Journal of Statistical Physics, Vol. 33, No. 2, 1983

Exact Solution of a Large Class of Interacting Quantum Systems Exhibiting Ground State Singularities

Bill Sutherland[1] and B. Sriram Shastry[1,2]

Received May 12, 1983

We demonstrate how to construct a large class of interacting quantum systems for which an exact solution may be found for the ground state wave function and ground state energy for some range of interaction parameters. It is shown that the ground state exhibits singularities in these cases, and in some simple instances the exact ground state phase diagram and critical indices are also found.

KEY WORDS: Ground state singularities; spin systems; exactly soluble models.

A large number of quantum spin systems have been discovered whose ground state wave function and energy can be found exactly. Examples exist in all dimensionality, and the zero-temperatures phase diagram is sufficiently complicated to exhibit singularities as parameters of the Hamiltonian are varied, and thus exhibit two or more phases. These models are elaborations based on the original observation of Majumdar[(1)] for the exact ground state of a one-dimensional spin chain.

It is the purpose of this paper to elucidate the special properties of a system required for such a solution, and thus delineate the class of problems which can be exactly solved by the general methods. To this aim we define the notion of superstability, and then prove a theorem which enables us to construct the large class of exactly soluble models. Various features are illustrated by simple examples.

---

[1] Department of Physics, University of Utah, Salt Lake City, Utah 84112.

[2] Permanent address: Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India.

0022-4715/83/1100-0477$03.00/0

We first introduce the important concept of superstability. We shall say that an eigenstate ψ of the Hamiltonian H is superstable (SS) with respect to the operator J at H if

$$(H + \alpha J)\psi \equiv H(\alpha)\psi = E(\alpha)\psi \tag{1}$$

for all $|\alpha| < \epsilon$, with ϵ a nonzero, positive number. The quantity α is the field conjugate to J. The set of all α for which ψ is an eigenstate of $H(\alpha)$ will be called the region of superstability of ψ with respect to J. Note that ψ is *not* to depend upon α.

We easily prove the following results:

1. If ψ is superstable with respect to J, then ψ is an eigenstate of J.
2. The region of superstability is all α.
3. The set of all J's for which ψ is superstable form an $[(n-1)^2+1]$-dimensional vector space, where n is the dimension of the original vector space. (The number of mutually commuting independent operators, on the other hand, form only an n-dimensional vector space.)

We henceforth normalize, unless otherwise indicated, so that $J\psi = 0$ by replacing J by $J - \lambda I$, where λ is the eigenvalue of J corresponding to ψ.

We are concerned with finding the ground state of certain interacting systems, so we define the following additional concepts:

If ψ is the ground state of $H(\alpha)$ for all $|\alpha| < \boldsymbol{\alpha}$, $\boldsymbol{\alpha}$ a nonzero positive number, then we say that ψ is superstable as a ground state (SSGS) with respect to J at H.

Likewise we define the region of superstability of ψ as a ground state (RSSGS) to be the set of all α for which ψ remains a ground state of $H(\alpha)$. This region of the—in general—multidimensional field space α includes, of course, the origin $\alpha = 0$, but otherwise it is a very complicated region usually difficult to determine exactly.

To settle on notation, ψ always indicates our SS state which may also be SSGS. We have normalized so that $J\psi = 0$, and thus the energy eigenvalue is E, independent of α for all α. The operators and fields J, α are, of course, multidimensional. The ground state is always written as $\psi_0(\alpha)$ with ground state energy $E_0(\alpha)$. ψ, E coincide with $\psi_0(\alpha), E_0(\alpha)$ for the RSSGS.

The following general results relevant for the ground state are easily shown:

1. $E_0(\alpha)$ as a function of α is concave downwards.
2. $dE_0(\alpha)/d\alpha = [\psi_0(\alpha), J\psi_0(\alpha)] \equiv J(\alpha)$.
3. Legendre transformation gives us the quantity $E_0(J) \equiv E_0(\alpha) - \alpha J(\alpha)$, which is concave upwards.
4. The RSSGS is a convex region. Thus the set of J's for which ψ is a superstable ground state also form a vector space of dimension less than or

equal to $(n-1)^2+1$. If we determine that the RSSGS includes $|\alpha_\sigma| \leqslant \boldsymbol{\alpha}_\sigma$ for a set of independent J_σ, then the RSSGS also includes the region generated by the $\boldsymbol{\alpha}_\sigma$, meaning the polyhedron with vertices at $(0, \ldots, 0, \pm \boldsymbol{\alpha}_\sigma, 0, \ldots, 0)$; or the convex hull.

We now give some examples to illustrate the concepts, and indicate they are not empty.

1. First, consider the simplest case of a vector space of dimension $n=2$. Then the most general Hamiltonian with a SS state is $H_{ij} = \delta_{i2}\delta_{j2}\alpha$, $(i, j = 1, 2)$. The RSSGS is then clearly $\alpha > 0$.

A slightly more complicated case is $n=3$. We take the Hamiltonian as

$$H = \begin{vmatrix} 0 & 0 & 0 \\ 0 & \alpha & \lambda \\ 0 & \lambda^* & \beta \end{vmatrix} \tag{2}$$

The condition which determines the RSSGS is that the nonzero eigenvalues be positive, or $\alpha\beta - |\lambda|^2 > 0$, $\alpha + \beta > 0$.

2. Consider now the two-spin Hamiltonian

$$H = \mathbf{S} \cdot \mathbf{S}', \qquad S(S+1) = \mathbf{S} \cdot \mathbf{S} \tag{3}$$

If we write the total spin as

$$\mathbf{L} = \mathbf{S} + \mathbf{S}', \qquad \mathbf{L} = 0, 1, 2, \ldots, 2S \tag{4}$$

then we may reexpress the Hamiltonian as $H = (1/2)L \cdot L - S(S+1)$. This immediately gives us the eigenvalues. The ground state is given by $L = 0$, $E_0 = -S(S+1)$ and the ground state wave function is a nondegenerate singlet.

First, let $J = L_z$; $[H, L_z] = 0$, and thus all states are SS. We may explicitly find the energies as

$$E(\alpha) = \tfrac{1}{2}L(L+1) - S(S+1) + \alpha L_z \tag{5}$$

For a given L, the lowest energy is always at $L_z = \pm L$. Thus the levels $L = 0$ and $L = 1$ cross at $\alpha = \pm 1$, and we find the RSSGS to be $|\alpha| \leqslant \boldsymbol{\alpha} = 1$.

Second, let $J = S_z S_z'$. This operator acting on the singlet state can only give a singlet contribution, and thus the singlet state is SS with respect to this J. The eigenvalue λ of J is determined by $3\lambda = -S(S+1)$, so if

$$H = \mathbf{S} \cdot \mathbf{S}' + \sum_{\sigma = x,y,z} S_\sigma S_\sigma' \alpha_\sigma \tag{6}$$

then

$$E(\alpha) = -S(S+1)\left(1 + \frac{\sum \alpha_\sigma}{3}\right) \tag{7}$$

The RSSGS, although nonzero, is a more complicated calculation.

3. Let us now consider the spin–1/2 Heisenberg–Ising chain with Hamiltonian

$$H(\alpha) \equiv H(\delta) + \alpha J = \sum_{n.n.} [\mathbf{S} \cdot \mathbf{S}' + \delta S_z S_z'] + \alpha \sum S_z \tag{8}$$

Since $[H(\delta), J] = 0$, all states are SS with respect to J. However, to answer the more interesting question of the RSSGS of the singlet ground state $\psi_0(\delta)$, it has been shown by Yang and Yang[2] that for $\delta > 1$ the RSSGS is given by

$$|\alpha| \leqslant 2(\sinh\lambda) \sum_{n=-\infty} \frac{(-1)^n}{2\cosh(n\lambda)}$$

$$= \frac{\pi \sinh\lambda}{\lambda} \sum_{n=-\infty}^{\infty} \operatorname{sech}\left[\frac{\pi^2}{2\lambda}(1+2n)\right] \equiv \boldsymbol{\alpha} \tag{9}$$

where $\cosh\lambda = \delta + 1$.

The operator J is an extensive parameter, and J/N is the intensive magnetization per spin. Then the field $-\alpha$ serves as a magnetic field. Yang and Yang also find that for $|\alpha|$ near $\boldsymbol{\alpha}$, the energy per spin is given by

$$E(\alpha) \approx |\alpha - \boldsymbol{\alpha}|^{3/2} \frac{2\alpha}{3\pi} \left[\frac{\sinh^3\lambda}{2} \sum_{n=-\infty}^{\infty} \frac{(-1)^n n^2}{\cosh n\lambda} \right]^{-1/2} \tag{10}$$

Thus the singularity of the ground state as a function of α is not simply first order at $|\alpha| = \boldsymbol{\alpha}$, but instead is continuous with an appropriate critical exponent.

4. If $[H, J] = 0$, then H and J can be simultaneously diagonalized, and all states are SS. If the dimension n of the vector space is finite, then the parameter space is covered by separate RSSGS regions of different SS states. On the other hand, if the dimension n of the vector space increases without limit, as for a thermodynamic system, the RSSGS regions usually do not remain finite. Example 3 illustrated a situation where in fact the RSSGS for the singlet state remains finite. In general, a ground state which is SS will be also SSGS if the dimension n of the vector space is finite, whether H and J commute or not.

We now wish to consider a more general case where the vector space V is the tensor product of two vector spaces $V^1 \times V^2$. The notation is as before with the addition of a superscript to indicate when an operator acts in a vector space V^j. The superscript will never indicate powers of an operator. As a first example, we treat the Hamiltonian:

$$H = H^1 \times I^2 + \alpha J^1 \times K^2 \equiv H^1 + \alpha J^1 K^2 \tag{11}$$

H^1 is the previous Hamiltonian SS with respect to J^1. The expression

$\alpha J^1 \times K^2$ in turn is shorthand for a generally more complicated expression

$$\alpha J^1 \times K^2 = \sum_{\sigma,\tau} \alpha_{\sigma\tau} J_\alpha^1 K_\tau^2 \tag{12}$$

Thus the fields α in general are multidimensional. We further assume that the operator K^2 is bounded so that the eigenvalues γ_j lie between $-\gamma$ and γ. This we indicate as $|K^2| \leqslant \gamma$. The corresponding eigenstates we write as ψ_j^2.

Let us look at the action of H on $\phi^1 \times \psi_j^2$, where ϕ^1 is any vector in V^1:

$$H\phi^1 \times \psi_j^2 = \left(H^1 + \alpha\gamma_j J^1\right)\phi^1 \times \psi_j^2 \tag{13}$$

Since $|\gamma_j| \leqslant \gamma$, we will be within the RSSGS if $|\alpha|\gamma \leqslant \boldsymbol{\alpha}$. Then all states $\psi^1 \times \psi_j^2$ are degenerate ground states with ground state energy E^1.

Let us now look at a more complicated situation where

$$H = H^1 \times I^2 + I^1 \times H^2 + \alpha J^1 \times K^2 \tag{14}$$

Consider the action of H on $\psi = \psi^1 \times \psi_0^2$:

$$H\psi = \left(E^1 + E_0^2\right)\psi \tag{15}$$

Thus ψ is SS with respect to $J^1 \times K^2$, as is any state $\psi^1 \times \psi_j^2$.

On the other hand,

$$E_0 \geqslant \min H^2 + \min(H^1 + \alpha J^1 K^2) = E_0^2 + \min(H^1 + \alpha J^1 K^2) \tag{16}$$

But by our previous argument, if $|\alpha|\gamma < \boldsymbol{\alpha}$, $E_0 \geqslant E_0^2 + E^1$. Thus considering ψ as a trial state, we have the upper bound equal to the lower bound, and conclude that $\psi = \psi^1 \times \psi_0^2$ is SSGS with ground state energy $E_0 = E_0^2 + E^1$. The RSSGS includes the region $|\alpha|\gamma \leqslant \boldsymbol{\alpha}$, but may easily be larger.

We remark that nowhere have we required that there exist a state SS with respect to K^2 at H^2.

The previous considerations lead us to the following:

Cluster Theorem. Let us consider a set of Hamiltonians H^j ($j = 1, \ldots, N$) acting on the vector spaces V^j. Assume these have states ψ^j SSGS with respect to operators J_σ^j. Let the RSSGS include the region generated by $|\alpha_\alpha^j| \leqslant \boldsymbol{\alpha}_\sigma^j$. Further assume K_τ^j to be bounded operators with $|K_\tau^j| \leqslant \gamma_\tau^j$. Then the following Hamiltonian,

$$H = \sum_j H^j + \sum_{\substack{j,l \\ \sigma,\tau}} J_\sigma^j K_\tau^l \alpha_{\sigma l}^{j\tau} \tag{17}$$

acting on $V = V^1 \times \cdots \times V^N$ has the state $\psi = \psi^1 \times \cdots \times \psi^N$ SSGS with respect to the interactions $J_\sigma^j K_\tau^l$. The ground state energy is $E = E^1 + \cdots + E^N$. The RSSGS includes the region in parameter space $R = R^1 \times \cdots \times R^N$, where R^j is generated by

$$\sum_{l,\tau} |\alpha_{\alpha\tau}^{jl}| \gamma_\tau^l \leqslant \boldsymbol{\alpha}_\sigma^j \tag{18}$$

If l ranges only over a finite number of neighbors, then the resulting RSSGS remains finite in the limit $N \to \infty$.

The proof is simply by induction on the previous case.

Because of limited space we can only offer a few simple examples of applications of the cluster theorem to specific systems. References 3 and 4 give two important examples to which the cluster theorem applies. Two further examples are offered to illustrate important aspects.

5. Let us consider a chain of spins $\mathbf{T}_j$ alternating with pairs of spins $\mathbf{S}_j, \mathbf{S}_j'$, $T = S$. The interaction is chosen to be

$$H = \sum_{j=1}^{N} 2\alpha \mathbf{S}_j \cdot \mathbf{S}_j' + (\mathbf{S}_j + \mathbf{S}_j') \cdot (\mathbf{T}_j + \mathbf{T}_{j+1}) \tag{19}$$

The pairs of spins $\mathbf{S}, \mathbf{S}'$ form a cluster, and the SS state is a product of singlet states for each of these N clusters. This state is SSGS for α sufficiently large. When a cluster is in the singlet state, the chain is broken at this point, and this system is representative of a large class of systems in which clusters act as "switches" causing the lattice to fall into independent pieces. The ground state has a degeneracy $(2T + 1)^N$ since the T spins are then independent. The ground state energy is $E_0 = -2\alpha NS(S + 1)$. We may also establish that the RSSGS includes the region $\alpha > 1$.

On the other hand, if $\alpha = 1$, we may consider the alternate cluster scheme $T_1S_1, S_1'T_2, S_2S_2', T_3S_3, S_3'T_4, S_4S_4', \ldots$. It is degenerate with the previous state, and if we consider it as a trial state, it gives us the estimate $E_0 \leqslant -[\alpha + 1]NS(S + 1)$. Thus, the RSSGS is $\alpha > 1$.

6. As a second example, let us consider a mean field model made up of N^2 chains, the chain being the cluster with the Heisenberg–Ising Hamiltonian of example 3. The interaction we take to be $\alpha mm'/N$ between all pairs of chains. Here $m = \sum S_z / N$ is the z component of magnetization of a chain. The ground state is a product of the singlet ground states of an individual chain as given in Ref. 2.

The RSSGS we determine by minimizing the mean field ground state energy per spin,

$$E_0/N^2 = E_0(m) - \frac{\alpha m^2}{2} \tag{20}$$

where $E_0(m)$ is the ground state energy per spin of an individual chain. The boundary of the RSSGS occurs at an $\boldsymbol{\alpha}$ which gives a second minimum of the energy at $\mathbf{m}$, where

$$E_0(\mathbf{m}) - \frac{\alpha\mathbf{m}^2}{2} = E_0(0) \tag{21}$$

This value of $\boldsymbol{\alpha}$ is considerably larger than the boundary value of the RSSGS of an individual chain as given in the previous example 3.

With the cluster theorem, we have given a procedure for constructing larger and more complicated systems, which in turn have a state which is SSGS. We will be most interested in thermodynamic systems which we have shown to have a nonzero RSSGS in the limit $N \to \infty$. In proving the cluster theorem, we were only concerned with the existence of the RSSGS. This is sufficient to also establish the existence of a singularity of the ground state energy as a function of the fields α, since a very simple trial function can give a lower energy than the SS cluster functions for sufficiently large $|\alpha|$. Another way of saying the same thing: The ground state cannot be independent of the external parameters α for all α, and thus a singularity must exist at the boundary of the RSSGS.

To locate the boundary of the RSSGS exactly is difficult. By better and better trial functions, we can enclose the boundary from the outside, and by better and better lower bounds on the Hamiltonian we may enlarge our estimate of the interior of the RSSGS. Depending on our diligence, this can give us quite a good approximation to the boundary of the RSSGS.

On the other hand, designation of the clusters and interactions is arbitrary, and it may happen that two different cluster schemes may give two different RSSGS with a common portion of boundary. Examples are Ref. 4 and our fifth example. In this case we can rigorously locate the singularity, and conclude that it is of first order with a discontinuity in the normal derivative upon crossing the common boundary. However, it would be a mistake to conclude that all singularities at the boundary of a RSSGS must be of first order, as the example of the Heisenberg–Ising chain showed.

A detailed discussion of the nature of the SSGS phase, the microscopic theory of the excitations above this phase, and the connection with the "standard" theory of phase transitions will be presented in an expanded paper. We simply remark here, that for a system built of finite clusters, it is reasonable to designate the RSSGS phase as a quantum fluid, as was done in Ref. 3.

ACKNOWLEDGMENT

This work was supported in part by National Science Foundation Grant No. DMR81-06223.

REFERENCES

1. C. K. Majumdar, Exact solution of an antiferromagnet, *J. Phys. C* **3**:911–914 (1970).
2. C. N. Yang and C. P. Yang, One-dimensional chain of anisotropic spin–spin interactions. III. Application. *Phys. Rev.* **151**:258–264 (1966).
3. B. S. Shastry and B. Sutherland, Exact ground state of a quantum mechanical ferromagnet, *Physica* **108B**:1069–1070 (1981).
4. B. S. Shastry and B. Sutherland, Excitation spectrum of a dimerized next-neighbor antiferromagnetic chain, *Phys. Rev. Lett.* **47**:964–967 (1981).