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Convergence condition of the TAP equation for the infinite-ranged Ising spin glass model†

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Abstract. It is shown that the power expansion of the Gibbs potential of the SK model up to second order in the exchange couplings leads to the TAP equation. This result remains valid for the general (including a ferromagnetic exchange) SK model. Theorems of power expansions and resolvent techniques are employed to solve the convergence problem. The convergence condition is presented for the whole temperature range and for general distributions of the local magnetisations.

1. Introduction

The infinite-ranged Ising spin glass model of Sherrington and Kirkpatrick (1975) (referred to hereafter as SK) is expected to give a mean field type description for spin glasses. SK originally employed the replication procedure of Edwards and Anderson (1975). To obtain physical results at low temperatures a breaking of the replica symmetry is necessary (de Almeida and Thouless 1978, Blandin 1978, Bray and Moore 1978, Parisi 1979). The ansatz for the symmetry breaking which leads to the solution of the SK model, however, is not known.

Thouless, Anderson and Palmer (1977) (referred to hereafter as TAP) gave an alternative approach to the solution of the SK model. These authors presented the free energy derived by diagram expansion of the partition function (see in addition Sommers (1978) and de Dominicis (1980)). Southern and Young (1977) showed that this TAP free energy can also be obtained from the spherical approximation of the Ising model.

TAP have presented the convergence condition of their expansion for temperatures near and above the critical temperature. Far below the critical temperature this condition is to the best of our knowledge not known and will be presented in this paper (§ 3). Our analysis is based on the results of § 2 where we show that the TAP equations can alternatively be obtained from the power expansion of the Gibbs potential up second order in the exchange couplings.

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2. The TAP equation as a power expansion

The highly idealised SK model of a spin glass is described by N Ising spins ($S_i = \pm 1$) whose interaction is given by

$$\mathcal{H}_{\text{int}} = -\tfrac{1}{2} \sum_{i \neq j} J_{ij} S_i S_j \tag{2.1}$$

where the random exchange interactions $J_{ij} = J_{ji}$ are infinitely long ranged (of the order $N^{-1/2}$). They are independent, but equally distributed according to gaussian distributions

$$P(J_{ij}) = \left(\frac{2\pi J^2}{N}\right)^{-1/2} \exp\left(-\frac{(J_{ij} - J_0/N)^2}{2J^2/N}\right) \tag{2.2}$$

with means J_0/N and standard deviations of $JN^{-1/2}$.

As we want to give a power expansion, let us introduce

$$\mathcal{H}(\alpha) = \alpha \mathcal{H}_{\text{int}} - \sum_i h_i^{\text{ex}} S_i \tag{2.3}$$

where h_i^{ex} are external magnetic fields and the parameter α describes the interaction strength. The value of $\alpha = 1$ has to be used at the end of the calculation to obtain the results for the actual SK model.

The Gibbs potential corresponding to the Hamiltonian (2.3) is given by

$$-\beta G(\alpha, \beta, \{m_i\}) = \ln \operatorname{Tr} \mathrm{e}^{-\beta \mathcal{H}(\alpha)} - \beta \sum_i h_i^{\text{ex}} m_i. \tag{2.4}$$

The independent thermodynamic variables are $\beta = (kT)^{-1}$ and the local magnetisations m_i. Note that by standard Legendre transformation techniques h_i^{ex} are functions of α, β and $\{m_i\}$, which can in principal be obtained by inverting the relations $m_i = \langle S_i \rangle_\alpha$. $\langle \ldots \rangle_\alpha$ denotes the canonical expectation value with respect to the Hamiltonian (2.3).

Suppressing the β and $\{m_i\}$ dependence of G, the power expansion is given by

$$G(\alpha) = G(0) + \left.\frac{\partial G}{\partial \alpha}\right|_{\alpha=0} \alpha + \frac{1}{2} \left.\frac{\partial^2 G}{\partial \alpha^2}\right|_{\alpha=0} \alpha^2 + \mathrm{O}(\alpha^3). \tag{2.5}$$

The derivatives are calculated to

$$\partial G / \partial \alpha = \langle \mathcal{H}_{\text{int}} \rangle_\alpha \tag{2.6}$$

and

$$\frac{\partial^2 G}{\partial \alpha^2} = -\beta \left\langle \mathcal{H}_{\text{int}} \left(\mathcal{H}_{\text{int}} - \langle \mathcal{H}_{\text{int}} \rangle_\alpha - \sum_i \frac{\partial h_i^{\text{ex}}}{\partial \alpha} (S_i - m_i) \right) \right\rangle_\alpha . \tag{2.7}$$

For the $\alpha = 0$ case the expectation values are those of a non-interacting system. As all m_i are held constant (implying $m_i = \langle S_i \rangle_\alpha = \langle S_i \rangle_{\alpha=0}$) we find

$$\left.\frac{\partial G}{\partial \alpha}\right|_{\alpha=0} = -\tfrac{1}{2} \sum_{i \neq j} J_{ij} m_i m_j \tag{2.8}$$

and

$$\left.\frac{\partial^2 G}{\partial \alpha^2}\right|_{\alpha=0} = -\tfrac{1}{2}\beta \sum_{i \neq j} J_{ij}^2 (1 - m_i^2)(1 - m_j^2). \tag{2.9}$$

To obtain equation (2.9)

$$\left.\frac{\partial h_i^{\mathrm{ex}}}{\partial \alpha}\right|_{\alpha=0} = \left.\frac{\partial^2 G}{\partial \alpha\, \partial m_i}\right|_{\alpha=0} = -\sum_{j(\neq i)} J_{ij} m_j$$

was used which results from the thermodynamic relation $h_i^{\mathrm{ex}} = \partial G/\partial m_i$.

In equation (2.5) $G(0)$ represents the Gibbs potential of non-interacting Ising spins. Thus this equation gives together with (2.8) and (2.9)

$$\beta G(\alpha) = \tfrac{1}{2}\sum_i \left[(1+m_i)\ln \tfrac{1}{2}(1+m_i) + (1-m_i)\ln \tfrac{1}{2}(1-m_i)\right]$$
$$-\frac{\beta\alpha}{2}\sum_{i\neq j} J_{ij} m_i m_j - \left(\frac{\beta\alpha}{2}\right)^2 \sum_{i\neq j} J_{ij}^2 (1-m_i^2)(1-m_j^2) + \mathrm{O}(\alpha^3). \tag{2.10}$$

For $\alpha = 1$ this is exactly the TAP expression if the higher-order terms $\mathrm{O}(\alpha^3)$ can be neglected. A term-by-term investigation basically identical (and thus not given here) to the treatments of Thouless, Anderson, Lieb and Palmer (unpublished report) and Sommers (1978) shows that these higher-order terms can be neglected in the $N \to \infty$ limit as long as α remains finite. To prove this, one has only to employ $\bar{J}_{ij}, \bar{J}_{ij}^2 \sim N^{-1}$. The exact form of the distribution (2.2) is not needed. Thus as a by-product of this study we find that the TAP equations remain valid for the full SK model including a non-zero mean J_0/N of the distribution $p(J_{ij})$.

In concluding this section we want to point out that the term-by-term treatment can only be justified in the region in which the power expansion is convergent. The convergence criterion of a power expansion, however, is simple and given by $|\alpha| < \rho$, where ρ is the radius of convergence. This radius ρ certainly depends on β and on all m_i. Thus after setting $\alpha = 1$ the relation $1 < \rho$ is the validity condition for the TAP equation.

3. The convergence condition

A direct determination of the radius of convergence seems to be difficult. Thus we will employ an indirect treatment. According to equation (2.6) the exact relation

$$\frac{\partial G}{\partial \alpha} = \langle \mathcal{H}_{\mathrm{int}} \rangle_\alpha = -\tfrac{1}{2}\sum_{i\neq j} J_{ij} m_i m_j - \frac{1}{2\beta}\sum_{i\neq j} J_{ij}\chi_{ij}(\alpha) \tag{3.1}$$

holds where $\chi_{ij}(\alpha) = \beta(\langle S_i S_j\rangle_\alpha - m_i m_j)$ is the susceptibility matrix. Next two standard theorems for power series are used. First the expansions of $G(\alpha)$ and $\partial G/\partial\alpha$ have the same radius of convergence. Secondly the distance from the origin ($\alpha = 0$) to the nearest singular point of the function $G(\alpha)$ is equal to the radius of convergence ρ of the expansion. From equation (3.1) we can conclude that the singularities of $G(\alpha)$ are given by the singular eigenvalues of the matrix $\chi_{ij}(\alpha)$ or by the vanishing eigenvalues of the inverse matrix $\chi_{ij}^{-1}(\alpha)$. Thus the minimum value of $|\alpha|$ for which $\chi_{ij}^{-1}(\alpha)$ has at least one eigenvalue zero determines the radius ρ.

To analyse the eigenvalues of χ_{ij}^{-1} we apply resolvent techniques and introduce

$$R(z) = \frac{1}{N}\mathrm{Tr}_i \frac{1}{z-\chi^{-1}} = \frac{1}{N}\sum_{i=1}^{N} (z-\chi^{-1})_{ii}^{-1}. \tag{3.2}$$

As the singularities of $R(z)$ are given by the eigenvalues of $\chi^{-1}(\alpha)$, we have to find out the special values of α for which the resolvent $R(z)$ is singular at the point $z=0$. The minimum of the absolute values of all these special α will then give us the radius ρ. To keep our analysis as simple as possible, let us treat the case $J_0=0$ first and give the generalisation for $J_0 \neq 0$ afterwards.

The elements of χ^{-1} can be calculated from the relation $\chi_{ij}^{-1} = \partial^2 G/\partial m_i \partial m_j$. The representation (2.10) of $G(\alpha)$ can be used as long as $|\alpha| < \rho$ and we find

$$\chi_{ij}^{-1}(\alpha) = A_{ij}(\alpha) - \alpha J_{ij}. \tag{3.3}$$

Replacing J_{ij}^2 by J^2/N†, the matrix A_{ij} is given by

$$A_{ij}(\alpha) = a_i(\alpha)\delta_{ij} - 2N^{-1}\alpha^2 \beta J^2 m_i m_j \tag{3.4}$$

with

$$a_i(\alpha) = [\beta(1-m_i^2)]^{-1} + \alpha^2 \beta J^2 (1-q_2) \tag{3.5}$$

and

$$q_r = \frac{1}{N}\sum_i m_i^r. \tag{3.6}$$

Note that the off-diagonal term of $A_{ij}(\alpha)$ is proportional to a projector. Such projector terms (even if they are of the order N^{-1}) may in general have an important influence on the spectrum (compare e.g. the modification of the semicircle law due to $J_0 \neq 0$ (Brody *et al* 1981)). This essential point has been overlooked in the treatment of the χ^{-1} spectrum given by Bray and Moore (1979). We further note that equations (3.3) and (3.4) contain all relevant terms for the spectrum of χ^{-1} in the $N \to \infty$ limit. No further relevant contributions are found from the higher-order terms of equation (2.10) (see Appendix).

Applying a theorem of Pastur (1974) (see also Brody *et al* (1981)) for random matrices of type (3.3), the resolvent $R(z)$ is determined by the functional equation $(N \to \infty)$

$$R(z) = R_0(z - \alpha^2 J^2 R(z)) \tag{3.7}$$

where the function $R_0(z)$ is defined as

$$R_0(z) = N^{-1}\,\mathrm{Tr}_i (z-A)^{-1} \tag{3.8}$$

The off-diagonal part of $A_{ij}(\alpha)$ is proportional to a projector. Thus $z-A$ can be inverted:

$$(z-A)_{ij}^{-1} = \frac{1}{z-a_i}\delta_{ij} - \frac{1}{N}\frac{2\alpha^2\beta J^2 m_i m_j/(z-a_i)(z-a_j)}{1+(2\alpha^2\beta J^2/N)\sum_k m_k^2/(z-a_k)}. \tag{3.9}$$

We obtain $R_0(z)$ by summing all diagonal elements, and equation (3.7) yields

$$R(z) = \frac{1}{N}\sum_i \frac{1}{z-\alpha^2 J^2 R(z) - a_i} - \frac{2\alpha^2 \beta J^2}{N}\frac{N^{-1}\sum_i m_i^2/(z-\alpha^2 J^2 R(z) - a_i)^2}{1+2\alpha^2\beta J^2 N^{-1}\sum_k m_k^2/(z-\alpha^2 J^2 R(z)-a_k)}. \tag{3.10}$$

† The deviations $J_{ij}^2 - J^2/N$ are random and of the order N^{-1}. This gives corrections to J_{ij} in equation (3.3) negligible for $N \to \infty$ (cf Appendix).

As shown by Pastur (1974), this equation for $R(z)$ always has a unique solution (in the class of functions analytic in z for $\mathrm{Im}\, z \neq 0$ and such that $\mathrm{Im}\, R(z) > 0$ for $\mathrm{Im}\, z < 0$).

For an arbitrary distribution of the m_i it is impossible to give this solution explicitly. As, however, the second term in equation (3.10) is of lower order in N than the first one, we can simplify the problem with the ansatz†

$$R(z) = \alpha^{-2}J^{-2}\gamma_0(z) + \gamma_1(z) \tag{3.11}$$

where $\gamma_0(z)$ is the solution of

$$\gamma_0(z) = N^{-1}\sum_j \frac{\alpha^2 J^2}{z - \gamma_0(z) - a_j}. \tag{3.12}$$

Equation (3.10) shows that $\gamma_1(z)$ is of the order of N^{-1} and is calculated in this order to

$$\gamma_1(z) = -\frac{2\alpha^2\beta J^2}{N}\frac{1}{N}\sum_j \frac{m_j^2}{(z-\gamma_0-a_j)^2} \times\left[1 - \frac{\alpha^2 J^2}{N}\sum_i \frac{1}{(z-\gamma_0-a_i)^2}\right]^{-1}\left[1 + \frac{2\alpha^2\beta J^2}{N}\sum_k \frac{m_k^2}{(z-\gamma_0-a_k)}\right]^{-1} \tag{3.13}$$

and the simpler problem remains of solving equation (3.12).

Again this is impossible for arbitrary distributions of the m_i. For our analysis, however, we need only the behaviour in the neighbourhood of $z=0$. According to (3.2) and the definition of χ_{ii} the relation

$$R(0) = -N^{-1}\sum_i \chi_{ii} = -\beta(1-q_2) \tag{3.14}$$

is exact for every N. The solution of equation (3.10) (being exact only in the limit $N \to \infty$ and under the condition $|\alpha| < \rho$) should give the same value of $R(z)$ for $z=0$. Again as long as $|\alpha| < \rho$ the resolvent $R(z)$ is not singular at $z=0$. Thus $R(z)$ and $\gamma_0(z)$ can be expanded at $z=0$. Using (3.5) and setting

$$\gamma_0(z) = -(\alpha J)^2\beta(1-q_2) + \eta(z), \tag{3.15}$$

equation (3.12) takes the form

$$\eta(z) = \alpha^2 J^2\beta(1-q_2) + N^{-1}\sum_i \frac{\alpha^2 J^2\beta(1-m_i^2)}{[z-\eta(z)]\beta(1-m_i^2) - 1}. \tag{3.16}$$

As $z - \eta(z)$ is small near $z=0$ the denominators can be expanded, yielding in first order of $[z-\eta(z)]$

$$\eta(z) = -(\alpha J\beta)^2[z-\eta(z)]N^{-1}\sum_i (1-m_i^2)^2 \tag{3.17}$$

or

$$\eta(z) = z\alpha^2(\alpha^2 - \alpha_0^2)^{-1} \tag{3.18}$$

where we have set

$$\alpha_0^{-2} = (\beta J)^2(1 - 2q_2 + q_4) \tag{3.19}$$

and where the q_r are given by equation (3.6).

† This method is analogous to the treatment of Brody *et al* (1981) to find the modification of the semicircle law resulting from $J_0 \neq 0$.

For $\alpha^2 < \alpha_0^2$ equation (3.18) shows that $\mathrm{Im}\,\eta(z) > 0$ for $\mathrm{Im}\,z < 0$ and $\eta(z)$ gives the leading behaviour of $R(z)$ near $z = 0$. This is, however, not the case for $\alpha^2 > \alpha_0^2$ and equation (3.18) represents a wrong branch of $\eta(z)$ for $\alpha^2 > \alpha_0^2$†. This behaviour shows that the values of $\alpha = \pm\alpha_0$ belong to those we are looking for to find the radius of convergence. These singularities correspond to the instability found in the replica procedure (de Almeida and Thouless 1978), in the diagram expansion (Sommers 1978) and in the spectrum of χ^{-1} (Bray and Moore 1979).

To finish our analysis for the $J_0 = 0$ case we have to investigate $\gamma_1(z)$ (given by (3.13)) near $z = 0$. As we are only interested in values of $\alpha^2 < \alpha_0^2$ we can use equation (3.18). Expanding the denominators again, we find for $z \to 0$

$$\gamma_1(z) \sim N^{-1}(\alpha_1^2 - \alpha^2 + \text{constant } z)^{-1} \tag{3.20}$$

with

$$\alpha_1^{-2} = (\beta J)^2 2(q_2 - q_4). \tag{3.21}$$

Equation (3.20) shows that $\gamma_1(z)$ is regular near $z = 0$ for $\alpha^2 \neq \alpha_1^2$, but has a pole singularity at $z = 0$ for $\alpha = \pm\alpha_1$.

From the arguments given above we are now able to conclude that for the $J_0 = 0$ case the radius of convergence of the power expansion in the limit $N \to \infty$ is‡

$$\rho = \min\{|\alpha_0|, |\alpha_1|\} \tag{3.22}$$

where α_0 and α_1 are given by equations (3.19) and (3.21). Setting $\alpha = 1$, the convergence condition $|\alpha| < \rho$ leads us to the region of validity of the TAP equations in the $J_0 = 0$ case:

$$(\beta J)^{-2} > \max\{(1 - 2q_2 + q_4); 2(q_2 - q_4)\}. \tag{3.23}$$

Condition (3.23) represents the fundamental result of this paper. As pointed out by TAP this convergence condition is useful to get a better understanding of the mean field approach to the spin glass problem. As a simple example we remark that the zero field solution of the TAP equations, $m_i = 0$, must be rejected for temperatures $kT < J$ as condition (3.23) does not hold for these temperatures. Moreover, as another simple application an exact lower bound for the spin glass order parameter q_2 can be obtained (Plefka 1982) from condition (3.23).

Let us now generalize to the $J_0 \neq 0$ case. This case can be obtained from the treated one if we replace J_{ij} by $J_{ij} + J_0 N^{-1}$. Then the term $-\alpha J_0 N^{-1}$ has to be added to the RHS of equation (3.4). This new term $-\alpha J_0 N^{-1}$ is similar to the other off-diagonal term of $A_{ij}(\alpha)$. Both terms are of order N^{-1} and both terms are proportional to projectors. Thus we can use the methods applied before to study $R(z)$ near $z = 0$. The behaviour of $\gamma_0(z)$ does not change and the modifications appear in $\gamma_1(z)$. For special values of α, $\gamma_1(z)$ again has poles at $z = 0$. There are in general three values of α called α_2, α_3, α_4 which are given by the solutions of

$$0 = [1 - \alpha\beta J_0(1 - q_2)][1 - 2\alpha^2(\beta J)^2(q_2 - q_4)] - 2\alpha^3\beta^3 J_0 J^2 (q_1 - q_3)^2 \tag{3.24}$$

† For $\alpha^2 - \alpha_0^2 \to +0$ the formal correct branch (having, however, no physical significance) can be found by expanding (3.16) up to $(z - \eta)^2$, which is possible as long as $\mathrm{Im}\, z \neq 0$.

‡ The theorem of Pastur (proved for real A_{ij}) restricts the given analysis to real α. The singular points in the complex α plane may give smaller values of $|\alpha|$. In this case $\rho < \min(|\alpha_0|, |\alpha_1|)$, but condition (3.23) is still necessary. Additional investigations (limited up to now to special distributions of the m_i), however, indicate that (3.23) is also sufficient.

and the condition (3.23) for the validity of the TAP equation has to be replaced for the $J_0 \neq 0$ case by

$$1 > \max\{\beta J(1-2q_2+q_4)^{1/2}; |\alpha_2|^{-1}; |\alpha_3|^{-1}; |\alpha_4|^{-1}\} \tag{3.25}$$

which is our most general result. In the limiting case $J=0$ and $J_0>0$ the condition (3.25) reduces to $1>\beta J_0(1-q_2)$. This is, as it must be, the well known restriction of the mean field theory of an Ising ferromagnet.

One may ask if the function $G(\alpha)$ is defined (in the limit $N\to\infty$) outside the convergence region of the power expansion. We do not believe this and our arguments are the following. Consider the set of equations $m_i = \langle S_i\rangle_\alpha(\{h_i^{\mathrm{ex}}\})$ and vary all fields h_i^{ex} from $-\infty$ to $+\infty$. If there is any phase transition (for $N\to\infty$) then there must be a restriction on the values of m_i. The inversion of $m_i=\langle S_i\rangle_\alpha$ is thus not defined for all values of m_i. As one needs this inversion to define $G(\alpha)$, one has to conclude that $G(\alpha)$ is in the limit $N\to\infty$ not defined for all values of m_i.

4. Conclusion

Summing up, we have shown that the TAP equation of the SK Ising model can be obtained by a power expansion of the Gibbs potential. This new derivation is transparent and has the advantage that the simple theorems for power expansions can be applied to study the convergence problem. For all temperatures the convergence condition of the TAP equation has been presented. This condition seems to us a key to a better understanding of the mean field theory of spin glasses.

In addition it has been shown that the TAP equations remain valid for the general SK model including a ferromagnetic interaction. Finally we emphasise that our treatment can be applied to other infinite-ranged spin glass models.

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Appendix

We will show that higher-order terms of equation (2.10) will not change our basic results.

Let $K_{ij}=k_i\delta_{ij}$ be a non-random matrix ($k_i \sim N^0$) and J_{ij} ($\overline{J_{ij}^2}=J^2N^{-1}$) a random matrix leading to the semicircle law. Then the resolvent $R(z)$ of $B_{ij}=K_{ij}+J_{ij}$ can be found for $N\to\infty$ from

$$R(z)=\frac{1}{N}\mathrm{Tr}_i[z-K-J^2R(z)]^{-1}=\frac{1}{N}\sum_i\frac{1}{z-k_i-J^2R(z)}. \tag{A1}$$

Now we consider $\mathrm{O}(1/N)$ 'perturbations' b_{ij} to B_{ij}. Each b_{ij} can contain a non-random part b_{ij}^0 and a random part b'_{ij} (with $\overline{b'_{ij}}=0$). For the resolvent $\hat{R}$ of $\hat{B}_{ij}=B_{ij}+b_{ij}^0+b'_{ij}$ again the theorem of Pastur holds.

As long as $b_{ij}^0 = 0$ (for $i \neq j$) the perturbations are (for finite N) corrections to the k_i and the J_{ij} which, however, are unimportant for $N \to \infty$, and in this case $\hat{R}(z) \to R(z)$. Thus only off-diagonal non-random perturbations may affect $R(z)$ for $N \to \infty$.

Next it is shown that there are no such corrections to χ^{-1} resulting from the higher-order terms of equation (2.10). Denoting the TAP terms by G_{TAP} and $(\chi_{ij}^{-1})_{\mathrm{TAP}}$, one finds

$$\overline{G - G_{\mathrm{TAP}}} = \sum_{n_1, n_2, \ldots = 0} C(n_1, n_2, \ldots) q_1^{n_1} q_2^{n_2} q_3^{n_3} \ldots \tag{A2}$$

where the bar denotes the J_{ij} average and where the q_r are given by equation (3.6). The coefficients C (which are independent of the m_i) certainly satisfy (as long as $|\alpha| < \rho$)

$$\lim_{N \to \infty} N^{-1} C = 0. \tag{A3}$$

$\chi_{ij}^{-1} = \partial^2 G / \partial m_i \partial m_j$ leads for $i \neq j$ to

$$\overline{\chi_{ij}^{-1} - (X_{ij}^{-1})_{\mathrm{TAP}}} = N^{-2} \sum_{n' n'' n_1, \ldots} \hat{C}(n', n'', n_1 \ldots) m_i^{n'} m_j^{n''} q_1^{n_1} \ldots \tag{A4}$$

where the $\hat{C}$ are linear combinations of the C. Employing (A3), we can conclude that

$$\lim_{N \to \infty} N[\overline{X_{ij}^{-1} - (X_{ij}^{-1})_{\mathrm{TAP}}}] = 0 \tag{A5}$$

and it has been shown that there are no perturbations which can affect our result for $N \to \infty$.

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