*Indian J. Phys.* **78 (6)**, 463-469 (2004)

AN INTERNATIONAL JOURNAL
IJP

# Study of bound states in Schrödinger equation of a particle using the Hopfield model of artificial neural network

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*Received 5 September 2003, accepted 21 April 2004*

**Abstract** : In the solution of Schrödinger equation for a particle, confined within one-dimensional infinitely hard boundaries, there are discrete energy states in which the particle can exist. The particle has finite probability of finding itself inside the boundaries for ground, first, second... $n$-th excited states (*i.e.* for quantum numbers $n$ = 1, 2, 3,...$n$). To explore the optimized possibility of finding a particle inside the boundaries for any quantum number, we use the Stochastic Hopfield Neural Network Model with Mean field Approximation of Simulated Annealing. In this process, the network activation dynamics at a given temperature, reaches the thermal equilibrium position. This equilibrium position is the steady state position of the network that is achieved only if the probability of visiting the global minimum energy states becomes maximum and it refers to the optimized probability of finding the particle inside the boundaries.

**Keywords** : Bound states, Schrödinger equation, Hopfield model, mean field approximation, simulated annealing.

**PACS Nos.** : 07.05.Mh, 03.65.Ge

## 1. Introduction

Now a days, the computer technology has led to belief that a machine can realize intelligent tasks. An intelligent system, capable of modeling the human behavior, has captured the attention of the world for years [1,2]. The approach of neural computing is to capture the guiding principles that underlie the brain's solution for many intelligent tasks and to apply them to computer systems. We do not know how the brain works for these intelligent tasks but we do know that it uses billions of slow units that are highly interconnected in immensely complex fashion, each being connected to thousands of others and working together to solve all the tasks. We call this structure a Biological Neural Network [3]. Brain's basic structure is intrinsically suited to parallel problems rather than serial ones. We can simulate this structure in a serial fashion, allowing the parallelism of the brain's structure. We call this structure an Artificial Neural Network [4]. It consists of numerous simple processing units [5] that can be globally programmed for computation and are enable to collectively solve complicated and ambiguous problems.

In problems such as Pattern Classification, Associative Memories, Optimization, Vector Quantization and Control Applications, the principles of neural network are directly applicable. The most successful application of neural network is for the optimization problems [6]. It is possible to capture such a problem with a feedback network, where the units and connection strengths are identified by comparing a cost function of the problem with the energy function of the network given by Hopfield [7,8], expressed in terms of processing elements and connection strengths. The solution of the problem can be achieved by determining the state of the network at the global minimum energy of the energy landscape. In this process, it is necessary to escape the network from the local minima of the energy landscape, which is accomplished by using a simulated annealing schedule of mean field approximation [9].

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In this paper, we observe the bound states for a particle confined in a finite one-dimensional box with infinitely hard boundaries. These bound states may be obtained by solving the Time Independent Schrödinger Equation [10] for the wave function confined within the finite boundaries $0 < x < l$. So, the particle has finite probabilities of finding itself in the bound states for ground, first, second... $n$-th excited states (*i.e.* for quantum numbers $n = 1, 2, 3...n$). A Hopfield-type feed back network can be used to store a pattern environment in the form of quantum numbers and the probabilities of finding the particle inside the boundaries for the quantum numbers. The trained network is capable of estimating the optimized probability of finding the particle inside the boundaries for any unknown quantum number for which the network has not been trained. As this unknown input pattern is represented to the network, it approaches the higher energy states. In order to achieve the global minimum energy states by escaping the local (false) minimum energy states, we are using Simulated Annealing in which the constraint parameter (temperature $T$) is reduced as per the annealing schedule [11] of mean field approximation [12]. At the allowable lower limit of constraint parameter (*i.e.* $T \approx 0$) or thermal equilibrium, the network achieves the global minimum energy states representing the optimized probability of finding the particle inside the boundaries.

## 2. Bound state condition and the Hopfield model

We may specify the particle's position with the assumption that it is confined to move along $x$-axis between finite boundaries $x = 0$ and $x = l$ of infinitely hard walls. For convenience, we may assume that the potential energy $V$ of the particle is infinite on both sides of the boundaries and zero inside. Therefore, the Time Independent Schrödinger Equation becomes,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0, \tag{2.1}$$

or,

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \tag{2.2}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

The solution of eq. (2.1) can be given as

$$\psi = A\sin(kx + \theta). \tag{2.3}$$

Using boundary condition $\psi \to 0$ as $x \to 0$ and $\psi \to 0$ as $x \to l$, we get

$$\theta = 0 \tag{2.4}$$

and

$$k_n = n\pi/l, \tag{2.5}$$

where $n$ is an integer.

Substituting the values of $\theta$ and $k_n$ from eqs. (2.4) and (2.5) in eq. (2.3), we get the plane wave solution within the boundaries as

$$\psi_n = A\sin\frac{nx\pi}{l} \tag{2.6}$$

Thus, the normalized wave function may be given as

$$\psi_n = \sqrt{\frac{2}{l}}\sin\frac{nx\pi}{l}. \tag{2.7}$$

The corresponding eigen values may be obtained from the eq. (2.5) as

$$k_n = \sqrt{\frac{2mE_n}{\hbar^2}} \tag{2.8}$$

and

$$E_n = \frac{\hbar^2 n^2\pi^2}{2ml^2}. \tag{2.9}$$

The integral of $|\psi_n|^2$ over the whole space within boundaries, is finite. The probability of finding the particle between the region $x_a$ and $x_b$ within the boundaries $x = 0$ and $x = l$ in the $n$-th excited state, can be defined as

$$\left(p_{x_a x_b}\right)_n = \int_{x_a}^{x_b} |\psi_n|^2 dx$$

and

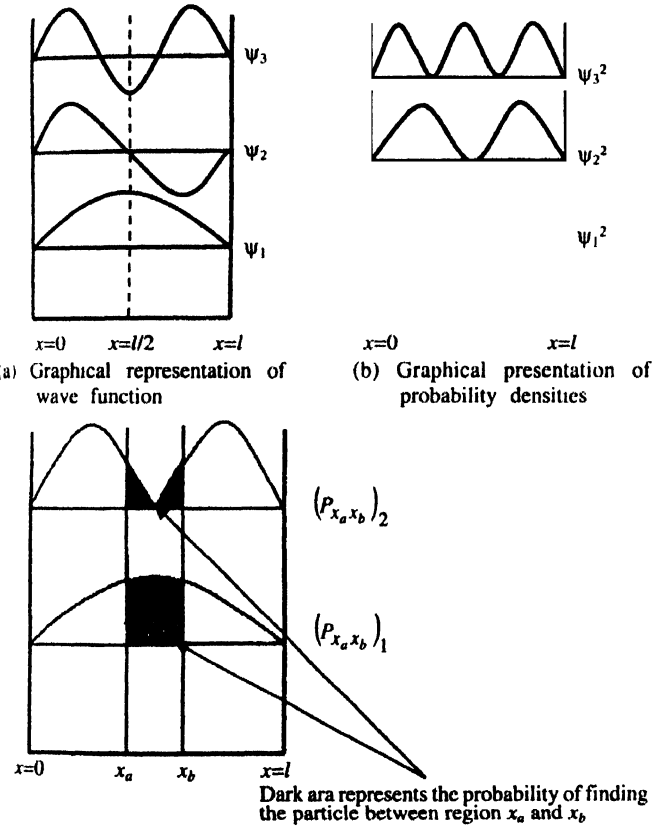
$$\left(p_{x_a x_b}\right)_n = A^2 \int_{x_a}^{x_b} \sin^2\left(\frac{nx\pi}{l}\right) dx$$

$$= \frac{2}{l}\int_{x_a}^{x_b} \sin^2\left(\frac{nx\pi}{l}\right) dx,$$

$$(p_{x_a x})_n = \left[\frac{x}{l} - \left(\frac{1}{2n\pi}\right)\sin\left(\frac{2nx\pi}{l}\right)\right]_{x_a}^{x_b}. \qquad (2.10)$$

On putting $n$ = 1, 2, 3.....$n$, we get the probabilities of finding the particle inside the region $x_a$ and $x_b$ as $(p_{x_a x_b})_1, (p_{x_a x_b})_2, \ldots\ldots\ldots (p_{x_a x_b})_n$ for ground, first....$n^{th}$ excited states.

The graphical representation for wave function $\psi_1$, $\psi_2$, ..... $\psi_n$, and the probability densities $(p_{x_a x_b})_1, (p_{x_a x_b})_2, \ldots\ldots\ldots (p_{x_a x_b})_n$ can be shown by the Figure 1. The $\psi_n$ may be negative or positive, but $|\psi_n|^2$




(a) Graphical representation of wave function

(b) Graphical presentation of probability densities

Dark ara represents the probability of finding the particle between region $x_a$ and $x_b$

(c) Graphical representation of probability densities between region $x_a$ and $x_b$

**Figure 1.** Graphical representation of wave function and probability densities of a particle confined in a box with rigid walls.

will always be positive and since $\psi_n$ will be normalized, its values at a given $x$ will be equal to the probability density for finding the particle there, by $|\psi_n|^2 \to 0$ as $x \to 0$ and $x \to l$. At a particular region in the box, the probability of finding the particle may be different for different quantum numbers. A particle in the lowest energy level *i.e.* $n$ = 1 (ground state) is most likely to be in the middle of the box, while a particle with the next higher energy levels can never be there.

The Hopfield network is a fully interconnected network [7,8] in which weights are symmetric and output function of each unit is bipolar. The input pattern can be applied to all of the nodes at once. It moves through the succession of states until it reaches the stable state. We can use this model with its energy function estimation and we assume that the energy associated with each output state depends on network parameter like weights, bias *etc*. This energy landscape refers to change in output state of the network with time and the hollows of the landscape represent the basins of attraction called global minima, which are the areas where the energy function of the landscape is minimum *i.e.* energy minima and can be used to store the input patterns. First of all we specify the limit of the region within the boundaries with the values of $x_a$, $x_b$ and in this region the network can estimate the probability of finding the particle for different quantum numbers with the help of eq. (2.10). Now, we have a pattern environment in the form of sample of quantum numbers $n$ = 1, 2, 3...$n$ and probabilities of finding the particle inside the boundaries $(p_{x_a x_b})_1, (p_{x_a x_b})_2, \ldots\ldots\ldots (p_{x_a x_b})_n$ for these quantum numbers and it can be represented to the network. The state of the network changes with time. This change in the state of the network continues until the network activation dynamics reaches a stable state (global minimum energy state). At the stable state, sample of quantum numbers and the probabilities of finding the particle inside the boundaries for these quantum numbers are stored in different global minima. The activation dynamics of the network can be expressed as

$$S_i(t+1) = \mathrm{sgn}\left(\sum_{i \neq j} S_j(t) W_{ij}\right) = S_i(t)$$

with

$$W_{ij} = S_i S_j, \qquad (2.11)$$

as the weights are symmetric and states are bipolar.

At the stable state, each minima of the energy landscape represents a different probability for a different quantum number. The number of input patterns that can be stored, depends on the number of units and the strength of connecting links. The energy function of global minimum of energy landscape can be given as

$$E(S) = -\frac{1}{2}\sum_{i \neq j} W_{ij} S_i S_j + \sum_i \theta_i S_i, \qquad (2.12)$$

where $\theta_i$ is the threshold function.

Now, as the unknown input pattern sample in the form of quantum numbers (which is not given earlier) is being presented to the network, it starts iterations and settles to a stable state. This state can be represented in the form of associated energy as

$$E'(S) = -\frac{1}{2}\sum_{i\neq j} W_{ij} S_i' S_j' + \sum \theta_i S_i' . \qquad (2.13)$$

The network can estimate the optimized probability of finding the particle inside the bound states for the given quantum number by minimizing the difference between the energy functions. The change in energy function due to update of $k$-th unit is given by

$$\Delta E = E'(S) - E(S)$$

$$= \left[ -\frac{1}{2}\sum_{i\neq j} W_{ij} S_i' S_j' + \frac{1}{2}\sum_{i\neq j} W_{ij} S_i S_j + \sum_i \theta_i (S_i' - S_i) \right]$$

$$- \left[ \frac{1}{2}\sum_i W_{ik} S_i' S_k' + \frac{1}{2}\sum_j W_{jk} S_i' S_k' - \theta_k S_k' \right]$$

$$+ \left[ \frac{1}{2}\sum_i W_{ik} S_i S_k + \frac{1}{2}\sum_j W_{jk} S_j S_k - \theta_k S_k \right]. \qquad (2.14)$$

Since $S_i = S_i'$ for $i \neq j$, eq. (2.14) becomes

$$\Delta E = -S_k' \left[ \frac{1}{2}\sum_i W_{ik} S_i' + \frac{1}{2}\sum_j W_{jk} S_j' - \theta_k \right]$$

$$+ S_i \left[ \frac{1}{2}\sum W_{ik} S_i + \frac{1}{2}\sum W_{jk} S_j - \theta_k \right] \qquad (2.15)$$

But we have assumed that the weights are symmetric *i.e.* $W_{ij} = W_{ji}$, so we have

$$\Delta E = -S_k' \left[ \frac{1}{2}\sum_i W_{ik} S_i' - \theta_k \right] + S_k \left[ \frac{1}{2}\sum_i W_{ik} S_i - \theta_k \right]. \qquad (2.16)$$

If in addition, $W_{ii} = 0$, then since $S_i = S_i'$ for $i \neq j$, we have

$$\Delta E = (S_k - S_k') \left| \frac{1}{2}\sum W_{ik} S_i - \theta_k \right. \qquad (2.17)$$

As the change in energy function becomes minimized, *i.e.* $\Delta E \leq 0$, the network settles to the minimum of energy landscape which represents the stable states. At the stable state, the optimized probability from the stored sample will be recalled.

Consider a case in which the number of desired patterns is less than the number of basins of attraction There will be so called local (false) minima due to the additional basins of attraction. During recall, it is likely that the state of the network, as it evolves from the initial state corresponding to the input pattern, may settle in a local (false) minimum. The recalled pattern corresponding to the false minimum may not be the correct pattern, thus resulting in an error in recalling of the desired pattern. Error in recalling of desired patterns due to false minima can be reduced by designing the energy minima for the given patterns in an optimal way, so that the given pattern corresponds to the lowest energy minimum in the network and further by using a stochastic update of the state of each unit instead of the deterministic update dictated by the activation values and the output function. In order to reduce the error in recalling the desired pattern and reach the global minimum energy states by escaping the local (false) minimum energy states, we can use Simulated Annealing in which the constraint parameter (temperature $T$) is reduced as per the annealing schedule [11] of mean field approximation [12]. As the temperature is reduced slowly, the probability of visiting the lower energy states increases and at the possible minimum energy state (global minimum energy state), the network will be in the thermal equilibrium (as shown by Figure 2).

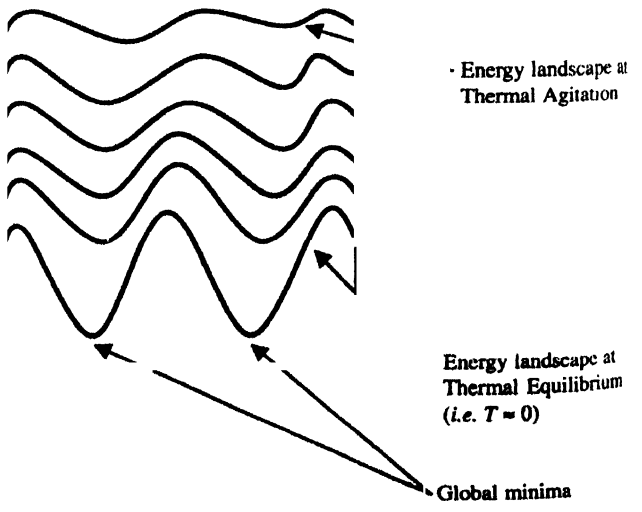



**Figure 2.** Achieving the global minima by reducing the temperature according to the annealing schedule.

At the thermal equilibrium, the network captures the approximately correct probability of finding the particle inside the boundaries.

## 3. Optimization for boundary state condition with simulated annealing

To explore the optimized probability of finding the particle inside the boundaries, a structure and learning algorithm similar to the Hopfield net with the probabilistic update rule can be used. The probabilistic distribution of states will be stationary or independent of time for a network to be in stochastic equilibrium. On decreasing the temperature according to the probabilistic annealing schedule, the network produces a new energy landscape, which contains the minimum energy states with respect to the previous one. This process continues until the network reaches the global minimum energy state. This state refers to the optimized probability of finding the particle inside the boundaries.

Now, after specifying the limit of the region within the boundaries with the values of $x_a$ and $x_b$ the network can estimate the probability of finding the particle for different quantum numbers with the help of eq. (2.10) and store them in the different global minima of energy function using the activation dynamics expressed by eq. (2.11).

As the new quantum number $n = m$ is being represented to the network, it approaches higher energy states, so that the probability of visiting the lower energy states decreases. The probability distribution of states can be given as

$$P(s) = \frac{1}{z} e^{-\frac{E(s)}{T}} \tag{3.1}$$

Here, $z$ represents the partition function.

Thus, we can see from eq. (3.1) that at high temperatures, the probability of visiting the lower energy states decreases. Now, as the temperature is reduced as per the annealing schedule of mean field approximation, the probability of visiting the lower energy states increases. Finally, at the allowable lower limit of temperature *i.e.* $T \approx 0$, the probability of visiting the lower energy states approaches 1 (*i.e.* highest probability), so that the network settles in the global minimum energy state, describing the optimized probability of finding the particle inside the boundaries for the unknown quantum number. The implementation of simulated annealing requires computation of stationary probabilities at thermal equilibrium for each annealing schedule. To speed up this process, we may use mean field approximation [12] in which the stochastic update of bipolar units is replaced with deterministic states. The basic idea of mean field approximation is to replace the fluctuating activation values of each unit by their average values

$$\langle y_i \rangle = \left\langle \sum_i W_{ij} S_i \right\rangle,$$

$$\langle y_i \rangle = \sum W_{ij} \langle S_i \rangle, \tag{3.2}$$

where $\langle S_i \rangle$ is the average of the states of $i$-th unit and

$$\langle S_i \rangle = \tanh\left(\frac{y_i}{T}\right). \tag{3.3}$$

In the mean field approximation, the activation of $i$-th unit $y_i$ is replaced by $\langle y_i \rangle$, so that using eq. (3.3), we have

$$\langle S_i \rangle = \tanh\left(\frac{1}{T}\sum_j W_{ij}\langle S_j \rangle\right). \tag{3.4}$$

The set of these equation is a result of minimization of an effective energy defined as a function of temperature [13]. Thus, eq. (3.7) may be expressed as

$$\langle S_i \rangle = \tanh\left(-\frac{1}{T}\frac{\partial E(\langle S \rangle)}{\partial(\langle S_i \rangle)}\right). \tag{3.5}$$

The change in energy function for the average states of $i$-th unit is given by

$$\frac{\partial E(\langle S \rangle)}{\partial(\langle S_i \rangle)} = -\frac{1}{2}\sum_{i \neq j} W_{ij} S_j + \theta_i. \tag{3.6}$$

So that from eq. (3.6), we have

$$\langle S_i \rangle = \tanh\left[-\frac{1}{T}\left(\frac{1}{2}\sum_{i \neq j} W_{ij} S_j + \theta_i\right)\right. \tag{3.7}$$

These nonlinear deterministic equations are solved iteratively. As the temperature is lowered to the minimum

value, the steady equilibrium values of $\langle S_i \rangle$ have been obtained. At the allowable lower temperature, the probability of visiting the global minima has the maximum value *i.e.* $P(s) = \frac{1}{z} e^{-\frac{E(s)}{T}} \approx 1$, so that the network will achieve one of the global minima, which represents the optimized probability of finding the particle inside the boundaries for the given quantum number. The average value of the state of the network is described in terms of the average value of the output of each unit of the network, which represents the optimized probability of finding the particle inside the boundaries for the given quantum number as the new energy function represents the global minimum of the landscape.

$$i.e.\ \langle S_i \rangle = k\left(p_{x_a x_b}\right)_m, \tag{3.8}$$

where $k$ is the proportionality constant.

The above procedure can be explained by following algorithmic steps.

## 4. Algorithm

(1) Initialize the weights and threshold by providing small random numbers and set the network to its average value.

(2) Calculate the probability of finding the particle inside the boundaries for different quantum numbers as

$$\left(p_{x_a x_b}\right)_n = \left[\frac{x}{l} - \left(\frac{1}{2n\pi}\right)\sin\left(\frac{2nx\pi}{l}\right)\right]_{x_a}^{x_b}$$

(3) Store the pattern environment in the form of quantum numbers and the probabilites of finding the particle inside the boundaries for these quantum numbers in different global minima of energy landscape by using the activation dynamics of the Hopfield neural network as

$$S_i(t+1) = \mathrm{sgn}\left[\sum_{i \neq j} S_j(t) W_{ij} \right] = s_i(t)$$

with

$$W_{ij} = S_i S_j.$$

(4) Present any unknown quantum number $n = m$ to the network for which the network has not been trained.

(5) Reduce the temperature as per the annealing schedule, so that the probability of achieving the global minima approaches 1 *i.e.* $P(s) = \frac{1}{z} e^{-\frac{E(s)}{T}} \approx 1$.

Thus, for each schedule

*(5.1) estimate the energy function for these stored patterns as*

$$E(S) = -\frac{1}{2}\sum_{i \neq j} W_{ij} S_i S_j + \sum_i \theta_i S_i.$$

*(5.2) calculate the average value of states as*

$$\langle S_i \rangle = \tanh\left(\frac{1}{T}\frac{\partial E(\langle S \rangle)}{\partial(\langle S_i \rangle)}\right)$$

*(5.3) calculate the change in energy function for the average value of states of i-th unit as*

$$\frac{\partial E(\langle S \rangle)}{\partial(\langle S_i \rangle)} = -\frac{1}{2}\sum_{i \neq j} W_{ij} S_j + \theta_i.$$

*(5.4) calculate the probability for achieving the global minima using equation*

$$P(s) = \frac{1}{z} e^{-\frac{E(s)}{T}}.$$

(6) End.

## 5. Conclusion

To estimate the optimized probability of finding the particle inside the boundaries for any given quantum number; we may use a structure and learning algorithm similar to the Hopfield Model with Mean field approximation of Simulated Annealing. In this outgoing Discussion, the following observations can be made

(i) We can train a network which is capable of storing a pattern environment in the form of quantum numbers $n$ = 1, 2, 3,...$n$ and the probabilities of finding the particle $\left(p_{x_a x_b}\right)_1, \left(p_{x_a x_b}\right)_2, \ldots\ldots\ldots \left(p_{x_a x_b}\right)_n$ for these quantum numbers.

(ii) Hopfield energy function can be used to represents the stored probability functions with their quantum numbers.

(iii) We can optimize the probability of finding the particle inside the boundaries for any given quantum number using a mean field approximation of the annealing

schedule. As the temperature gradually reduces according to the annealing schedule, the probability of visiting the minimum energy states increases. Each schedule determines a new energy function of the network and the network estimates the energy function for this state. At the thermal equilibrium, the network produces the stable states according to the annealing schedule, which represents the optimized probability of finding the particle inside the boundaries.

(iv) In this way, the network which satisfies the bound state condition of a particle confined within finite hard boundaries, is capable of estimating the optimized probability of finding the particle inside the boundaries for any given quantum number.

(v) Ever since the Schrödinger equation was conceived in 1926, quantum mechanics, at least in estimation of non-specialists, has been bedeviled by the mathematical complexity of its formulation. The central problem is to solve the Schrödinger equation and explore its applications to understand the modern physics. A particle trapped in a box with infinitely hard walls is the simplest quantum mechanical application of Schrödinger equation. The last 70 years have seen many elegant solutions of different applications of this kind. The advantage of using the optimization technique of ANN in aspect of solving this problem is that we can get the most elegant solution for this problem. The result of optimization technique with Artificial Neural Network, may be used to solve such kind of quantum mechanical problems in future.

**References**


[1] T Kohonen *Biol. Cybernet* **43** 59 (1982)

[2] T Kohonen *Self Organization and Associative Memory* (Berlin : Springer-Verlag) 3rd edn (1989)

[3] B Muller and J Reinhardt in *Neural Networks An Introduction, Physics of Neural Networks* (New York : Springer-Verlag) (1991)

[4] P K Simpson *Artificial Neural Systems* (Elmsford N Y : Pergamon Press) (1990)

[5] W S Mculloch and W Pitts *Bull. Math. Bio. Phys.* **5** 115 (1943)

[6] C Peterson and B Sodenberg *Neural Optimization in the Hand Book of Brain Theory and Neural Networks* (ed.) M A Arbib (Cambridge, MA : MIT Press) p617 (1995)

[7] J J Hopfield *Proc. National Acad. Sci.* (USA) **79** 2554 (1982)

[8] J J Hopfield *Proc. National Acad. Sci.* (USA) **81** 3088 (1984)

[9] S Kirkpatrick, C D Gelatt and M P Vecchi *Science* **220** 671 (1983)

[10] E Schrödinger *Ann. der Physik* **81** 109 (1926)

[11] Harold Szu *Neural Networks for Computing* (ed.) J S Denker (American Institute of Physics, New Yourk : Snowbird) p420 (1986)

[12] C Peterson and J R Anderson *Complex Systems* **1** 995 (1987)

[13] S Haykin *Neural Networks : A Comprehensive Foundation* (New York : Macmillan College) p338 (1994)