frac{1}{2}\right) = -0.4040\ J\,, \\ \mathcal{E}_2 &= \frac{1}{6}E^{06}\left(\frac{1}{2}\right) = -0.4156\ J\,, \\ \mathcal{E}_3 &= \frac{1}{8}E^{08}\left(\frac{1}{2}\right) = -0.4219\ J \end{aligned}\right\} \tag{17}$$

respectively in the cases of 4 sites, 6 sites and 8 sites, in which the energy of ground state of per site of the case with 8 sites is very close to the result

$$E_0 = -0.443\ J$$

for infinite site chain given by Hulthens[8]. In fact, as the site number of the calculation becomes large, the result of calculation will approach the exact result E. The fact

$$\frac{|\mathcal{E}_1 - \mathcal{E}_2|}{\mathcal{E}_2} = 2.78\%\,,$$

$$\frac{|\mathcal{E}_2 - \mathcal{E}_3|}{\mathcal{E}_3} = 1.49\%$$

tells us that the 8-site case is good enough for the calculation of the ground state. We would like to point out that Tavan has obtained the nearly exact variational wave function for the ground state in the case with 8-site ring[9], but what we obtained is just an exact eigenfunction of the Hamiltonian.

The method used in this paper is expected to approach other problems about many-mode coupling.

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