Transverse Ising Model, Glass and Quantum Annealing

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I. INTRODUCTION

In many physical systems, cooperative interactions between spin-like (two-state) degrees of freedom tend to establish some kind of order in the system, while the presence of some noise effect (due to temperature, external transverse field etc.) tends to destroy it. Transverse Ising model can quite successfully be employed to study the order-disorder transitions in many of such systems.

An example of the above is the study of ferro-electric ordering in Potassium Dihydrogen Phosphate (KDP) type systems (see, e.g., [1]). To understand such ordering, the basic structure can be viewed as a lattice, where in each lattice point there is a double-well potential created by an oxygen atom and the hydrogen or proton resides within it in any of the two wells. In the corresponding Ising (or pseudo-spin) picture the state of a double-well with a proton at the left-well and that with one at the right-well are represented by, say, $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively (see, for a portion of the lattice, Fig. 1.1). The protons at neighbouring sites have mutual dipolar repulsions. Hence had proton been a classical particle, the zero-temperature configuration of the system would be one with either all the protons residing at their respective left-well or all residing at the right-well (corresponding to the all-up or all-down configuration of the spin system in presence of cooperative interaction alone, at zero-temperature). Considering no fluctuation at zero temperature, the Hamiltonian for the system in the corresponding pseudo-spin picture will just be identical to the classical Ising Hamiltonian (without any transverse term). However, proton being a quantum particle, there is always a finite probability for it to tunnel through the finite barrier between two wells even at zero-temperature due to quantum fluctuations. To formulate the term for the tunnelling in the corresponding spin-picture, we notice that $\sigma^x$ is the right operator. This is because

$$\sigma^x|\uparrow\rangle = |\downarrow\rangle \quad \text{and} \quad \sigma^x|\downarrow\rangle = |\uparrow\rangle, \quad (1)$$

where $|\uparrow\rangle$ represents the state where the proton is in the left well, while $|\downarrow\rangle$ represents that with the proton in the right well. Hence the tunnelling term will exactly be represented by the transverse field term in the transverse Ising Hamiltonian. Here the transverse field coefficient $\Gamma$ will represent the tunnelling integral, which depends on the width and height of the barrier, mass of the particle, etc.

II. TRANSVERSE ISING MODEL (TIM)

Such a system as discussed above, can be represented by a quantum Ising system, having Hamiltonian

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma^z_i \sigma^z_j - \Gamma \sum_i \sigma^x_i. \quad (2)$$

Here, $J_{ij}$ is the coupling between the spins at sites $i$ and $j$, where $\sigma^\alpha$'s ($\alpha = x, y, z$) are the Pauli spins satisfying the commutation relations

$$[\sigma^\alpha_i, \sigma^\beta_j] = 2i\delta_{ij} \epsilon_{\alpha\beta\gamma} \sigma^\gamma_i \quad (3)$$

Here, $\delta_{ij}$ is the Krönecker’s $\delta$, and $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol, and $\langle i, j \rangle$ in (1) represents neighbouring pairs.

The Pauli spin matrices being representatives of spin-1/2, $\sigma^z$ has got two eigenvalues ($\pm 1$) corresponding to spins aligned either along $z$-direction or along the opposite direction respectively. The eigenstate corresponding to
FIG. 1: The double wells at each site (e.g., provided by oxygen in KDP) provide two (low-lying) states of the proton (shown by each double well) indicated by the Ising states $|\uparrow\rangle$ and $|\downarrow\rangle$ at each site. The tunnelling between the states are induced by the transverse field term ($\Gamma \sigma^x$). The dipole-dipole interaction $J_{ij}$ here for the (asymmetric) choice of one or the other well at each site induces the ‘exchange’ interaction as shown.

eigenvalue (+1) is symbolically denoted by $|\uparrow\rangle$, while that corresponding to $(-1)$ is denoted by $|\downarrow\rangle$.

If we represent

$$|\uparrow\rangle \Leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$|\downarrow\rangle \Leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

then taking these two eigen-vectors as basis, Pauli spins have following matrix representations

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

With these, one can see that relations in (3) are easily satisfied and the tunnelling required in (1) can be easily accommodated. The order parameter for such a system is generally taken to be the expectation value of z-component of the spin, i.e. $\langle \sigma^z \rangle$. Needless to say that in such a system absolute ordering (complete alignment along z-direction) is not possible even at zero-temperature, i.e., $\langle \sigma^z \rangle_{T=0} \neq 1$, when $\Gamma \neq 0$. In general, therefore, the order ($\langle \sigma^z \rangle \neq 0$) to disorder $\langle \sigma^z \rangle = 0$ transition can be brought about by tuning either of, or both of the tunnelling field $\Gamma$ and the temperature $T$ (see Fig. 1.2).

III. MEAN FIELD THEORY (MFT)

(a) For $T = 0$
Let,

\[ \sigma^z_i = |\vec{\sigma}| \cos \theta, \quad \text{and} \quad \sigma^x_i = |\vec{\sigma}| \sin \theta, \]  

where \( \theta \) is the angle between \( \vec{\sigma} \) and z-axis. This renders the two mutually non-commuting part of the Hamiltonian (2) commuting, since both are expressed in terms of \( |\vec{\sigma}| \) operator only. If \( \sigma \) is the eigen-value of \( |\vec{\sigma}| \) (\( \sigma = 1 \) for Pauli spin), then the energy per site of the semi-classical system is given by

\[ E = -\sigma \Gamma \sin \theta - \sigma^2 J(0) \cos^2 \theta, \]  

(7)

\( J(0) = J_i(0) = \sum_{(i,j)} J_{ij} \), where \( j \) indicates the \( j \)-th nearest neighbour of the \( i \)-th site. And the average of the spin-components are given by

\[ \langle \sigma^z \rangle = \cos \theta \]
\[ \langle \sigma^x \rangle = \sin \theta. \]

The energy (7) is minimized for

\[ \sin \theta = \Gamma / J(0) \quad \text{or} \quad \cos \theta = 0. \]  

(8)

Thus we see that if \( \Gamma = 0 \), \( \langle \sigma^z \rangle = 0 \) and the order parameter \( \langle \sigma^z \rangle = 1 \), indicating perfect order.

On the other hand, if \( \Gamma < J(0) \), then the ground state is partially polarized, since none of \( \langle \sigma^z \rangle \) or \( \langle \sigma^x \rangle \) is zero. However, if \( \Gamma \geq J(0) \), then we must have \( \cos \theta = 0 \) for the ground state energy, which means \( \langle \sigma^z \rangle = 0 \), i.e., the state is a completely disordered one. Thus, as \( \Gamma \) increases from 0 to \( J(0) \), the system undergoes a transition from ordered (ferro)- phase with order parameter \( \langle \sigma^z \rangle = 1 \) to disordered (para)-phase with order parameter \( \langle \sigma^z \rangle = 0 \) (see Fig. 1.2).

(b) For \( T \neq 0 \)

The mean field method can also be extended to obtain the behaviour of this model at non-zero temperature. In this case we define a mean field \( \vec{h}_i \) at each site \( i \), which is, in some sense, a resultant of the average cooperative enforcement in z-direction and the applied transverse field in x-direction. Precisely, we take, for general random case,

\[ \vec{h}_i = \Gamma \hat{x} + \left( \frac{1}{2} \sum_j J_{ij} \langle \sigma^z_j \rangle \right) \hat{z}, \]  

(9)
and the spin-vector at the \( i \)-th site follows \( \vec{h}_i \). The spin-vector at \( i \)-th site is given by

\[
\vec{\sigma}_i = \sigma^x_i \hat{x} + \sigma^z_i \hat{z},
\]

and Hamiltonian thus reads

\[
\mathcal{H} = -\sum_i \vec{h}_i \cdot \vec{\sigma}_i. \tag{10}
\]

For non-random case, all the sites have identical ambience, hence \( \vec{h}_i \) is replaced by \( \vec{h} = \Gamma \hat{x} + \langle \sigma^z \rangle J(0) \). And the resulting Hamiltonian takes the form

\[
\mathcal{H} = -\vec{h} \cdot \sum_i \vec{\sigma}_i.
\]

The spontaneous magnetization can readily be written down as

\[
\vec{\sigma} = \tanh(\beta |\vec{h}|) \frac{\vec{h}}{|\vec{h}|}
\]

\[
|\vec{h}| = \sqrt{\Gamma^2 + (J(0)\langle \sigma^z \rangle)^2}. \tag{11}
\]

Now if \( \vec{h} \) makes an angle \( \theta \) with \( z \)-axis, then 
\[
\cos \theta = \frac{J(0)\langle \sigma^z \rangle}{|\vec{h}|} \quad \text{and} \quad \sin \theta = \Gamma |\vec{h}|,
\]

and

\[
\langle \sigma^x \rangle = \tanh(\beta |\vec{h}|) \frac{\Gamma}{|\vec{h}|} \tag{12}
\]

Here, \( \beta = (1/k_B T) \). Equation (12) is the self-consistency equation which can be solved or graphically or otherwise, to obtain the order parameter \( \langle \sigma^z \rangle \) at any temperature \( T \) and transverse field \( \Gamma \). Clearly, the order-disorder transition is tuned both by \( \Gamma \) and \( T \) (see Fig. 1.2).

\( \Gamma = 0 \) (Transition driven by \( T \)):

Here,

\[
\langle \sigma^z \rangle = \tanh \left( \frac{J(0)\langle \sigma^z \rangle}{k_B T} \right)
\]

and

\[
\langle \sigma^x \rangle = 0
\]

One can easily see graphically, that the above equations has a nontrivial solution only if \( k_B T < J(0) \), i.e.,

\[
\langle \sigma^z \rangle \neq 0 \quad \text{for} \quad k_B T < J(0)
\]

\[
\langle \sigma^z \rangle = 0 \quad \text{for} \quad k_B T > J(0).
\]

This shows that there is a critical temperature \( T_c = J(0) \) above which, there is no order.

\( \Gamma \to 0 \) (Transition driven by \( \Gamma \)): 

For \( k_B T \to 0 \) (Transition driven by \( \Gamma \)): 

Here,

\[ \langle \sigma^z \rangle = \frac{J(0)\langle \sigma^z \rangle}{\sqrt{(\Gamma)^2 + (J(0)\langle \sigma^z \rangle)^2}} \quad \text{(since, } \tanh x \bigg|_{x \to \infty} = 1 \text{)} \]

From this equation we easily see that in the limit \( \Gamma/J(0) \to 1 \), the only real nontrivial solution is

\[ \langle \sigma^z \rangle \to 0 \]

and

\[ \langle \sigma^x \rangle = \frac{\Gamma}{\sqrt{(\Gamma)^2 + (J(0)\langle \sigma^z \rangle)^2}} \to 1, \quad \text{as} \quad \frac{\Gamma}{J(0)} \to 1. \]

Thus we see that their is a critical transverse field \( \Gamma_c = J(0) \) such that for any \( \Gamma > \Gamma_c \) there is no order even at zero temperature. In general one sees that at any temperature \( T < T_c \), there exist some transverse field \( \Gamma_c \) at which the transition from the ordered state \( (\langle \sigma^z \rangle \neq 0) \) to the disordered state \( (\langle \sigma^z \rangle = 0) \) occurs. The equation for the phase boundary in the \( (\Gamma - T) \) - plane is obtained by putting \( \langle \sigma^z \rangle \to 0 \) in equation (12). The equation gives the relation between \( \Gamma_c \) and \( T_c \) as follows

\[ \tanh \left( \frac{\Gamma_c k_B T}{\beta} \right) = \frac{\Gamma_c}{J(0)}. \]

One may note that for ordered phase, since \( \langle \sigma^z \rangle \neq 0 \),

\[ \frac{1}{|H|} \tanh(\beta|H|) = \frac{1}{J(0)} = \text{Constant}. \]

Hence, \( \langle \sigma^x \rangle = \left( \frac{\Gamma}{|H|} \right) \tanh(\beta|H|) = \Gamma/J(0) \); independent of temperature in the ordered phase. While for the disordered phase, since \( \langle \sigma^z \rangle = 0 \),

\[ \langle \sigma^x \rangle = \tanh(\beta\Gamma). \]

Using magnetic mapping, mean field theory of this type was indeed applied to (the BCS theory of) superconductivity \[5\], as shown in appendix A.

**IV. DYNAMIC MODE-SOFTENING PICTURE**

The elementary excitations in such a system as described above are known as spin waves, and they can be studied using Heisenberg equation of motion for \( \sigma^z \) using the Hamiltonian. The equation of motion is then given by

\[ \dot{\sigma}^z_i = (i\hbar)^{-1}[\sigma^z_i, \mathcal{H}] \]

or,

\[ \dot{\sigma}^z_i = 2\Gamma \sigma^y_i \quad \text{(with} \quad \hbar = 1) \]

Hence,

\[ \dot{\sigma}^z_i = 2\Gamma \sigma^y_i = 4\Gamma \sum_j J_{ij} \sigma^z_i \sigma^z_j - 4\Gamma^2 \sigma^z_i. \]

With Fourier transforms and random phase approximation \( (\sigma^z_i \sigma^z_j = \sigma^z_i \langle \sigma^z_j \rangle + \langle \sigma^z_i \rangle \sigma^z_j, \text{ with} \ (\sigma^z) = 0 \text{ in para phase}) \), we get

\[ \omega^2 = 4\Gamma(\Gamma - J(q)\langle \sigma^z \rangle), \]

for the elementary excitations (where \( J(q) \) is the Fourier transform of \( J_{ij} \)). The mode corresponding to \( (q = 0) \) softens, i.e., \( \omega_0 \) vanishes at the same phase boundary given by equation (13).
FIG. 3: The Suzuki-Trotter equivalence of quantum one dimensional chain and a (1+1) dimensional classical system. $J'$ indicates the additional interaction in the Trotter direction.

V. SUZUKI-TROTTER FORMALISM

Exact analysis for the quantum fluctuation can indeed be tackled by using renormalization group theory; see appendix B for real space quantum RG theory for one dimensional chain (cf [6]). However, such formalisms have serious limitations in applicability and the Suzuki-Trotter formalism to map the quantum problem to a classical one has been of enormous practical importance (e.g. in simulations).

Suzuki-Trotter formalism [7] is essentially a method to transform a $d$-dimensional quantum Hamiltonian into a $(d+1)$-dimensional effective classical Hamiltonian giving the same canonical partition function. Let us illustrate this by applying it to transverse Ising system. We start with Transverse Ising Hamiltonian

$$H = -\Gamma \sum_{i=1}^{N} \sigma_i^x - \sum_{(i,j)} J_{ij} \sigma_i^z \sigma_j^z = H_0 + V$$

The canonical partition function of $H$ reads

$$Z = Tr e^{-\beta (H_0 + V)}.$$  

Now we apply the Trotter formula

$$\exp (A_1 + A_2) = \lim_{M \to \infty} [\exp A_1/M \exp A_2/M]^M,$$

even when $[A_1, A_2] \neq 0$. On application of this, $Z$ reads

$$Z = \sum_{i} \lim_{M \to \infty} \langle s_i | \exp (-\beta H_0/M) \exp (-\beta V/M)^M | s_i \rangle.$$  

(18)

Here $s_i$ represent the $i$-th spin configuration of the whole system, and the above summation runs over all such possible configurations denoted by $i$. Now we introduce $M$ number of identity operators

$$I = \sum_{i} \sum_{k=1}^{M} | s_{i,k} \rangle \langle s_{i,k} |, \quad k = 1, 2, \ldots M.$$  

in between the product of $M$ exponentials in $Z$, and have

$$Z = \lim_{M \to \infty} Tr \prod_{k=1}^{M} (\sigma_{1,k} \ldots \sigma_{N,k} | \exp \left( \frac{-\beta H_0}{M} \right) \exp \left( \frac{-\beta V}{M} \right) | \sigma_{1,k+1} \ldots \sigma_{N,k+1} \rangle),$$
and periodic boundary condition would imply $\sigma_{N+1,p} = \sigma_{1,p}$. Now,

$$\prod_{k=1}^{M} \langle \sigma_{1,k}...\sigma_{N,k} | \exp \left( \frac{\beta}{M} \sum_{i,j} \sigma_{i,k}^{z} \sigma_{j,k}^{z} \right) | \sigma_{1,k+1}...\sigma_{N,k+1} \rangle$$

$$= \exp \left[ \sum_{i,j=1}^{N} \sum_{k=1}^{M} \frac{\beta J_{ij}}{M} \sigma_{i,k} \sigma_{j,k} \right], \quad (19)$$

where $\sigma_{i,k} = \pm 1$ are the eigenvalues of $\sigma^z$ operator. Also,

$$\prod_{k=1}^{M} \langle \sigma_{1,k}...\sigma_{N,k} | \exp \left[ \frac{\beta \Gamma}{M} \sum_{i} \sigma_{i,k}^{x} \right] | \sigma_{1,k+1}...\sigma_{N,k+1} \rangle$$

$$= \left( \frac{1}{2} \sinh \left[ \frac{2 \beta \Gamma}{M} \right] \right)^{\frac{N M}{2}} \exp \left[ \frac{1}{2} \ln \coth \left( \frac{\beta \Gamma}{M} \right) \sum_{i=1}^{N} \sum_{k=1}^{M} \sigma_{i,k} \right]. \quad (20)$$

The last step follows because

$$e^{\alpha \sigma^x} = e^{-i(ia\sigma^x)} = \cos (ia\sigma^x) - i \sin (ia\sigma^x) = \cosh (a) + \sigma^x \sinh (a),$$

and therefore

$$\langle \sigma | e^{\alpha \sigma^x} | \sigma' \rangle = \left[ \frac{1}{2} \sinh (2a) \right]^{1/2} \exp [(\sigma \sigma' / 2) \ln \coth (a)],$$

since

$$\langle \uparrow | e^{\alpha \sigma^x} | \uparrow \rangle = \langle \downarrow | e^{\alpha \sigma^x} | \downarrow \rangle = \cosh (a) = \left[ \frac{1}{2} \sinh (2a) \right] / \coth (a) \right]^{1/2}$$

and

$$\langle \uparrow | e^{\alpha \sigma^x} | \downarrow \rangle = \langle \downarrow | e^{\alpha \sigma^x} | \uparrow \rangle = \sinh (a) = \left[ \frac{1}{2} \sinh (2a) / \coth (a) \right]^{1/2}.$$

Thus the partition function reads

$$Z = C^{\frac{N M}{2}} Tr_{\sigma} \left( -\beta \mathcal{H}_{eff}[\sigma] \right) \quad C = \frac{1}{2} \sinh \left( \frac{2 \beta \Gamma}{M} \right)$$

where the effective classical Hamiltonian is

$$\mathcal{H}_{eff}(\sigma) = \sum_{(i,j) k=1}^{N} \sum_{k=1}^{M} \left[ - \frac{J_{ij}}{M} \sigma_{ik} \sigma_{jk} - \frac{\delta_{ij}}{2 \beta} \ln \coth \left( \frac{\beta \Gamma}{M} \right) \sigma_{ik} \sigma_{ik+1} \right]. \quad (21)$$

The Hamiltonian $\mathcal{H}_{eff}$ is a classical one, since the variables $\sigma_{i,k}$’s involved are merely the eigenvalues of $\sigma^z$, and hence there is no non-commuting part in $\mathcal{H}_{eff}$. It may be noted from (21) that $M$ should be at the order of $\hbar \beta$ (we have taken $\hbar = 1$ in the calculation) for a meaningful comparison of the interaction in the Trotter direction with that in the original Hamiltonian (see Fig. 1.3). For $T \to 0$, $M \to \infty$, and the Hamiltonian represents a system of spins in a $(d+1)$-dimensional lattice, which is one dimension higher than the original $d$-dimensional Hamiltonian, as is evident from the appearance of one extra label $k$ for each spin variable (see Fig. 1.3). Thus corresponding to each single quantum spin variable $\sigma_i$ in the original Hamiltonian we have an array of $M$ number of classical replica spins $\sigma_{ik}$. This new (time-like) dimension along which these classical spins are spaced is known as Trotter dimension. From the explicit form of $\mathcal{H}_{eff}$, we see that in addition to the previous interaction ($J$) term ($-\sum_{i,j}^N J_{ij} \sigma_i \sigma_j$), there is an additional nearest neighbour interaction ($J'$) between the Trotter replicas corresponding to the same original
spin, along the Trotter direction, given by the term \((\sum_{i,j} \sum_{k=1}^{M} -\frac{\delta_{ij}/2}{\beta} \ln \coth(\beta \Gamma/M) \sigma_{ik} \sigma_{iK+1})\) (as shown in Fig. 1.3). For finite temperature, the optimal width of the lattice in the Trotter direction is finite and the critical behaviour remains \(d\)-dimensional.

The calculations, and consequently the effective Hamiltonian (21), is valid for any general interaction \(J_{ij}\); of course, \(\Gamma\) has been taken to be nonrandom. Fig. 1.4 describes a situation where \(J_{ij}\) were nonrandom (we had \(J_{ij} = J\)). For random \(J_{ij}\), where \(J_{ij}\) were nonrandom (we had \(J_{ij} = J\)). For random \(J_{ij}\), remain identical (\(J'\)) whereas the spatial randomness in interactions for various Trotter slices get correlated as indicated in Fig. 1.4. Such equivalence of \(d\)-dimensional quantum system with a \((d+1)\)-dimensional classical model can also be seen from the renormalization group study of the quantum models (say, one-dimensional transverse Ising model and its equivalent critical behaviour of two-dimensional classical Ising system) as shown in Appendix B.

VI. CLASSICAL SPIN GLASSES: A SUMMARY

Spin glasses are magnetic systems with randomly competing (frustrated) interactions. Frustration is a situation where all of the spins present in the system cannot energetically satisfy every bond associated to them. Here the frustration arises due to competing (ferromagnetic and anti-ferromagnetic) quenched random interactions between the spins. As a result there arise huge barriers \(O(N)\), \(N = \text{system size}\) in the free-energy landscape of the system. In thermodynamic limit, height of such barriers occasionally go to infinity. These barriers strongly separate different configurations of the system, so that once the system gets stuck in a deep valley in between two barriers, it practically gets trapped around that configuration for a macroscopically large time. Because of frustration, the ground state is largely degenerate; degeneracy being of the order of \(\exp(N)\). As discussed above, different ground state configurations are often separated by \(O(N)\) barriers, so that once the system settles down in one of them, it cannot visit the others equally often in course of time, as predicted by the Boltzmann probability factor. The system thus becomes “nonergodic” and may be described by a nontrivial order parameter distribution in the thermodynamic limit (unlike the unfrustrated cooperative systems, where the the distribution becomes trivially delta function-like). The spins in such a system thus get frozen in random orientations below a certain transition temperature. Although there is no long range magnetic order, i.e., the space average of spin moments vanishes, the time average of any spin is nonzero below the transition (spin-glass) temperature. This time average is treated as a measure of spin freezing or spin glass order parameter.

Several spin glass models have been studied extensively using both analytic and computer simulation techniques. The Hamiltonian for such models can be written as

\[
\mathcal{H} = -\sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z
\]  

(22)

where \(S_i^z = \pm 1, 2, ..., N\), denote the Ising spins, interacting with random quenched interactions \(J_{ij}\), which differs in various models. We will specifically consider three extensively studied models.

(a) In Sherrington-Kirkpatrick (S-K) model \(J_{ij}\) are long-ranged and are distributed with a Gaussian probability (centered around zero), as given by

\[
P(J_{ij}) = \left(\frac{N}{2\pi J^2}\right)^{1/2} \exp\left(-\frac{-N J_{ij}^2}{2 J^2}\right)
\]  

(23)
(b) In Edward-Anderson (EA) model, the $J_{ij}$'s are short-ranged (say, between the nearest neighbours only), but similarly distributed with Gaussian probability (23)

$$P(J_{ij}) = p\delta(J_{ij} - J) + (1 - p)\delta(J_{ij} - J).$$

The disorder in the spin system being quenched, one has to perform configurational averaging (denoted by overhead bar) over $\ln Z$, where $Z(= Tr \exp -\beta\mathcal{H})$ is the partition function of the system. To evaluate $\ln Z$, one usually employs replica trick based on the representation $\ln Z = \lim_n \rightarrow 0 [Z^n - 1]/n$. Now for classical Hamiltonian (with all commuting spin components), $Z^n = \prod_{\alpha=1}^{n} Z_\alpha = Z(\sum_{\alpha=1}^{n} H_\alpha)$, where $H_\alpha$ is the $\alpha$-th replica of the Hamiltonian $\mathcal{H}$ in equation (22) and $Z_\alpha$ is the corresponding partition function. The spin freezing can then be measured in terms of replica overlaps, and Edward-Anderson order parameter takes the form

$$q = \frac{1}{N} \sum_{i=1}^{N} \langle S_i^z(t)S_i^z(0) \rangle_{t \rightarrow \infty} \simeq \frac{1}{N} \sum_{i=1}^{N} \langle \tilde{S}_{i\alpha}^z \tilde{S}_{i\beta}^z \rangle,$$

where $\alpha$ and $\beta$ corresponds to different replicas.

Extensive Monte Carlo studies, together with the analytical solutions for the mean field of S-K and EA models, have revealed the nature of spin glass transition. It appears that the lower critical dimension $d^c_l$ for EA model, below which transition ceases to occur (with transition temperature $T_c$ becoming zero), is between 2 and 3: $2 < d^c_l < 3$. The upper critical dimension $d^c_u$, at and above which mean field results (e.g., those of S-K model) apply, appears to be 6: $d^c_u = 6$. Within these dimensions ($d^c_l < d < d^c_u$), the spin glass transitions occur (for Hamiltonians with short-ranged interactions) and the transition behaviour can be characterized by various exponents. Although the linear susceptibility shows a cusp at the transition point, the nonlinear susceptibility $\chi_{SG} = (1/N) \sum_r g(r)$, diverges at the spin glass transition point:

$$\chi_{SG} \sim (T - T_c)^{-\gamma_c}, \quad g(r) \sim r^{-(d-2+\eta_c)} f\left(\frac{r}{\xi}\right), \quad \xi \sim |T - T_c|^{-\nu_c}$$

Here $\xi$ denotes the correlation length which determines the length scaling in the spin correlation function $g(r)$ (in $g(r)$ denotes the scaling function). Numerical simulation gives $\nu_c = 1.3 \pm 0.1, 0.80 \pm 0.15, 1/2$ and $\gamma_c = 2.9 \pm 0.5, 1.8 \pm 0.4, 1$ for $d = 2, 3$ and 6 respectively for the values of exponents. One can define the characteristic relaxation time $\tau$ through the time dependence of spin auto-correlation

$$g(t) = \langle S_i^z(t)S_i^z(0) \rangle \sim t^{-x} \bar{q} \left(\frac{t}{\tau}\right), \quad \tau \sim \xi^z \sim |T - T_c|^{-\nu_c/z_c}$$

where $x = (d-2+\eta_c)/2z_c$, and $z_c$ denotes the classical dynamical exponent. Numerical simulations give $z_c = 6.1 \pm 0.3$ and $4.8 \pm 0.4$ in $d = 3$ and 4 dimensions respectively. Of course, such large values of $z_c$ (particularly in lower dimensions) also indicates the possibility of the failure of power law variation (26) of $\tau$ with $T - T_c$ and rather suggests a Vogel-Fulcher like variation: $\tau \sim \exp[A/(T - T_c)]$. In the $\pm J$ spin glasses (type (c) above), some exact results are known along the ‘Nishimori Line’ $\bar{S}$, and the nature of the phase transition there is precisely known.

VII. QUANTUM SPIN GLASSES

Quantum spin glasses have the interesting feature that the transition in randomly frustrated (competing) cooperatively interacting systems can be driven both by thermal fluctuations or by quantum fluctuations. Quantum spin glasses can be of two types: vector spin glasses introduced by Bray and Moore (see Figures), where of course quantum fluctuation cannot be tuned, or a classical spin glass perturbed by some tunable quantum fluctuations e.g., as induced by a non commutative transverse field. The amount of quantum fluctuation being tunable, this Transverse Ising Spin Glass (TISG) model is perhaps simplest model in which the quantum effects in a random system can be and has been studied extensively and systematically. Precise realization of TISG in LiHo$_x$Y$_{1-x}$F$_4$, with magnetic Holonium ion concentration around $x = 0.167$, has led to several important developments.

The interesting in such quantum spin glass models is about the possibility of tunnelling through the (infinitely high) barriers of the free energy landscape in the classical spin glass models (e.g., S-K model) due to the quantum
fluctuations induced by the transverse field. In classical system, the overriding of an infinitely high barrier is infinitely hard for thermal fluctuations at any finite temperature. But quantum fluctuation can make a system tunnel through such a barrier, if its width is infinitessimally small. The barrier widths are actually seen to decrease with system size indicating to an ergodic (replica symmetric) picture for the free-energy landscape.

A. Models

1. Sherrington-Kirkpatrick Model in a Transverse Field

The sherrington-Kirkpatrick (S-K) model in presence of a non-commuting tunnelling field, given by the Hamiltonian

$$H = - \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x,$$

where the follows the Gaussian distribution

$$P(J_{ij}) = \left( \frac{N}{2\pi \Delta^2} \right)^{1/2} \exp \left( -\frac{N J_{ij}^2}{a \Delta^2} \right)$$

was first studied by Ishi and Yamamoto [9].

Phase Diagram

Several analytical studies have been made to obtain the phase diagram of the transverse Ising S-K model (giving in particular the zero-temperature critical field). The problem of S-K glass in transverse field becomes a nontrivial one due to the presence of noncommuting spin operators in the Hamiltonian. This leads to a dynamical frequency dependent (spin) self-interaction.

(i) Mean field estimates:

One can study an effective spin Hamiltonian for the above quantum many body system within the mean field framework. A systematic mean field theory for the above model was first carried out by Kopec (see e.g., [9]), using the thermofield dynamical approach and the short time approximation for the dynamical spin self-interaction. Before going into the discussion of this approach, we shall briefly review the replica-symmetric solution of the classical S-K model ($\Gamma = 0$) in a longitudinal field given by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^z$$

where $J_{ij}$ follows the Gaussian distribution given by (56). Using the replica trick, one obtains for configuration averaged $n$-replicated partition function $\bar{Z}^n$, given by

$$\bar{Z}^n = \sum_{\{\sigma_i = \pm 1\}} \int_{-\infty}^{\infty} P(J_{ij}) dJ_{ij} \exp \left[ \beta \sum_{\langle ij \rangle} J_{ij} \sum_{\alpha} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^z \right].$$

Performing the Gaussian integral, using Hubbard-Stratonovich transformation and finally using the method of steepest descent to evaluate integrals for thermodynamically large system, one obtains free energy per site $f$, given by

$$-\beta f = \lim_{n \to 0} \left[ \beta \frac{\Delta^2}{4} \left( 1 - \frac{1}{n} \sum_{\alpha, \beta} q_{\alpha, \beta}^2 + \frac{1}{n} \ln \text{Tr} (\exp L) \right) \right],$$

where $L = (\beta J)^2 \sum_{\alpha, \beta} q_{\alpha, \beta} \sigma_\alpha^z \sigma_\beta^z + \beta \sum_{\alpha=1}^n \sigma_\alpha^z$ and $q_{\alpha, \beta}$ is self-consistently given by the saddle point condition $(\partial f / \partial q_{\alpha, \beta}) = 0$. Considering the replica symmetric case ($q_{\alpha, \beta} = q$), one finds

$$-\beta f = \frac{(\beta \Delta)^2}{2} (1 - q) + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dr \ e^{-r^2/2} \ln \left[ 2 \cosh \{ \beta h(r) \} \right]$$
where \( r \) is the excess static noise arising from the random interaction \( J_{ij} \) and the spin glass order parameter \( q \) is self-consistently given by

\[
q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dr \ e^{-\frac{r^2}{2}} \tanh^2 \{\beta h(r)\}
\]

and \( h(r) = \Delta \sqrt{qr} + h \) can be interpreted as a local molecular field acting on a site. Different sites have different fields because of disorder, and the effective distribution of \( h(r) \) is Gaussian with mean 0 and variance \( \Delta^2 q \).

At this point we can introduce quantum effect through transverse field term \(-\Gamma \sum_i \sigma_i^x\) (with longitudinal field \( h = 0 \)). The effective single particle Hamiltonian in the transverse Ising quantum glass can be written as

\[
H_s = -h_z(r) \sigma_z - \Gamma \sigma_x,
\]

where \( h_z(r) \), as mentioned earlier, is the effective field acting along the z direction arising due to nonzero value of the the spin glass order parameter. Treating \( h_z(r) \) and \( \sigma \) as classical vectors in pseudo-spin space, one can write the net effective field acting on each spin as

\[
h_0(r) = h_z(r) \hat{z} - \Gamma \hat{x}; \quad |h_0(r)| = \sqrt{h_z(r)^2 + \Gamma^2}.
\]

One can now arrive at the mean field equation for the local magnetisation, given by

\[
m(r) = p(r) \tanh [\beta h_0(r)]; \quad p(r) = \frac{|h_z(r)|}{|h_0(r)|},
\]

and consequently, the spin glass order parameter can be written as

\[
q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dr \ e^{-r^2/2} \tanh^2 \{\beta h_0(r)\} p^2(r).
\]

The phase boundary can be found from the above expression by putting \( q \to 0 \) (\( h_z(r) = J \sqrt{qr} \) and \( h_0 = \Gamma \)), when it gives

\[
\frac{\Gamma}{\Delta} = \tanh \left( \frac{\Gamma}{k_B T} \right).
\]

From above we get \( \Gamma_c = J \). Ishi and Yamamoto used the “reaction field” technique to construct “TAP” like equation for free energy of the Hamiltonian (27) and perturbatively expanded the free energy in powers of \( \Gamma \) upto the order \( \Gamma^2 \) to obtain

\[
k_B T_c = \Delta [1 - 0.23(\Gamma/\Delta)^2].
\]

(ii) Monte Carlo Studies:

Several Monte Carlo studies have been performed \cite{9,13} for S-K spin glass in transverse field. Applying Suzuki-Trotter formulation (as discussed earlier) of effective partition function, one can obtain the effective classical Hamiltonian in \( M \)th Trotter approximation as

\[
H_{eff} = - \frac{1}{M} \sum_{i,j=1}^{N} \sum_{k=1}^{M} J_{ij} \sigma_{ik} \sigma_{jk} - \frac{1}{2\beta} \ln \coth \left( \frac{\beta \Gamma}{M} \right) \sum_{i=1}^{N} \sum_{k=1}^{M} \sigma_{ik} \sigma_{ik+1} - \frac{NM}{2} \ln \left[ \frac{1}{2} \sinh \frac{2\beta \Gamma}{M} \right],
\]

where \( \sigma_{ik} \) denotes the Ising spin defined on the lattice \((i, k)\), \( i \) being the position in the in the original S-K model and \( k \) denoting the position in the additional Trotter dimension.

Ray et al \cite{10} took \( \Gamma << J \) and their results indeed indicate a sharp lowering of \( T_C(\Gamma) \). Such sharp fall of \( T_c(\Gamma) \) with large \( \Gamma \) is obtained in almost all theoretical studies of the phase diagram of the model.
2. Edward-Anderson Model in a Transverse Field

The Hamiltonian for the Edward-Anderson spin glass in presence of transverse field is that given by (27), where the random interaction this time is restricted among the nearest neighbours and satisfies a Gaussian distribution with zero mean and variance $J$, as given by

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{J_{ij}^2}{2J^2}\right).$$

With $\Gamma = 0$, the above model represents the E-A model with order parameter $q = \langle \sigma_z^2 \rangle = 1$ (at $T = 0$). When the transverse field is introduced, $q$ decreases, and at a critical value of the transverse field the order parameter vanishes.

To study this quantum phase transition using quantum Monte Carlo techniques, one must remember that the ground state of a $d$-dimensional quantum model is equivalent to the free energy of a classical model with one added dimension which is the imaginary time (Trotter) dimension. The effective classical Hamiltonian can be written as

$$\mathcal{H} = \sum_k \sum_{ij} K_{ij} \sigma_i \sigma_j - \sum_k \sum_i K \sigma_i \sigma_{i+1}, \quad (32)$$

with

$$K_{ij} = \frac{\beta J_{ij}}{M}; \quad K = \frac{1}{2} \ln \coth \left(\frac{\beta \Gamma}{M}\right),$$

where $\sigma_i$ are classical Ising spins and $(i, j)$ denotes the original $d$-dimensional lattice sites and $k = 1, 2, ..., M$ denotes a time slice. Although the equivalence between classical and the quantum model holds exactly in the limit $M \rightarrow \infty$, one can always make an optimum choice for $M$. The equivalent classical Hamiltonian has been studied using standard Monte Carlo technique. The numerical estimates of the phase diagram etc. are reviewed in details in [13].

### B. Replica Symmetry in Quantum Spin Glasses

The question of existence of replica-symmetric ground states in quantum spin glasses has been studied extensively in recent years. Replica symmetry restoration is a quantum phenomena arising due to the quantum tunnelling between the classically ‘traped’ states separated by infinitely high (but infinitesimally narrow) barriers in the free energy surface, which is possible as the tunnelling probability is proportional to the barrier area, which remains finite. To investigate this aspect of quantum glasses, one has to study the overlap distribution function $P(q)$ given by

$$P(q) = \sum_{l,l'} P_l P_{l'} \delta(q - q^{(l,l')}), \quad (33)$$

where $P_l$ is the Boltzam weight associated with the state $l$ and $q^{(l,l')}$ is the overlap between the states $l$ and $l'$

$$q^{(l,l')} = \frac{1}{N} \sum_{i=1}^N \langle \sigma_i \rangle^{(l)} \langle \sigma_i \rangle^{(l')}.$$  

One can also define the overlap distribution in the following form (for a finite system of size $N$)

$$P_N(q) = \langle \delta(q - q^{(12)}) \rangle,$$

where $q^{(12)}$ is the overlap between two sets of spins $\sigma_i^{(1)}$ and $\sigma_i^{(2)}$, with identical bond distribution but evolved with different dynamics,

$$q^{(12)} = \frac{1}{N} \sum_{i=1}^N \sigma_i^{(1)} \sigma_i^{(2)}. \quad (36)$$

$P_N(q) \rightarrow P(q)$ in the thermodynamic limit. In quantum glass problem one can study similarly this overlap distribution $P_N(q)$; and if the replica symmetric ground states exists, the above function must tend to a delta function in
thermodynamic limit. In para-phase, the distribution will approach a delta function at \( q = 0 \) for the infinite system.

Ray, Chakrabarti and Chakrabarti \[10\], performed Monte Carlo simulations, mapping the \( d \)-dimensional transverse S-K spin glass Hamiltonian to an equivalent \((d + 1)\)-dimensional classical Hamiltonian and addressed the question of stability of the replica symmetric solution, with the choice of order parameter distribution function given by

\[
P_N(q) = \langle \delta \left( q - \frac{1}{NM} \sum_{i=1}^{N} \sum_{k=1}^{M} \sigma_k^{(1)} \sigma_k^{(2)} \right) \rangle, \tag{37}
\]

where, as mentioned earlier, subscripts \((1)\) and \((2)\) refer to the two identical samples but evolved through different Monte Carlo dynamics. It may be noted that a similar definition for \( q \) (involving overlaps in identical Trotter indices) was used by Guo et al \[11\]. Lai and Goldschmidt performed Monte Carlo studies with larger system size \((N \leq 100)\) and studied the order parameter distribution function

\[
P_N(q) = \langle \delta \left( q - \frac{1}{N} \sum_{i=1}^{N} \sigma_k^{(1)} \sigma_k^{(2)} \right) \rangle, \tag{38}
\]

where the overlap is taken between different (arbitrarily chosen) Trotter indices \( k, k' \); \( k \neq k' \). Their studies indicate that \( P_N(q) \) does not depend upon the choice of \( k \) and \( k' \) (Trotter symmetry). Rieger and Young (see \[3\]) also defined \( q^{(12)} \) in similar way \((q^{(12)} = 1/(NM) \sum_k \sum_{kk'} \sigma_k^{(1)} \sigma_k^{(2)} \)\). There are striking differences between the results Lai and Goldschmidt obtained with the results of Ray et al \[10\]. For \( \Gamma \ll \Gamma_c \), \( P(q) \) is found to have a oscillatory dependence on \( q \) with a frequency linear in \( N \) (which is probably due to the formation of standing waves for identical Trotter overlaps). However, with increase in \( N \), the amplitude of oscillation decreases and the magnitude of \( P(q = 0) \) decreases, indicating that \( P(q) \) might go over to a delta function in thermodynamic limit. The envelope of this distribution function appears to have an increasing \( P(q = 0) \) value as the system size is increased. Ray et al \[10\] argued that the whole spin glass phase is replica symmetric due to quantum tunnelling between the classical trap states. Lai and Goldschmidt on the other hand, do not find any oscillatory behaviour in \( P(q) \). In contrary they get a replica symmetry breaking (RSB) in the whole spin glass phase from the nature of \( P(q) \), which in this case, has a tail down to \( q = 0 \) even as \( N \) increases. According to them their results are different from Ray et al \[10\] because of different choices of the overlap function. Goldschmidt and Lai have also obtained replica symmetry breaking solution at first step RSB, and hence the phase diagram.

Büttner and Usadel (see e.g., Chakrabarti et al \[4\]), have shown that the replica symmetric solution is unstable for the effective classical Hamiltonian \((58)\) and also estimated the order parameter and other thermodynamic quantities like susceptibility, internal energy and entropy by applying Parisi’s replica symmetry breaking scheme to the above effective Hamiltonian. Using static approximation, Thirumalai et al (see \[4\]), found stable replica symmetric solution in a small region close to the spin glass freezing temperature near the phase boundary. But as mentioned earlier, in the region close to the critical line, quantum fluctuations are subdued by the thermal fluctuations. Thus the restoration of replica symmetry breaking, which is essentially a quantum effect, perhaps cannot be prominent there.

All these numerical studies are for equivalent classical Hamiltonian, obtained by applying the Suzuki-Trotter formalism to the original quantum Hamiltonian, where the interactions are anisotropic in the spatial and Trotter direction and the interaction in the Trotter direction becomes singular in the limit \( T \rightarrow 0 \). Obviously one cannot extrapolate the finite temperature results in zero temperature limit. The results of exact diagonalization of finite systems \((N \leq 10)\) at \( T = 0 \) itself do not indicate any qualitative difference in the behaviour of the (configuration average) mass gap \( \Delta \) and the internal energy \( E_q \) from that of a ferromagnetic transverse Ising case, indicating the possibility that the system might become “ergodic”. On the other hand, the zero temperature distribution for the order parameter does not appear to go to delta function with increasing \( N \) as is clearly found for the corresponding ferromagnet (random long range interaction without competition). In this case the order parameter distribution \( P(q) \) is simply the number of ground state configuratons having the order parameter value as \( q \). This perhaps indicate broken ergodicity for small values of \( \Gamma \). The order parameter distribution also shows oscillations similar to that obtained by Ray et al \[10\].

Kim and Kim \[14\] have very recently investigated the S-K model in transverse field using imaginary time replica formalism, under static approximation. They have shown that the replica-symmetric quantum spin glass phase is stable in most of the area of the spin glass phase, as have been argued by Ray et al, in contrary to the results of Lai et al and Thirumalai et al (see e.g., Chakrabarti et al \[4\]).
Multivariable optimization problems consist of finding the maximum or minimum values of a function (known as cost function) of very many independent variables. A given set of values for the whole set of independent variables defines a configuration. The value of the cost function depends on the configurations, and one has to find the optimum configuration that minimizes or maximizes the cost function. The explicit evaluation of the cost function for all possible configurations in this context, generally turns out to be absolutely impracticable for most systems.

One can therefore start from an arbitrary state and go on changing the configuration following some stochastic rule, unless an extremum is reached. For example, in a minimization problem, one may start from an arbitrary configuration, change the configuration according to some stochastic rule, evaluate the cost function of the changed configuration, and then compare its value with that of the original configuration. If the new cost function is lower, the change is retained, i.e., the new configuration is accepted. Otherwise the change is not accepted. Such steps may be repeated for times unless a minimum is reached. But in most cases of multivariable optimization problem, there are many local extrema in the cost function landscape, and one cannot be sure that the extremum that has been reached is the global one. Kirkpatrick et al. [15] proposed a very ingenious physical solution to this mathematical problem, now known by the name simulated annealing. The basic underlying principle of simulated annealing as follows. It is known that an ergodic physical system, at any finite temperature resides in the global minimum of its free energy. The minimum of the free energy is a thermodynamic macro-state corresponding to a maximum number of accessible microscopic configuration. Hence at thermal equilibrium an ergodic system explores its configuration space randomly with equal apriori probability of visiting any configuration, and consequently is found most of the time at one or other of the configurations that corresponds to the free energy minimum (since the number of configurations corresponding to such minimum is overwhelmingly large compared to that of any other macro-state). Now if the system starts from an arbitrary macrostate (not the minimum of free energy) then due to thermal fluctuation it reaches the free energy minimum within some time $\tau$ known as the thermal relaxation time of the system.

For an ergodic system (away from critical point) this relaxation time increases linearly with system size (which is logarithmically smaller a number compared to the corresponding number of all possible configurations). Hence if one follows the random dynamics of the thermal relaxation of a system, then he will be able to reach the minimum of cost function (zero temperature free energy) in a substantially smaller time. What one needs to do is to view the cost function $E$ as the internal energy of some system and start from an arbitrary configuration. Then one changes the configuration according to some stochastic rule, just as before. Now if the energy is lowered by the change, the change is accepted, but if it is not, the change is not thrown away with certainty. Instead it is accepted with a probability equal to the Boltzmann factor $e^{-\Delta E/k_B T}$, where $\Delta E = E_{\text{after change}} - E_{\text{before change}}$ (since this is the way how systems relax thermally to their free energy minimum). Temperature $T$ here is an artificially introduced parameter which has a high value initially, and is reduced slowly as time goes on, finally tending towards zero. At zero temperature the free energy is nothing but the internal energy of the system, and thus at the end of the final stage of annealing the system can be expected to be found, with a very high probability, in a configuration that minimizes the internal energy (cost function).

However this simulated annealing technique can suffer severe setback when the system is “nonergodic”, like the spin glasses we discussed earlier. In such cases configurations corresponding to minimum of the cost function are separated by $O(N)$ sized barriers, and at any finite temperature thermal fluctuations will take practically infinite time to relax the system to the global minimum crossing these barriers in thermodynamic limit $N \to \infty$.

### B. Ergodicity of Quantum Spin Glasses and Quantum Annealing

The non-ergodicity problem makes the search of the ground state of a classical spin glass a computationally hard problem (no algorithm bounded by some polynomial in system size exists for such NP-hard problems). The problems of simulated annealing of spin glass-like systems can be overridden (atleast partially) by employing the method of quantum annealing [16, 17]. The basic idea is as follows: First the problem has to be mapped to a corresponding physical problem, where the cost function is represented by some classical Hamiltonian (say $\mathcal{H}_0$) of the form (22). Then a suitably chosen noncommuting quantum tunnelling term (say $\mathcal{H}'(t)$) is to be added so that the Hamiltonian takes the form of (27). One can then solve the time dependent Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = [\mathcal{H}_0 + \mathcal{H}'(t)]\psi$$

(39)
for the wave-function $\psi(t)$ of the entire system $\mathcal{H}_0 + \mathcal{H}'(t)$. The solution of the time dependent Schrödinger equation approximately describes a tunnelling dynamics of the system between different eigenstates of $\mathcal{H}_0$. Like thermal fluctuations in (classical) simulated annealing, the quantum (tunnelling) fluctuations owing to $\mathcal{H}'$ in (39) help the system to come out of the local 'trap' states. If $\mathcal{H}'(t) \to 0$ for $t \to \infty$, the system eventually settles in one of the eigenstates of $\mathcal{H}_0$, hopefully the ground state. The introduction of such a quantum tunnelling is supposed to make the infinitely high (but infinitessimally thin) barriers transparent to the system (see, e.g., Appendix C), and it can make transitions to different configurations trapped between such barriers, in course of annealing. In other words, it is expected that application of a quantum tunnelling term will make the free energy landscape ergodic, and the system will consequently be able to visit any configuration with finite probability. Finally the quantum tunnelling term is tuned to zero ($\mathcal{H}'(t) \to 0$) to get back the classical Hamiltonian. It may be noted that the success of quantum annealing is directly connected to the replica symmetry restoration in quantum spin glass [10], [14] due to tunnelling through barriers (see Fig. 1.5 and the discussion in the preceding section).

Here, the $d$-dimensional quantum Hamiltonian (27) (to be annealed) is mapped to the $(d+1)$-dimensional effective Hamiltonian

$$\mathcal{H}_{d+1} = -\frac{M}{k+1} \left( \sum_{i,j} J_{ij} \sigma_i^k \sigma_j^k + J' \sum_{i=1}^{N} \sigma_i^k \sigma_i^{k+1} \right),$$

where

$$J' = \frac{MT}{2} \ln \tanh \left( \frac{\Gamma}{MT} \right) > 0$$

is the nearest neighbour ferromagnetic coupling in Trotter direction, between the Trotter replicas of the same spin. In course of annealing, the temperature is kept constant at a low but nonzero value, and the tunnelling field $\Gamma$ is tuned slowly from a high initial value to zero. The decrease in $\Gamma$ amounts to the increase in $J'$ (as can be seen from above expression of $J'$). Initially at high $\Gamma$, $J'$ is low, and each Trotter replica behaves almost like an independent classical spin system. The tunnelling field is then lowered in small steps. In each such step, the system is annealed in presence of the small temperature. Finally as $\Gamma \to 0$, $J' \to \infty$, forcing all replicas to coincide at the end. As mentioned already, quantum annealing possibility directly rests on the replica symmetry restoration feature of quantum spin glasses, discussed in earlier section. In fact ergodicity in quantum spin glasses, as suggested in Fig. 1.5 was attributed by Ray et al to the "quantum fluctuations due to transverse field. Quantum tunnelling between the classical ‘trap’ states, separated by infinite (but narrow) barriers in the free-energy surface, is possible as quantum tunnelling probability is proportional to the barrier area which is finite." (Sec. V, Ref. [10]).
C. Quantum Annealing in Kinetically Constrained Systems

It is largely believed that apart from the complexity associated to the non-trivial ground state structure of a glassy system, the occurrence of certain kinetic constraints (blockings) during relaxation also contributes substantially to the slowness of its low temperature dynamics. The Kinetic constraints or blockings can be viewed as infinitely high energy barriers appearing in the relaxation path of the system. In order to relax to the minimum of the free energy, the system has to jump over these high barriers thermally, which they fail to do at any finite temperature. However if such barriers are infinitessimally narrow, then the system might be able to tunnel through them quantum mechanically if sufficient quantum fluctuation $\Gamma$ is present in the system. Thus if one tries to anneal such a system down to its ground state starting from an arbitrary state, then quantum annealing might turn out to be much superior to the thermal annealing (see e.g., [18, 19]).

We have studied [20] the annealing of a kinetically constrained Ising spin chain of $N$ spins, starting from a disordered state (with negligible initial magnetization), to its (external field induced) fully ordered ground state. At any finite temperature $T$ (in the classical model) the system takes an exponentially long time to relax to the ordered state because of the kinetic constraints, which act like an infinite potential barrier, depending on the neighbouring spin configurations. Quantum mechanically, this infinite barrier is taken to be penetrable, ie with finite tunnelling probability, depending on the barrier height $\chi$ and width $a$ ($a \to 0$ faster than $\chi^{-2}$). The introduced noise, required for the annealing, is reduced following an exponential schedule in both the cases: $T = T_0 e^{-t/\tau_0}$, $\Gamma = \Gamma_0 e^{-t/\tau_0}$, with $T_0 \approx \Gamma_0$. For our simulation for the quantum case, we have taken the tunnelling probabilities $P$ (for cases I-IV) and employed them in a semi-classical fashion for the one dimensional spin chain considered. We observe that for similar achievement in final order ($m_f \simeq 0.92$ starting from $m_i = 10^{-3}$), $\tau_C \sim 10^3 \tau_Q$ for $N = 5 \times 10^3$. For even larger order ($m_f \sim 1$), quantum annealing works even better ($\tau_C \sim 10^3 \tau_Q$, for the same value of $N$). These comparison are for $\chi = 10^2$ and $\chi = 10^3$ for the constraint barriers [20].

In this picture, we considered the collective dynamics of a many particle system, where each one is confined in a (field) induced asymmetric double well potential for which we considered only the low lying two states (the wave packet localized in one well or the other), representing the two states (up and down) of an Ising spin discussed above. The tunnelling of the wave packet from one well to the other was taken into account by employing a scattering picture and we used the tunnelling probabilities as the flip probabilities for the quantum Ising spins. As such, the reported simulation for the one dimensional quantum East model is a semiclassical one. It may be noted however that, because of the absence of inter-spin interaction, the dimensionality actually plays no role in this model except for the fact that the kinetic constraints on any spin depend only on the left nearest neighbour (directedness in one dimension). Hence the semiclassical one dimensional simulation, instead of a proper quantum Monte Carlo simulation (equivalent to a higher dimensional classical one [4]), is quite appropriate here.

IX. SUMMARY AND DISCUSSIONS

We have introduced the transverse Ising model for discussing the order-disorder transition (at zero temperature) driven by quantum fluctuations. Mean field theories are discussed next in sections 1.3 and 1.4. Application to BCS superconductivity theory is discussed in appendix A. Renormalization group technique for study of critical behaviour in such quantum systems is discussed in appendix B (for a chain). Next we have discussed the Suzuki-Trotter mapping of the $d$-dimensional quantum system to $d + 1$ dimensional classical system (in section 1.6). We introduce then the transverse Ising spin glass models, namely, the S-K model in transverse field and the E-A model in transverse field (Sec. 1.8.2). The existing studies on their phase diagrams are discussed briefly. We then discuss about the problem of replica symmetry restoration in quantum spin glasses (in Sec. 1.8.3). The application of the quantum annealing technique to capture the near-global minima of NP-hard problems is then discussed, and the effectiveness of quantum tunnelling over the thermal barrier hopping is discussed (Sec. 1.9).

It may be noted in this connection that some recent attempts have been made to apply similar annealing, induced by quantum fluctuations, to the optimization problems like the travelling salesman problem, image restoration, etc. [18, 19]. Like the near-global minima in free energy landscape of such spin glasses, the barriers are often globally contributed and these barrier heights grow as the system size grows (unlike the locally optimized configurations and the barriers between them). Classically, the system becomes nonergodic due to these macroscopically high barriers (NP-hard to reach the ground state), as thermal fluctuations have to wait until they can scale such macroscopically high barriers. Quantum tunnelling does not necessarily look for barrier height [10] to overcome them (by tunnelling through; see appendix C, see Fig. 1.5) and helps restoring replica symmetry as well as annealing [16, 17].

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Appendix A:

MFT of TIM and BCS Theory of Superconductivity

The phonon mediated effective attractive interaction between electrons give rise to a cooperative quantum Hamiltonian. Although the quantum phase transition in such a system is not physical or meaningful, the finite temperature superconducting phase transition can be studied easily following the mean field theory discussed here (using a pseudo-spin mapping \[5\]). The relevant part of the Hamiltonian of electrons that take part in superconductivity has the following form

$$H = \sum_k \epsilon_k (c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) - V \sum_{kk'} c_k^\dagger c_{-k'} c_{-k} c_k$$

(A1)

Here the suffix \(k\) indicates a state with momentum \(\vec{k}\) and spin up, while \((-k)\) indicates a state with momentum \(-\vec{k}\) and spin down and \(V\) is a positive constant that models the attractive coupling between electrons through phonons.

We will solve this equation following spin-analog method \[4\]. Here we are considering low-lying states containing pair of electrons \((k, -k)\). For a given \(k\), there are two possible states that come into consideration: either the pair exists, or it does not. Thus we enter into a spin-like two-state picture as follows.

Let us introduce the number operator \(\hat{n}_k = c_k^\dagger c_k\). This reduces the Hamiltonian (A1) to

$$H_{red} = \sum_k \epsilon_k (1 - \hat{n}_k - \hat{n}_{-k}) - V \sum_{kk'} c_k^\dagger c_{-k'} c_{-k} c_k.$$

(A2)

Here we have introduced a term \(-\sum_k \epsilon_k\) with the choice \(\sum_k \epsilon_k = 0\) in mind, for all \(k\)'s (basically these sums are over the states within energy \(\pm \omega_D\) about the fermi level, where \(\omega_D\) is the Debye energy) that participate in pair formation. As stated earlier, if \(n_k\) denotes the number of electrons in \(k\)-state, then we are considering only a subspace of states defined by \(n_k = n_{-k}\), where either the both of the states in the pair \((k, -k)\) are occupied, or both are empty. Now if we denote by \(|1_k1_{-k}\rangle\) a \((k, -k)\) pair-occupied state and by \(|0_k0_{-k}\rangle\) an unoccupied one, then

\[
(1 - \hat{n}_k - \hat{n}_{-k})|1_k1_{-k}\rangle = (1 - 1 - 1)|1_k1_{-k}\rangle = -|1_k1_{-k}\rangle,
\]

and

\[
(1 - \hat{n}_k - \hat{n}_{-k})|0_k0_{-k}\rangle = (1 - 0 - 0)|0_k0_{-k}\rangle = |0_k0_{-k}\rangle.
\]

Thus we switch over to our good old pseudo-spin picture through the following correspondences

\[
|1_k1_{-k}\rangle \leftrightarrow |\downarrow\rangle_k,
\]

\[
|0_k0_{-k}\rangle \leftrightarrow |\uparrow\rangle_k,
\]

and

\[
(1 - n_k - n_{-k}) \leftrightarrow \sigma_z^k.
\]

(A3)

Since

\[
c_k^\dagger c_{-k} |\downarrow\rangle_k = |\downarrow\rangle_k, \quad c_k^\dagger c_{-k} |\uparrow\rangle_k = 0 \quad \text{&} \quad c_{-k} c_k |\downarrow\rangle_k = |\uparrow\rangle_k, \quad c_{-k} c_k |\uparrow\rangle_k = 0,
\]

we immediately identify its correspondence with raising and lowering operator \(\sigma^+ / \sigma^-\):

\[
\sigma^- = \sigma^x - i\sigma^y = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}
\]

and

\[
\sigma^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}
\]
and therefore
\[ c^+_k c^+_{-k} = \frac{1}{2} \sigma^+_k, \quad c_{-k} c^+_k = \frac{1}{2} \sigma^+_k. \] (A4)

Hence in terms of these spin operators, Hamiltonian (A2) takes the form
\[ \mathcal{H} = - \sum_k \epsilon_k \sigma^z_k - \frac{1}{4} V \sum_{kk'} \sigma^x_k \sigma^y_{k'}. \] (A5)

Since the term \( \sum_{kk'} (\sigma^x_k \sigma^y_{k'} - \sigma^y_k \sigma^x_{k'}) \) vanishes due to symmetric summing done over \( k \) and \( k' \), the Hamiltonian finally reduces to
\[ \mathcal{H} = - \sum_k \epsilon_k \sigma^z_k - \frac{1}{4} V \sum_{kk'} (\sigma^x_k \sigma^x_{k'} + \sigma^y_k \sigma^y_{k'}). \] (A6)

To obtain the energy spectrum of the pseudo-spin BCS Hamiltonian (A6) we apply now the mean field theory developed in earlier section.

**Weiss’ Mean Field Solution**

Just as we did in case of TIM (see sec 1.3), here also we introduce an average effective field \( \vec{h}_k \) for each pseudo-spin \( \sigma^z_k \) as
\[ \vec{h}_k = \epsilon_k \hat{z} + \frac{1}{2} V \sum_{k'} \langle \sigma^x_{k'} \hat{x} + \sigma^y_{k'} \hat{y} \rangle \]
and consequently the Hamiltonian (A6) takes the form
\[ \mathcal{H} = - \sum_k \vec{h}_k \cdot \vec{\sigma}_k. \]

Here for each \( k \) there is an independent spin \( \vec{\sigma}_k \) which interacts only with some effective field \( \vec{h}_k \), and our system is a collection of such mutually non-interacting spins under a field \( \vec{h}_k \).

Now if redefine our x-axis along the projection of \( \vec{h}_k \) on the x-y plane for each \( k \), then with all \( \langle \sigma^y_{k'} \rangle = 0 \) we get
\[ \tan \theta_k = \frac{h^x_k}{h^z_k} = \frac{1}{2} V \sum_{k'} \langle \sigma^x_{k'} \rangle \frac{\sin \theta_{k'}}{\epsilon_k} , \] (A7)
where \( \theta_k \) is the angle between z-axis and \( \vec{h}_k \).

**Excitation spectra at \( T = 0 \)**

Since at \( T = 0 \) \( \langle \sigma^x \rangle = 1 \),
\[ \langle \sigma^x_k \rangle = |\vec{\sigma}| \sin \theta_{k'} = \sin \theta_{k'} \] (A8)

Thus from (A7) we get
\[ \tan \theta_k = (\sqrt{2} \epsilon_{k'}) \sum_k \sin \theta_{k'} \]

Now let us define
\[ \Delta = \frac{1 \sqrt{2} V}{2} \sum_k \sin \theta_{k'} , \]
so that \( \tan \theta_k = \Delta / \epsilon_k \). Then simple trigonometry gives -
\[ \sin \theta_k = \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_k^2}} ; \quad \cos \theta_k = \frac{\epsilon_k}{\sqrt{\Delta^2 + \epsilon_k^2}}. \] (A9)
Substituting for \( \sin \theta_{k'} \) into the above equation we get

\[
\Delta = \frac{1}{2} V \sum_{k'} \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_{k'}^2}}.
\]

Assuming the spectrum to be nearly continuous, we replace the summation by an integral and note that \( V \) is attractive for energy within \( \pm \omega_D \) on both sides of fermi level; \( \omega_D \) being of the order of Debye energy. then the last equation becomes

\[
1 = \frac{1}{2} V \rho_F \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{\sqrt{\Delta^2 + \epsilon^2}} = V \rho_F \sinh^{-1}(\omega_D/\Delta).
\]

Here \( \rho_F \) is the density of states at fermi level. Thus

\[
\Delta = \frac{\omega_D}{\sinh(1/V \rho_F)} \approx 2\omega_D e^{-1/V \rho_F}, \quad (\text{if } \rho_F V << 1)
\]

We see that \( \Delta \) is positive if \( V \) is positive. To interpret the parameter \( \Delta \), one may notice that at first approximation, the excitation spectrum is obtained as the energy \( E_k \) to reverse a pseudo- spin in the field \( \vec{h}_k \), i.e.,

\[
E_k = 2 |\vec{h}_k| = 2 (\epsilon_k^2 + \Delta_k^2)^{1/2}.
\]

From this expression we clearly see that the minimum excitation energy is \( 2\Delta \), i.e., \( \Delta \) gives the energy gap in the excitation spectrum.

**Estimating transition temperature \( T_c \)**

To find the critical temperature for BCS transition, we just extend here the non-zero temperature version of mean field theory done for Ising case. We should have (unlike that in (A11), where \( \langle \sigma_k \rangle = 1 \) for \( T = 0 \):

\[
\langle \sigma_k^z \rangle = \tanh \left( \beta |\vec{h}_k| \right).
\]

Equation (23) accordingly modifies to

\[
\tan \theta_k = \left( \frac{V}{2\epsilon_k} \right) \sum_{k'} \tanh \left( \beta |\vec{h}_{k'}| \right) \sin \theta_{k'} = \frac{\Delta(T)}{\epsilon_k},
\]

where \( \Delta(T) = \frac{V}{2} \sum_{k'} \tanh \left( \frac{|\vec{h}_{k'}|}{T_c} \right) \sin \theta_{k'} \). From equation (A11) we have

\[
|\vec{h}_k| = [\epsilon_k^2 + \Delta^2(T)].
\]

The BCS transition is characterized by the vanishing of the gap \( \Delta \), since without such a gap in the spectrum, infinite conductance would not be possible except at \( T = 0 \). Hence, as \( T \to T_c \), \( \Delta \to 0 \), i.e., using (A11), \( |\vec{h}_k| = \epsilon_k \) and putting this and relations like (A9) in (A13), we get

\[
1 = V \sum_{k'} \frac{1}{2\epsilon_{k'}} \tanh \left( \frac{\epsilon_{k'}}{T_c} \right). \quad (A14)
\]

Above relation is correct if we consider an excited pair as a single entity. However, if we extend our picture to incorporate single particles excited symmetrically in momentum space, then we double the number of possible excitations, thereby doubling the overall entropy. This is exactly equivalent to a doubling of the temperature in free energy. The energy contribution to the free energy, however, remains unaltered, since two single particle excitations of same \( |\vec{k}| \) have same energy as that of a pair of equal \( |\vec{k}| \). Hence we replace \( T_c \) by \( 2T_c \), and in the continuum limit, get

\[
\frac{2}{V \rho_F} = \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{\epsilon} \tanh \left( \frac{\epsilon}{2T_c} \right) = 2 \int_0^{\omega_D/2T_c} \frac{\tanh x}{x} dx.
\]
with \((x = \epsilon/2T_c)\) This is the equation from which we obtain \(T_c\) on integration. If \(T_c << \omega_D\), then we may approximate \(\tanh x \approx 1\), for \(x \geq 1\), and for \(x << 1\), we set \(\tanh x \approx x\). This readily reduces the integral to the value \(1 + \log(\omega_D/2T_c)\), from which we have

\[
T_c = (e/2)\omega_D e^{-1/V F}.
\]

Grphical integration gives a closer result

\[
T_c = 1.14\omega_D e^{-1/V F}. \tag{A15}
\]

Comparing equations (A10) and (A15) we get the approximate relat ionship

\[
2\Delta \simeq 3.5T_c. \tag{A16}
\]

This result is quite consistent with the exprimental values for a number of materials. For example, the value of \(2\Delta/T_c\) are 3.5, 3.4, 4.1, 3.3 for Sn, Al, Pb, and Cd superconductors respectively.

Appendix B:

Real Space Renormalization for Transverse Ising Chain

Here the basic idea of real space block renormalization [6], [4] is illustrated by applying it on an Ising chain in transverse field. Taking the cooperative interaction along x-axis, and the transverse field along z-axis, the Hamiltonian reads

\[
H = -\Gamma N \sum_{i=1}^{N} \sigma_z^i - J \sum_{i=1}^{N-1} \sigma_z^i \sigma_x^{i+1}. 
\]

\[
= H_B + H_{IB} \quad \text{(say)}. \tag{B1}
\]

Here

\[
H_B = \sum_{p=1}^{N/b} H_p ; \quad H_p = -\Gamma \sigma_z^{i,p} - \sum_{i=1}^{b-1} J \sigma_x^{i,p} \sigma_x^{i+1,p} \tag{B2}
\]

and

\[
H_{IB} = \sum_{p=1}^{N/(b-1)} H_{p,p+1} ; \quad H_{p,p+1} = -J \sigma_x^{i,p} \sigma_x^{i+1,p+1}. \tag{B3}
\]

The above rearrangement of the Hamiltonian recasts the picture of \(N\) spins with nearest-neighbour interaction into one in which there are \(N/(b-1)\) blocks, each consisting of \(b\) number of spins. The part \(H_B\) represents the interaction between the spins within the blocks, while \(H_{IB}\) represents the interactions between the blocks through their terminal spins (see Fig. 1.6).

Here we will consider \(b = 2\), as shown in the figure. Now \(H_p\) has got 4 eigen-states, and one can express them in terms of the linear superposition of the eigen-states of \(\sigma_z^{i,p} \otimes \sigma_x^{i,p}\); namely,

\[
| \uparrow\uparrow \rangle, \quad | \downarrow\downarrow \rangle, \quad | \uparrow\downarrow \rangle, \quad \text{and} \quad | \downarrow\uparrow \rangle.
\]

Considering the orthonormality of the eigen-states, one may easily see that the eigenstates of \(H_p\) can be expressed as

\[
|0\rangle = \frac{1}{\sqrt{1 + a^2}}(| \uparrow\uparrow \rangle + a| \downarrow\downarrow \rangle) \quad |1\rangle = \frac{1}{\sqrt{2}}(| \uparrow\downarrow \rangle + | \downarrow\uparrow \rangle) \quad |2\rangle = \frac{1}{\sqrt{2}}(| \uparrow\downarrow \rangle - | \downarrow\uparrow \rangle) \quad |3\rangle = \frac{1}{\sqrt{1 + a^2}}(a| \uparrow\uparrow \rangle - | \downarrow\downarrow \rangle). \tag{B4}
\]
FIG. 6: The linear chain is broken up into blocks of size $b$ (= 2 here) and the Hamiltonian (B1) can be written as the sum of block Hamiltonians $H_p$ and inter-block Hamiltonians $H_{p,p+1}$. The Hamiltonian $H_p$ is diagonalized exactly and the lowest lying two states are identified as the renormalized spin states in terms of which the inter-block Hamiltonian is rewritten to get the RG recursion relation.

Here $a$ is a coefficient required to be chosen properly, so that $|0\rangle$ and $|3\rangle$ are eigenstates of $H_p$. One gets,

$$H_p|0\rangle = H_p \left[ \frac{1}{\sqrt{1 + a^2}} |\uparrow\uparrow\rangle + a |\downarrow\downarrow\rangle \right] = \frac{1}{\sqrt{1 + a^2}} \left[ -\Gamma(\sigma_1^z + \sigma_2^z) - J(\sigma_1^x \sigma_2^x) \right] |\uparrow\uparrow\rangle + \frac{1}{\sqrt{1 + a^2}} \left[ -\Gamma(2 |\uparrow\uparrow\rangle - 2a |\downarrow\downarrow\rangle) - J(|\downarrow\downarrow\rangle + a |\uparrow\uparrow\rangle) \right]$$

Thus $|0\rangle$ to be an eigenstate of $H_p$, one must have

$$-\frac{2\Gamma - J/a}{2\Gamma + Ja} = 1$$

$$=> \quad Ja^2 - 4\Gamma a - J = 0$$

or,

$$a = \pm \sqrt{\frac{4\Gamma^2 + J^2 - 2\Gamma}{J}}. \quad (B5)$$

To minimize the energy, we have to choose,

$$a = \frac{\sqrt{4\Gamma^2 + J^2 - 2\Gamma}}{J}.$$  

One can now see, applying $H_p$ on its eigenstates,

$$H_p|0\rangle = E_0|0\rangle, \quad E_0 = -\sqrt{4\Gamma^2 + J^2}$$
$$H_p|1\rangle = E_1|1\rangle, \quad E_1 = -J$$
$$H_p|2\rangle = E_2|2\rangle, \quad E_2 = +J$$
$$H_p|3\rangle = E_3|3\rangle, \quad E_3 = +\sqrt{4\Gamma^2 + J^2}. \quad (B6)$$
Now we define our new renormalized spin variables $\sigma^\prime$s, each replacing a block in the original Hamiltonian. We retain only the two lowest lying states $|0\rangle$ and $|1\rangle$ of a block and define corresponding $\sigma^\prime_Z$ to have them as its two eigenstates, $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$. We also define

$$\sigma^\prime_x = \frac{\sigma_x \otimes I + I \otimes \sigma^2}{2},$$

where $I$ is the $2 \times 2$ identity matrix. Now since

$$(0|\sigma^\prime_x|1) = \frac{1 + a}{\sqrt{2(1 + a^2)}},$$

we take our renormalized $J$ to be

$$J^\prime = J\frac{(1 + a)^2}{2(1 + a^2)}, \quad (B7)$$

and since the energy gap between $|0\rangle$ and $|1\rangle$ must be equal to $2\Gamma^\prime$ (This gap was $2\Gamma$ in the unrenormalized states), we set

$$\Gamma^\prime = \frac{E_1 - E_0}{2} = \frac{\sqrt{4\lambda^2 + J^2} + J}{2} = \frac{J}{2}\left[\sqrt{4\lambda^2 + 1} + 1\right], \quad (B8)$$

where $a = \sqrt{4\lambda^2 + 1 - 2\lambda}$, defining the relevant variable $\lambda = \Gamma/J$.

The fixed points of the recurrence relation (rewritten in terms of $\lambda$) are

$$\lambda^* = 0 \quad \lambda^* \rightarrow \infty \quad \text{and} \quad \lambda^* \simeq 1.277. \quad (B9)$$

Now if correlation length goes as

$$\xi \sim (\lambda - \lambda_c)^\nu,$$

in the original system, then in the renormalized system we should have

$$\xi^\prime \sim (\lambda^\prime - \lambda_c)^\nu$$

$$=> \quad \frac{\xi^\prime}{\xi} = \left(\frac{\lambda^\prime - \lambda_c}{\lambda - \lambda_c}\right)^{-\nu} = \left(\frac{\xi}{\xi}\right)^{-1/\nu} = \left|\frac{d\lambda^\prime}{d\lambda}\right|_{\lambda = \lambda_c = \lambda^*}. \quad (B10)$$

Now since the actual physical correlation length should remain same as we renormalize, $\xi^\prime$ (correlation length in the renormalized length scale) must be smaller by the factor $b$ (that scales the length), than $\xi$ (correlation length in original scale). i.e., $\xi^\prime/\xi = b$, or,

$$b^{-1/\nu} = \left|\frac{d\lambda^\prime}{d\lambda}\right|_{\lambda = \lambda_c = \lambda^*} \equiv \Omega \quad \text{(say)},$$

hence,

$$\nu = \frac{\ln \Omega}{\ln b} \bigg|_{\lambda = \lambda^*} = \frac{\ln \Omega}{\ln 2} \simeq 1.47, \quad \text{(for } b = 2), \quad (B11)$$

compared to the exact value $\nu = 1$ for $(d + 1 =) 2$ dimensional classical Ising system. Similarly $E_g \sim \omega \sim (\text{time})^{-1} \sim \xi^{-z}$; $z = 1$. But for $b = 2$, we donot get $z = 1$. Instead, $\lambda^\prime/\lambda \sim b^{-z}$ gives $z \simeq 0.55$. Energy gap

$$\Delta(\lambda) \sim |\lambda_c - \lambda|^s \sim \xi^{-z} \sim |\lambda^\prime - \lambda|^\nu \quad (B12)$$

Hence $s = \nu z = 0.55 \times 1.47 \simeq 0.81$ (compared to the exact result $s = 1$). Results improve rapidly for large $b$ values.
Appendix C:
Tunnelling Through Asymmetric Barrier

Let us consider an asymmetric potential energy barrier in one dimension, (as shown in Fig. 1.7). It is essentially a rectangular barrier of height $\chi$ and width $a$ between two different energy levels with a potential difference $h$ between them. The potential energy $V$ is zero at the left of the barrier ($x < 0$), and it is $h$ ($h$ may be negative as well) at the right of the barrier ($x > a$). If a beam of free particles of mass $m$ with kinetic energy $\Gamma$ incidents on the barrier from the left, then one can calculate the probability for a particle in the beam to get transmitted through (or reflected by) the barrier by solving the time-independent Schrödinger equation (with a time-independent $V$). The transmission coefficient $T$ (defined below) describes the probability of transmission for a single particle, as well as the average transmission of the incident beam.

The incident wave function $\psi_1(x)$, the intermediate wave function $\psi_2(x)$ and the transmitted wave function $\psi_3(x)$ then takes the form

$$\psi_1(x) = Ae^{-ik_1x}, \quad x < 0,$$
$$\psi_2(x) = Be^{k_2x} + Ce^{-k_2x}, \quad 0 \leq x \leq a$$
$$\psi_3(x) = De^{ik_3x}, \quad x > a$$

where,

$$k_1^2 = \Gamma; \quad k_2^2 = \Gamma - \chi \quad \text{and} \quad k_3^2 = \Gamma - h,$$

setting $2m/\hbar^2 = 1$. Here $A$ and $D$ are the amplitudes of the incident and the transmitted wave respectively. At this point one may note that for $\Gamma < h$ transmission is trivially zero. Hence we consider the case for $\Gamma > h$ i.e., for real $k_3$. In that case, applying the condition of continuity of the wave function and its space derivatives at the boundaries, one obtains the relation (cf. [21])

$$A = \frac{1}{2}De^{ik_3a}[(1 + k_3/k_1) \cosh \kappa a + i(k/k_1 - k_3/k) \sinh \kappa a],$$

where $\kappa^2 = -k_2^2 = \chi - \Gamma$. We now consider the limit of very high but narrow barrier, such that $\chi \to \infty$, $a \to 0$, with $g = \chi a$ finite. We also assume that $\chi \gg \Gamma$, so that $\kappa^2 \approx \chi$, and of course $\kappa$ is real. Since $\Gamma \geq 0$, $k_1$ is also real. Hence under this condition the transmission coefficient defined as $T = |D|^2k_3/|A|^2k_1$ is given by (cf. [21])

$$T = \frac{4k_3/k_1}{(1 + k_3^2/k_1^2) \cosh^2 (\kappa a) + \left( \frac{\kappa}{k_1} - \frac{k_3}{\kappa} \right)^2 \sinh^2 (\kappa a)}.$$
In the limit of high but narrow barrier specified above, one has $\kappa a \ll 1$. Hence neglecting terms quadratic or of higher order in $\kappa a$ and linear in $1/\kappa$, one gets

$$T \approx \frac{4k_3/k_1}{\left(1 + \frac{k_1}{\Gamma}\right)^2 + \left(\frac{\kappa}{k_1}\right)^2 (\kappa a)^2} = \frac{4\sqrt{\Gamma(\Gamma - h)}}{(\sqrt{\Gamma} + \sqrt{\Gamma - h})^2 + g^2},$$

putting $k_1 = \sqrt{\Gamma}$, $k_3 = \sqrt{\Gamma - h}$ and $\kappa^2 a \approx \chi a = g$. The transmission coefficient $T$ is thus finite even when the barrier height $\chi$ diverges keeping $g = \chi a$ finite.

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