AIMS - Nepomechie - Quantum Mechanics and Quantum Spin Chains

Problem Set #3 Due 6:00 p.m. December 19, 2009

You cannot teach a man anything; you can only help him discover it within himself

- Galileo Galilei (1564 - 1642)

1. Recall from the lectures that the one-site shift operator for a closed chain of N sites, $U(N)$, can be constructed recursively as follows

$$U(N) = (U(N-1) \otimes \mathbb{I}(1))\,(\mathbb{I}(N-2) \otimes \mathcal{P})\,, \qquad U(2) = \mathcal{P}\,, \tag{1}$$

where $\mathbb{I}(N)$ is the identity operator for N-sites, i.e., the $2^N \times 2^N$ unit matrix; and $\mathcal{P}$ is the 4×4 permutation matrix,

$$\mathcal{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\,. \tag{2}$$

Similarly, the Heisenberg Hamiltonian $H(N)$ can be constructed recursively as follows

$$H(N) = h(N) + l(N)\,, \tag{3}$$

where $h(N)$ is given by

$$h(N) = h(N-1) \otimes \mathbb{I}(1) + \mathbb{I}(N-2) \otimes h(2)\,, \qquad h(2) = -\frac{1}{2}\,(\mathbb{I}(2) - \mathcal{P})\,, \tag{4}$$

and the last term $l(N)$ can be expressed as

$$l(N) = U(N)\,(\mathbb{I}(N-2) \otimes h(2))\,U(N)^{-1}\,. \tag{5}$$

Moreover, the three spin operators $S^i(N)$ can be constructed recursively as follows,

$$S^i(N) = S^i(N-1) \otimes \mathbb{I}(1) + \mathbb{I}(N-1) \otimes S^i(1)\,, \qquad S^i(1) = \frac{1}{2}\sigma^i\,, \qquad i = 1, 2, 3\,. \tag{6}$$

(We set $\hbar = 1$.)

   (a) Write *Sage* code which constructs $U(N)$, $H(N)$, $S^z(N)$ and $\vec{S}^2(N) = \sum_{i=1}^{3} S^i(N)^2$ using the above recipe. Display the matrices for $N = 4$.

   (b) Using *Sage*, explicitly verify for the case $N = 4$ that $\{H(N)\,, U(N)\,, \vec{S}^2(N)\,, S^z(N)\}$ form a set of mutually commuting operators.

2. $N = 4$ case

   (a) According to the Clebsch-Gordon theorem, what values of spin s should you expect for a Heisenberg chain with 4 sites? Hint:

$$\mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} = (\mathbf{0} \oplus \mathbf{1}) \otimes (\mathbf{0} \oplus \mathbf{1}) \,. \tag{7}$$

   (b) Use *Sage* to compute the eigenvalues and eigenvectors of the Heisenberg Hamiltonian $H(N)$ for the case $N = 4$.

   (c) Find $2^4 = 16$ (linearly independent) linear combinations of these vectors which are simultaneous eigenvectors of $\{H(N)\,, U(N)\,, \vec{S}^2(N)\,, S^z(N)\}$. Construct a table (similar to the one given in lecture for the case $N = 2$) with four columns for the corresponding quantum numbers: E (eigenvalue of $H(N)$), P (momentum; you may use instead the eigenvalue of $U(N)$), s (where $s(s+1)$ is the eigenvalue of $\vec{S}^2(N)$), and m (eigenvalue of $S^z(N)$). Your table should have 16 rows, one for each vector.

3. $N = 6$ case

   (a) Use *Sage* to compute just the eigenvalues of the Heisenberg Hamiltonian $H(N)$ for the case $N = 6$.

   (b) What is the ground-state (lowest) energy?

   (c) Do you expect that this approach is practical for much higher values of N (say, 20 or 30) ?

4. As discussed in lecture, unlike generic quantum spin chains, the Heisenberg chain is "integrable": it can be solved by Bethe ansatz. The main purpose of this problem is to verify that the Bethe ansatz correctly reproduces your $N = 4$ results.

   (a) Solve the Bethe ansatz equations

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^N = \prod_{k \neq j}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}\,, \qquad j = 1, 2, \ldots, M\,, \qquad M = 0, 1, \ldots, \frac{N}{2}\,, \tag{8}$$

   for $N = 4$ directly using *Sage*.

   (b) Evaluate the quantum numbers using

$$E = -\frac{1}{2} \sum_{j=1}^{M} \frac{1}{\lambda_j^2 + \frac{1}{4}}\,, \tag{9}$$

$$P = \frac{1}{i} \sum_{j=1}^{M} \ln\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right) \pmod{2\pi}\,, \tag{10}$$

$$s = m = \frac{N}{2} - M\,, \tag{11}$$

and then match your solutions to the "highest-weight" states (i.e., those states with $s = m$) in your table from Problem 2. You should have one solution (i.e., one set of Bethe roots $\{\lambda_j\}$) for each of the highest-weight states.

Hint: For the solution $\{\frac{i}{2}, -\frac{i}{2}\}$, the energy and momentum seem to be divergent. Proceed by "deforming" this solution: compute the energy and momentum using instead $\{\frac{i}{2}+\epsilon, -\frac{i}{2}+\epsilon\}$, and then take the limit $\epsilon \to 0$.

(c) Do you expect that this approach is practical for much higher values of N (say, 20 or 30) ?

5. Note that, for both $N = 2$ and $N = 4$, the *ground state* is described by a set of $M = N/2$ Bethe roots (i.e., $s = m = 0$), and all the Bethe roots are real. This in fact is true for all even values of N. As discussed in lecture, the corresponding "counting" function $Z(\lambda\,; \{\lambda_k\})$ is given by

$$Z(\lambda\,; \{\lambda_k\}) = N q_1(\lambda) - \sum_{k=1}^{\frac{N}{2}} q_2(\lambda - \lambda_k)\,, \tag{12}$$

where $q_n(\lambda)$ is given by

$$q_n(\lambda) = 2\arctan(2\lambda/n)\,. \tag{13}$$

(a) For the case $N = 4$, plot the ground-state counting function $Z(\lambda\,; \{\lambda_k\})$ as a function of λ, and verify that it is monotonic increasing. (Use the Bethe roots for the ground state which you found in Problem 4.)

(b) Again for the case $N = 4$, verify that the ground-state counting function evaluated at the Bethe roots is equal to

$$Z(\lambda_j\,; \{\lambda_k\}) = 2\pi J_j\,, \qquad j = 1, 2, \ldots, \frac{N}{2}\,, \tag{14}$$

where

$$J_1 = -J^{max}\,, \quad J_2 = -J^{max} + 1\,, \ldots\,, \quad J_{\frac{N}{2}} = J^{max}\,, \tag{15}$$

and

$$J^{max} = \frac{N}{4} - \frac{1}{2}\,. \tag{16}$$

6. As discussed in lecture, Eqs. (14)-(16) are equivalent to the Bethe ansatz equations (8) for the ground state; and they are particularly convenient to solve numerically by iteration. Indeed, an initial (zeroth) solution $\{\lambda_j^{(0)}\}$ can be obtained by dropping the second term in (12),

$$N q_1(\lambda_j^{(0)}) = 2\pi J_j\,, \tag{17}$$

which implies

$$\lambda_j^{(0)} = \frac{1}{2} \tan\left(\frac{\pi J_j}{N}\right) , \qquad j = 1, 2, \ldots, \frac{N}{2} . \tag{18}$$

Subsequent iterations can be obtained by solving

$$Z(\lambda_j^{(n+1)} ; \{\lambda_k^{(n)}\}) = 2\pi J_j , \qquad j = 1, 2, \ldots, \frac{N}{2} , \qquad n = 0, 1, \ldots \tag{19}$$

(a) Write a program in *Sage* for determining the ground-state Bethe roots based on (18), (19). Use Newton's method (Problem Set #1 !) to help find the roots. Note that

$$\frac{d}{d\lambda} q_n(\lambda) = \frac{n}{\lambda^2 + \frac{n^2}{4}} .$$

Test your code for the case $N = 6$, and make sure that you obtain the same ground-state energy which you found by brute-force diagonalization in Problem 3.

(b) Demonstrate that this approach is practical for much larger values of N by computing the ground-state energy for $N = 32$.