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Towards an exact solution for the three-dimensional Ising model: A method of the recurrence equations for partial contractions

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ABSTRACT

We find the exact solutions for the main steps in the analysis of the three-dimensional Ising model. A method is based on a recently found rigorous theory of magnetic phase transitions in a mesoscopic lattice of spins, described as the constrained spin bosons in a Holstein–Primakoff representation.

An exact solution of a famous three-dimensional (3D) Ising model (or any other nontrivial 3D model) of a phase transition was not found, despite almost a century of intensive effort. Only the 1D [1] and 2D Ising models with zero [2] or non-zero [3] external field were solved (see [4,5] and references therein). That 3D problem remains one of the major unsolved problems in physics.

1. A rigorous theory of the constrained spin bosons in a Holstein–Primakoff representation

We start with a rigorous theory, that follows from a recently developed exact approach to the critical phenomena [6] and offers an exact solution for the 3D Ising model. Let us consider a cubic lattice of N interacting immovable spins $s = \frac{1}{2}$ with a period a in a box with volume $V = L^3$ and periodic boundary conditions. The lattice sites are enumerated by a position vector $\mathbf{r}$. A dimensionality of the lattice is arbitrary $d = 1, 2, 3, \ldots$. According to a Holstein–Primakoff representation [7], worked out also by Schwinger [8], each spin is a system of two spin bosons, which are constrained to have a fixed total occupation $\hat{n}_{0\mathbf{r}} + \hat{n}_{\mathbf{r}} = 2s$; $\hat{n}_{\mathbf{r}} = \hat{a}^\dagger_{\mathbf{r}}\hat{a}_{\mathbf{r}}$, $\hat{n}_{0\mathbf{r}} = \hat{a}^\dagger_{0\mathbf{r}}\hat{a}_{0\mathbf{r}}$. The $\hat{a}_{\mathbf{r}}$ and $\hat{a}_{0\mathbf{r}}$ are the annihilation operators. A vector spin operator $\hat{\mathbf{S}}_{\mathbf{r}}$ at a site $\mathbf{r}$ is given by its components as

$$\hat{S}^x_{\mathbf{r}} = \frac{\hat{a}^\dagger_{0\mathbf{r}}\hat{a}_{\mathbf{r}} + \hat{a}^\dagger_{\mathbf{r}}\hat{a}_{0\mathbf{r}}}{2}, \; \hat{S}^y_{\mathbf{r}} = \frac{\hat{a}^\dagger_{0\mathbf{r}}\hat{a}_{\mathbf{r}} - \hat{a}^\dagger_{\mathbf{r}}\hat{a}_{0\mathbf{r}}}{2i}, \; \hat{S}^z_{\mathbf{r}} = s - \hat{a}^\dagger_{\mathbf{r}}\hat{a}_{\mathbf{r}}.$$

By means of a many-body Hilbert space reduction [6], we can prove that this system is isomorphic to a system of N spin-boson excitations, described by annihilation operators $\hat{\beta}_{\mathbf{r}}$ at each site $\mathbf{r}$ and obeying the Bose canonical commutation relations $[\hat{\beta}_{\mathbf{r}}, \hat{\beta}^\dagger_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'}$, if we cutoff them by a step-function $\theta(2s - \hat{n}_{\mathbf{r}})$. This isomorphism is valid on an entire physically allowed Hilbert space and is achieved by equating the annihilation operators $\hat{\beta}'_{\mathbf{r}} = \hat{\beta}_{\mathbf{r}}\theta(2s - \hat{n}_{\mathbf{r}})$ of those constrained, true excitations to the cutoff Holstein–Primakoff's transition operators:

$$\hat{\beta}'_{\mathbf{r}} = \hat{a}^\dagger_{0\mathbf{r}}(1 + 2s - \hat{n}_{\mathbf{r}})^{-1/2}\hat{a}_{\mathbf{r}}\theta(2s - \hat{n}_{\mathbf{r}}). \tag{1}$$

The vector components of the spin operator become

$$\hat{S}^x_{\mathbf{r}} = \tfrac{1}{2}(S^-_{\mathbf{r}} + \hat{S}^+_{\mathbf{r}}), \; \hat{S}^y_{\mathbf{r}} = \frac{i}{2}(S^-_{\mathbf{r}} - \hat{S}^+_{\mathbf{r}}), \; \hat{S}^z_{\mathbf{r}} = s - \hat{n}_{\mathbf{r}};$$
$$\hat{S}^+_{\mathbf{r}} = \sqrt{2s - \hat{n}_{\mathbf{r}}}\,\hat{\beta}'_{\mathbf{r}}, \; \hat{S}^-_{\mathbf{r}} = \hat{\beta}'^\dagger_{\mathbf{r}}\sqrt{2s - \hat{n}_{\mathbf{r}}}; \; \hat{n}_{\mathbf{r}} = \hat{\beta}'^\dagger_{\mathbf{r}}\hat{\beta}'_{\mathbf{r}}.$$

A free Hamiltonian of a system of N spins in a lattice

$$H_0 = \sum_{\mathbf{r}} \varepsilon \hat{n}_{\mathbf{r}}, \quad \hat{n}_{\mathbf{r}} = \hat{\beta}^\dagger_{\mathbf{r}}\hat{\beta}_{\mathbf{r}}, \quad \varepsilon = g\mu_B B_{ext}, \tag{2}$$

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is determined by a Zeeman energy $-g\mu_B B_{ext}\hat{S}^z$ of a spin in an external magnetic field B_{ext} (which is assumed homogeneous and directed along the axis z) via a g-factor and a Bohr magneton $\mu_B = \frac{e\hbar}{2Mc}$. T is a temperature.

An interaction Hamiltonian in the Ising model becomes

$$H' = -\sum_{\mathbf{r}\neq\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'}[s-\theta(2s-\hat{n}_{\mathbf{r}})\hat{n}_{\mathbf{r}}][s-\theta(2s-\hat{n}_{\mathbf{r}'})\hat{n}_{\mathbf{r}'}], \quad (3)$$

where a coupling between spins is a symmetric function $J_{\mathbf{r},\mathbf{r}'} = J_{\mathbf{r}-\mathbf{r}'}$ of a vector $\mathbf{r}-\mathbf{r}'$, connecting spins. For a spin at a site $\mathbf{r_0}$ there are only the coordination number p of the nonzero couplings $J_{\mathbf{r_0},\mathbf{r_l}} \neq 0$ with the neighboring spins at sites $\mathbf{r_l} = \mathbf{r_0} + \mathbf{l}$; $l = 1, \ldots, p$. The result in Eq. (3) generalizes the Holstein–Primakoff's one [7] by including the nonpolynomial operator $\theta(2s-\hat{n}_{\mathbf{r}})$-cutoff functions, which add a spin-constraint nonlinear interaction and are crucially important in a critical region.

A total Hamiltonian $H = H_0 + H'$ makes any operator $\hat{A}$, evolving in an imaginary time $\tau \in [0, \frac{1}{T}]$ in a Heisenberg representation, the Matsubara operator $\tilde{A}_\tau = e^{\tau H}\hat{A}e^{-\tau H}$. A symbol $\tilde{A}_{j\tau}$ stands for an operator itself $\tilde{A}_{1\tau} = \tilde{A}_\tau$ at $j=1$ and a Matsubara-conjugated operator $\tilde{A}_{2\tau} = \tilde{\bar{A}}_\tau$ at $j=2$. Let $x = \{\tau, \mathbf{r}\}$ be a 4D coordinate and $\hat{\theta} = \prod_{\mathbf{r}} \theta(2s-\hat{n}_{\mathbf{r}})$ – a product of all N cutoff factors.

The unconstrained and true Matsubara Green's functions for spin excitations are defined by a T_τ-ordering:

$$G^{j_2\tau_2\mathbf{r_2}}_{j_1\tau_1\mathbf{r_1}} = -\langle T_\tau \tilde{\beta}_{j_1\tau_1\mathbf{r_1}} \tilde{\bar{\beta}}_{j_2\tau_2\mathbf{r_2}}\rangle, \ \langle\ldots\rangle \equiv \frac{\mathrm{Tr}\{\ldots e^{-\frac{H}{T}}\}}{\mathrm{Tr}\{e^{-\frac{H}{T}}\}}, \quad (4)$$

$$G'^{j_2\tau_2\mathbf{r_2}}_{j_1\tau_1\mathbf{r_1}} = -\langle T_\tau \tilde{\beta}'_{j_1\tau_1\mathbf{r_1}} \tilde{\bar{\beta}}'_{j_2\tau_2\mathbf{r_2}}\hat{\theta}\rangle/P_s; \quad P_s = \langle\hat{\theta}\rangle. \quad (5)$$

In the Ising model there is no coherence, $\langle\beta_{\mathbf{r}\tau}\rangle = 0$, and the unconstrained Green's functions obey the usual Dyson equation with a total irreducible self-energy $\Sigma^{j_2x_2}_{j_1x_1}$,

$$G^{j_2x_2}_{j_1x_1} = G^{(0)j_2x_2}_{j_1x_1} + \check{G}^{(0)}[\check{\Sigma}[G^{j_2x_2}_{j_1x_1}]]. \quad (6)$$

Here the integral operators $\check{\Sigma}$ or $\check{G}^{(0)}$, applied to any function f_{jx}, stand for a convolution of that function f_{jx} over the variables $j, \tau, \mathbf{r}$ with the total irreducible self-energy Σ or a free propagator $G^{(0)}$, respectively:

$\check{K}[f_{jx}] \equiv \sum_{j'=1}^{2}\sum_{\mathbf{r}'}\int_0^{1/T} K^{j'x'}_{jx} f_{j'x'} d\tau'$ for $\check{K} = \check{\Sigma}, \check{G}^{(0)}$.

The total irreducible self-energy is defined by equation

$$\langle T_\tau[\tilde{\beta}_{j_1x_1}, \tilde{H}'_{\tau_1}]\tilde{\bar{\beta}}_{j_2x_2}\rangle = (-1)^{j_1}\sum_{j=1}^{2}\int_0^{\frac{1}{T}}\sum_{\mathbf{r}}\Sigma^{jx}_{j_1x_1}G^{j_2x_2}_{jx}d\tau. \quad (7)$$

The constrained, true Green's functions (5) do not obey the equations of a Dyson type due to a presence of the nonpolynomial functions $\theta(2s-\hat{n}_{\mathbf{r}})$. A standard diagram technique is not suited to deal with them.

2. A method of the recurrence equations for the partial operator contractions

We employ the recurrence equations, derived via a nonpolynomial diagram technique [6], to solve that problem and find the true, constrained Green's functions:

$$G'^{J_2}_{J_1} = -\langle\tilde{b}^{J_2}_{J_1}[\tilde{\theta}_{\tau_1}\tilde{\theta}_{\tau_2}]\rangle/P_s. \quad (8)$$

Here a basis partial two-operator contraction

$$\tilde{b}^{J_2}_{J_1}[f(\{\tilde{n}_{x_1}, \tilde{n}_{x_2}\})] \equiv \mathcal{A}_{\tau_{i_1}\tau_{i_2}} T_\tau\{\tilde{\beta}^c_{J_1}\tilde{\bar{\beta}}^c_{J_2} f^c(\{\tilde{n}_{\tau_1}, \tilde{n}_{\tau_2}\})\} \quad (9)$$

is an operator-valued functional, evaluated for an operator function f and defined as a sum of all possible partial connected contractions, denoted by the superscripts "c". We consider a generic case of an arbitrary operator function $f(\{\tilde{n}_{x_1}, \tilde{n}_{x_2}\})$, which depends on the two sets $\{\tilde{n}_{\mathbf{r_1}\tau_1}\}$ and $\{\tilde{n}_{\mathbf{r_2}\tau_2}\}$ of the spin-excitation occupation operators at all lattice sites at two different times τ_1, τ_2. An anti-normal ordering $\mathcal{A}_{\tau_{i_1}\tau_{i_2}}$ prescribes only positions of the external operators $\tilde{\beta}_{J_1}$ and $\tilde{\bar{\beta}}_{J_2}$ relative to the function $f(\{\tilde{n}_{x_1}, \tilde{n}_{x_2}\})$ and does not affect any other operators' positions, set by T_τ-ordering. We use the short notations for the combined indexes $J = \{ji\mathbf{r_i}\}$ and $J_l = \{j_l i_l \mathbf{r_{i_l}}\}$. An index $i = 1, 2$ (or i_l) enumerates different times τ_i (or τ_{i_l}) in the external operator $\tilde{\beta}_{j\tau_i\mathbf{r_i}}$ (or $\tilde{\beta}_{j_l\tau_{i_l}\mathbf{r_{i_l}}}$).

The exact closed recurrence (difference) equations for the basis partial operator contraction $\tilde{b}^{J_2}_{J_1}[f(\{m_{J'}\})]$ for an arbitrary function $f(\{m_{J'}\}) = f(\{\tilde{n}_{x_1} + 2s + 1 - m_{x_1}, \tilde{n}_{x_2} + 2s + 1 - m_{x_2}\})$, where a set $\{m_{J'}\}$ consists of two sets of integers $\{m_{x_1}\}$, $\{m_{x_2}\}$, are derived in [6]:

$$\tilde{b}^{J_2}_{J_1}[f] = g^{J'_1}_{J_1}\Delta_{m_{J'_1}}\Delta_{m_{J'_2}}\tilde{b}^{J'_2}_{J'_1}[f]g^{J_2}_{J'_2} - g^{J'}_{J_1}\Delta_{m_{J'}} f g^{J_2}_{J'} - g^{J_2}_{J_1} f. \quad (10)$$

Here a matrix $g^{J'}_J$ is the unconstrained Green's function $G^{J'}_J$ for $\tau_i \neq \tau_{i'}$ and its limit at $\tau' \to \tau - (-1)^{j'}0$ for equal times in accord with an anti-normal ordering of operators $\tilde{\beta}_J$, $\tilde{\bar{\beta}}_{J'}$. The latter is dictated by the anti-normal ordering in the definition of the basis contractions in Eq. (9). In Eq. (10), a symbol $\Delta_{m_{J'}}$ means a partial difference operator [9–11] ($\Delta_{m_1} f(m_1, m_2) = f(m_1+1, m_2) - f(m_1, m_2)$ and $\Delta_{m_2} f(m_1, m_2) = f(m_1, m_2+1) - f(m_1, m_2)$), and we assume an Einstein's summation over the repeated indexes J', J'_1, J'_2. The sums run over $j' = 1, 2$ and all different arguments $\tilde{n}_{x'_{i'}}$ of f for J' and similarly for J'_1, J'_2.

A linear system (10) of the integral equations over the spin positions' variables and discrete (recurrence) equations over variables $\{m_{J'}\}$ can be solved by well-known methods [9–11], such as a Z-transform, a characteristic function, or a direct recursion. The partial contraction in Eq. (8) is given by those solutions at $m_{J'} = 2s + 1$.

3. The exact total irreducible self-energy

A formula for the exact total irreducible self-energy

$$\Sigma^J_{J_0} = -\delta(\tau - \tau_0)\sum_{l=1}^{p}\sum_{I'} J_{\mathbf{r_0},\mathbf{r_l}}\bar{b}^{I'}_{I_0}[f(\tilde{n}_{\mathbf{r_0}} - 1, \tilde{n}_{\mathbf{r_l}})](g^{-1})^{I}_{I'} \quad (11)$$

follows from Eqs. (7) and (10). Here $\bar{b}^{I'}_{I_0}[f] = \langle\tilde{b}^{I'}_{I_0}[f]\rangle$, $f(\tilde{n}_{\mathbf{r_0}}, \tilde{n}_{\mathbf{r_l}}) = (\delta_{0,\tilde{n}_{\mathbf{r_0}}} - \delta_{1,\tilde{n}_{\mathbf{r_0}}})(1 - 2\delta_{1,\tilde{n}_{\mathbf{r_l}}})$, and $(g^{-1})^{I}_{I'}$ is a matrix, inverse to the equal-time anti-normally ordered correlation matrix $g^{I'}_I$ over the combined indexes $I = \{j, \mathbf{r}\}$ and $I' = \{j', \mathbf{r}'\}$. The self-energy matrix has a pure $(p+1)$-banded diagonal structure in indexes $\mathbf{r_0}, \mathbf{r}$,

$$\Sigma^J_{J_0} = \delta(\tau - \tau_0)\sum_{l=0}^{p}\delta_{\mathbf{r},\mathbf{r_l}}\Sigma^{j\mathbf{r_l}}_{j_0\mathbf{r_0}}(l), \quad \mathbf{r_l} = \mathbf{r_0} + \mathbf{l}. \quad (12)$$

For a given spin $\mathbf{r_0}$, it is not zero only for the neighboring spins $\mathbf{r} = \mathbf{r_l}$; $l = 0, 1, \ldots, p$. We find each 2×2-matrix block $\Sigma^j_{j_0}(l)$ by solving the recurrence Eq. (10). That result is crucial for the exact solution of the Ising model.

We consider a homogeneous phase, when the Green's function $G^{j_2\tau_2\mathbf{r_2}}_{j_1\tau_1\mathbf{r_1}}$ depends on $\mathbf{r_1}$ and $\mathbf{r_2}$ only via $\mathbf{r_2} - \mathbf{r_1}$. So, it is a Toeplitz matrix with respect to indexes $\mathbf{r_1}$ and $\mathbf{r_2}$. A general case will be presented elsewhere. We find the 2×2-matrices $\bar{b}^{j'}_{j_0}(l) = \bar{b}^{j'\mathbf{r_l}}_{j_0\mathbf{r_0}}[f(\tilde{n}_{\mathbf{r_0}} - 1, \tilde{n}_{\mathbf{r_l}})]$ as follows