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OF BOGOLUBOV TO THE ISING MODEL

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Применение функционального аналога
вариационного метода Боголюбова

Функциональный аналог вариационного метода Боголюбова применяется к модели Изинга. В качестве вариационного функционала берется четный полином порядка $2p$. Вычисляются значения критических индексов в этом приближении. Получается уравнение для критической температуры в зависимости от спина. Дается решение и приводятся численные результаты.

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Application of a Functional Analog of the Variational
Method of Bogolubov to the Ising Model

A functional analog of the variational method of Bogolubov is applied to the Ising model. A well known path integral representation for the free energy and pair correlation function is derived and the variational method is applied using a class of trial functionals with non-coupled modes. The values of critical indices and a general equation for the critical temperature in a simple cubic lattice are obtained. The last is solved for different values of the spin, and the numerical results are presented.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. Introduction

In ^{1/} a functional analog of the variational method of Bogolubov for path integral applications in statistical mechanics was developed. As an illustration we will apply it here to the simplest nontrivial model used to describe second order phase transitions, the well studied Ising model.

2. Integral Representation for the Free Energy and Correlation Functions

In order to illustrate the systematic procedure of application of our variational method, we will briefly derive a well known path integral representation (see, e.g., ^{2/}) for the partition function and the pair correlation function of Ising model.

The Hamiltonian of Ising model for a system of N spins S in a lattice is

$$H = -h \sum_{f=1}^N S_f^z - \frac{1}{2} \sum_{f,g=1}^N J_{fg} S_f^z S_g^z, \quad (2.1)$$

where J_{fg} is the exchange interaction between spins in sites f and g , h is the external magnetic field multiplied by $\frac{e\hbar}{mC}$, and S_f^z can take the values $-S, -S+1, \dots, S$. By defining

$$S(\vec{r}) = \sum_{f=1}^N S_f^z \delta[\vec{r} - \vec{r}_f]$$

the Hamiltonian can be rewritten.

$$\hat{H} = -h \int d\vec{r} S(\vec{r}) - \frac{1}{2} \int d\vec{r} d\vec{r}' J(\vec{r} - \vec{r}') S(\vec{r}) S(\vec{r}'). \quad (2.2)$$

We introduce the generating functional

$$Z_g(\ell) = \text{Sp} \left\{ e^{\beta \left[\int d\vec{r} [h + \ell(\vec{r})] S(\vec{r}) + \frac{g}{2} \iint d\vec{r} d\vec{r}' J(\vec{r} - \vec{r}') S(\vec{r}) S(\vec{r}') \right]} \right\} \quad (2.3)$$

which satisfies the functional differential equation

$$\frac{\partial Z_g(\ell)}{\partial g} = \frac{1}{2\beta} \iint d\vec{r} d\vec{r}' J(\vec{r} - \vec{r}') \frac{\delta^2 Z_g(\ell)}{\delta \ell(\vec{r}) \delta \ell(\vec{r}')} \quad (2.4)$$

with the initial condition

$$\left. Z_g(\ell) \right|_{g=0} = Z_0(\ell) = \text{Sp} e^{\beta \int d\vec{r} [h + \ell(\vec{r})] S(\vec{r})} \quad (2.5)$$

The solution of (2.4), (2.5) is given by the path integral

$$Z_g(\ell) = \frac{\int \mathcal{D}m e^{-\Phi_0(m)} Z_0(\ell+m)}{\int \mathcal{D}m e^{-\Phi_0(m)}} \quad (2.6)$$

Then, for the partition function $Z = \text{Sp} e^{-\beta \hat{H}}$ we obtain

$$Z = \frac{\int \mathcal{D}\ell e^{-\Phi_0(\ell)} Z_0(\ell)}{\int \mathcal{D}\ell e^{-\Phi_0(\ell)}} \quad (2.7)$$

the magnetization $\sigma = \langle S(\vec{r}) \rangle$ and the pair correlation func-

tion $\Gamma(\vec{r} - \vec{r}') = \langle S(\vec{r}) S(\vec{r}') \rangle$ can be obtained from (2.6) by taking the variational derivative with respect to ℓ and making $\ell = 0$ $g = 1$, the result being :

$$\sigma = \int d\vec{r}' J^{-1}(\vec{r} - \vec{r}') \frac{\int \mathcal{D}\ell e^{-\Phi_0(\ell)} Z_0(\ell) \ell(\vec{r}')}{\int \mathcal{D}\ell e^{-\Phi_0(\ell)} Z_0(\ell)} \quad (2.8)$$

$$\Gamma(\vec{r} - \vec{r}') = -\frac{1}{\beta} J(\vec{r} - \vec{r}') + \iint d\vec{r}_1 d\vec{r}_2 J^{-1}(\vec{r} - \vec{r}_1) J^{-1}(\vec{r}_1 - \vec{r}_2) \frac{\int \mathcal{D}\ell e^{-\Phi_0(\ell)} Z_0(\ell) \ell(\vec{r}_1) \ell(\vec{r}_2)}{\int \mathcal{D}\ell e^{-\Phi_0(\ell)} Z_0(\ell)}, \quad (2.9)$$

where

$$\Phi_0(\ell) = \frac{\beta}{2g} \int d\vec{r} d\vec{r}' J(\vec{r} - \vec{r}') \ell(\vec{r}) \ell(\vec{r}') \quad (2.10)$$

and in formulae (2.7), (2.8), (2.9) we put $g = 1$. Now, coming back to discrete variables

$$Z = \frac{\int \mathcal{D}\ell e^{-\Phi(\ell)}}{\int \mathcal{D}\ell e^{-\Phi_0(\ell)}} \quad (2.11a)$$

$$\sigma = \sum_{f=1}^N J_{ff}^{-1} \langle l_f \rangle_{\Xi} \quad (2.11b)$$

$$\Gamma_{fg} = \sum_{f_1, g_1=1}^N J_{ff_1}^{-1} J_{g_1g}^{-1} \langle l_{f_1} l_{g_1} \rangle_{\Xi} - \sigma J_{fg}^{-1} \quad (2.11c)$$

where we have introduced the notation

$$l = \{l_1, \dots, l_N\}; \int Dl \dots = \int \prod_{f=1}^N dl_f \dots$$

$$\langle \dots \rangle_{\Phi} = \frac{\int Dl e^{-\Phi(l)} \dots}{\int Dl e^{-\Phi(l)}}$$

$$\Phi(l) = \Phi_0(l) + \Phi_1(l) \quad (2.12)$$

$$\Phi_0(l) = \frac{\beta}{2} \sum_{f,g=1}^N J_{fg}^{-1} l_f l_g$$

$$\Phi_1(l) = - \sum_{f=1}^N Q_s [\beta(h+l_f)]$$

$$Q_s(x) = \ln \sum_{m=-s}^{m=s} e^{mx}$$

The mean field approximation is obtained making

$$\bar{l} = e^{-\Phi(\bar{l})}, \quad (2.13)$$

where \bar{l} is determined from the condition

$$\left. \frac{\delta \Phi}{\delta l_f} \right|_{l_f = \bar{l}} = 0 \quad (2.14)$$

which gives for the magnetization σ the equation

$$\sigma = Q'_s(\beta J \sigma) \quad (2.15)$$

and the critical temperature $T_c^0 = \frac{Q_c^0}{J}$ results

$$T_c^0 = \frac{S(S+1)}{3}. \quad (2.16)$$

Here and in what follows we will consider a simple cubic lattice and interaction only with near neighbours, then

$$J(\vec{k}) = \sum_f J_{f0} e^{-i\vec{k} \cdot \vec{r}_f} \quad (2.17)$$

$$J(\vec{k}) = \frac{J}{3} [\cos k_x a + \cos k_y a + \cos k_z a], \quad (2.18)$$

where a is the lattice constant and $J = J(0)$

3. Application of the Variational Principle

Let us consider the system in the paramagnetic region and $h = 0$. We introduce the trial functional

$$\Psi[\eta] = \sum_{n=1}^P \sum_{\vec{k}} A_n(\vec{k}) |\eta(\vec{k})|^{2n}, \quad (3.1)$$

where

$$\eta(\vec{k}) = \frac{1}{\sqrt{N}} \sum_{f=1}^N l_f e^{i\vec{k} \cdot \vec{r}_f} \quad (3.2)$$

and \vec{k} belongs to the first Brillouin zone. We also suppose that $A_n(\vec{k}) = A_n(-\vec{k})$ and $A_p(\vec{k}) > 0$ for all \vec{k} .

Using (2.11), the following inequality for the free energy

$F = -\theta \ln Z$ is easily obtained^{1/1}

$$F \leq F(\Psi) = \theta \langle \Phi[l(\eta)] - \Psi[\eta] \rangle_{\Psi} + \theta \ln \frac{\int D\eta e^{-\Phi_0[l(\eta)]}}{\int D\eta e^{-\Psi[\eta]}}. \quad (3.3)$$

Now, the condition of minimum of the right-hand side of (3.3)

$$\frac{\delta F(\Psi)}{\delta A_n(\vec{k})} = 0 \quad n=1, \dots, P$$

gives a set of P equations determining the functions $A_n(\vec{k})$

$$\langle \Psi, |\eta(\vec{k})|^{2n} \rangle_{\Psi} = \langle \Phi_0; |\eta(\vec{k})|^{2n} \rangle_{\Psi} + \frac{\delta}{\delta A_n(\vec{k})} \langle \Phi_1 \rangle_{\Psi}, \quad (3.4)$$

where $\langle\langle A; B \rangle\rangle_{\psi} = \langle A \rangle_{\psi} \langle B \rangle_{\psi} - \langle AB \rangle_{\psi}$.

The correlators $\langle\langle \Phi_0; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi}$ and $\langle\langle \Psi; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi}$ are very easily obtained whereas $\langle \Phi_1 \rangle_{\psi}$ can be found in the following formal way

$$\langle \frac{\Phi_1}{N} \rangle_{\psi} = -\frac{1}{N} \sum_{f=1}^N \langle Q_S(\beta l_f) \rangle \quad (3.5)$$

$$\langle \frac{\Phi_1}{N} \rangle_{\psi} = -\sum_{m=0}^{\infty} \frac{Q_S^{(2m)}}{(2m)!} \beta^{2m} \frac{1}{N^m} \sum_{\vec{k}_1, \dots, \vec{k}_{2m}} \Delta(\vec{k}_1 + \dots + \vec{k}_{2m}) \langle \eta(\vec{k}_1) \dots \eta(\vec{k}_{2m}) \rangle,$$

where $Q_S(x) = \sum_{m=0}^{\infty} \frac{Q_S^{(2m)} x^{2m}}{(2m)!}$ for $|x| < x_0$.

For $N \rightarrow \infty$ defining

$$\omega^2 = \frac{\beta^2}{N} \sum_{\vec{k}} \langle |\eta(\vec{k})|^2 \rangle_{\psi}$$

we obtain

$$\langle \frac{\Phi_1}{N} \rangle_{\psi} = -\sum_{m=0}^{\infty} \frac{Q_S^{(2m)}}{2^m (m-1)!} \omega^{2m} \quad (3.6)$$

Since x_0 is finite the series (3.5) is divergent but can be summarized by a moment constant method. (See ¹³) with

$$\mu_n = \frac{1}{2} \Gamma(n + \frac{1}{2}).$$

$$\langle \frac{\Phi_1}{N} \rangle_{\psi} = -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{t^2}{2}} Q_S(\omega t) dt \quad (3.7)$$

The correctness of this summation procedure is determined by the analytic properties of $\langle \frac{\Phi_1}{N} \rangle_{\psi}$ which must be an analytic function of β (and hence of ω) except on the imaginary axis. For the case $p=1$ formula (3.7) can be directly obtained

without series expansion (see next section).

Now,

$$\frac{\delta}{\delta A_n(\vec{k})} \langle \Phi_1 \rangle_{\psi} = \frac{\delta \omega^2}{\delta A_n(\vec{k})} \frac{1}{2\omega} \frac{\partial}{\partial \omega} \langle \Phi_1 \rangle_{\psi}$$

$$= \beta^2 \frac{\delta \langle |\eta(\vec{k})|^2 \rangle_{\psi}}{\delta A_n(\vec{k})} \cdot \frac{1}{2\omega} \frac{\partial}{\partial \omega} \langle \frac{\Phi_1}{N} \rangle_{\psi}$$

$$\frac{\delta \langle \Phi_1 \rangle_{\psi}}{\delta A_n(\vec{k})} = -\beta^2 \langle\langle |\eta(\vec{k})|^2; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi} \frac{1}{2\omega} \frac{\partial}{\partial \omega} \langle \frac{\Phi_1}{N} \rangle_{\psi}.$$

Taking into account (3.7) we obtain

$$\frac{\delta \langle \Phi_1 \rangle_{\psi}}{\delta A_n(\vec{k})} = -\beta^2 \langle\langle |\eta(\vec{k})|^2; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi} I(\omega), \quad (3.8)$$

where

$$I(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{-\frac{t^2}{2}} Q_S''(\omega t) \quad (3.9)$$

Now, equations (3.4) can be explicitly written

$$\sum_{r=1}^p U_{rn}(\vec{k}) A_r(\vec{k}) = \frac{\beta}{2} [J'(\vec{k}) - \beta I(\omega)] \quad (3.10)$$

with

$$U_{rn}(\vec{k}) = \frac{\langle\langle |\eta(\vec{k})|^{2r}; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi}}{\langle\langle |\eta(\vec{k})|^2; |\eta(\vec{k})|^{2n} \rangle\rangle_{\psi}}.$$

We look for solutions in the form $A_r(\vec{k}) = Q_r A_1^r(\vec{k})$ so that:

$$U_{rn}(\vec{k}) = C_{rn} A_1^{-r+1}(\vec{k})$$

$$\langle |\eta(\vec{k})|^2 \rangle_{\psi} = C_0 A_1^{-1}(\vec{k}),$$

where C_{rn} and C_0 are functions of a_2, \dots, a_p which are determined by the set of equations

$$\sum_{r=1}^p C_{r1} a_r = \sum_{r=1}^p C_{r2} a_r = \dots = \sum_{r=1}^p C_{rp} a_r = A. \quad (3.11)$$

The main quantity is $\langle |\eta(\vec{r})|^2 \rangle_\psi$ which, making $C = 2C_0 A$ is given by

$$\langle |\eta(\vec{r})|^2 \rangle_\psi = \frac{C \theta}{J^2(\vec{r}) - \beta I(\omega)}. \quad (3.12)$$

The pair correlation function (in \vec{r} space) $\Gamma(\vec{r})$ and the susceptibility $\chi(\theta)$ are expressed in terms of $\langle |\eta(\vec{r})|^2 \rangle_\psi$ as follows

$$\Gamma(\vec{r}) = \frac{\langle |\eta(\vec{r})|^2 \rangle_\psi - \theta J(\vec{r})}{J^2(\vec{r})} \quad (3.13)$$

$$\chi(\theta) = \frac{\beta \langle |\eta(0)|^2 \rangle_\psi J}{J^2}. \quad (3.14)$$

The condition determining the critical temperature $\tau_c = \frac{\theta_c}{J}$ is

$$\frac{1}{\chi(\theta_c)} = 0. \quad (3.15)$$

Then, from (3.12) and (3.14)

$$\tau_c = I[\omega(\tau_c)]. \quad (3.16)$$

For $\theta = \theta_c$ and $\vec{r} \neq 0$

$$\langle |\eta(\vec{r})|^2 \rangle_\psi = \frac{C \theta_c J J(\vec{r})}{J - J(\vec{r})} \quad (3.17)$$

then

$$\omega^2(\tau_c) = \frac{C}{\tau_c} \frac{1}{N} \sum_{\vec{k}} \frac{J(\vec{k})}{J - J(\vec{k})} = \frac{C}{\tau_c} \frac{a^3}{(2\pi)^3} \int d^3 \vec{k} \frac{J(\vec{k})}{J - J(\vec{k})}$$

$$\omega^2(\tau_c) = \frac{Cg}{\tau_c}. \quad (3.18)$$

Using (2.18), the value $g = 0.516386$ is obtained^{14/}. The number C can only depend on p . The explicit equation for τ_c is

$$\tau_c^{1/2} = \frac{1}{\sqrt{2\pi Cg}} \int_{-\infty}^{\infty} dt e^{-\frac{\tau_c t^2}{2Cg}} Q_S''(t). \quad (3.19)$$

In order to determine the critical indices γ, η, ν we note that for $ka \ll 1$ and $\theta \gtrsim \theta_c$

$$\Gamma(\vec{r}) \approx \frac{6C\tau_c}{k^2 a^2 + \frac{1}{r_0^2}}. \quad (3.20)$$

This means that $\eta = 0$ and $\gamma = 2\nu$. The correlation length (in units of a) r_0 is given by

$$\frac{1}{r_0^2} = 6 \frac{\tau - I(\omega)}{\tau}. \quad (3.21)$$

As $I(\omega)$ is an analytic function for $\text{Re} \omega > 0$, for $\tau \gtrsim \tau_c$ we have

$$\frac{1}{r_0^2} = \frac{6(\tau - \tau_c)}{\tau_c} + \frac{6 I'(\omega)(\omega_c - \omega)}{\tau_c}. \quad (3.22)$$

Now, taking into account (3.11) and (3.18)

$$\omega^2(\theta) = \frac{C}{Z} \frac{1}{N} \sum_{\vec{k}} \frac{J(\vec{k})}{J - J(\vec{k}) + \frac{J(\vec{k})}{6r_c^2}} \quad (3.23)$$

and for $Z \rightarrow Z_c$ ($r_0 \rightarrow \infty$) we obtain

$$\omega_c - \omega \approx \frac{3}{4\pi\omega_c r_c} \quad (3.24)$$

Substituting (3.21) into (3.19), the following equation

for $r(\tau)$ is obtained

$$\frac{1}{r_0^2} - \frac{9I(\omega_c)}{2\pi\omega_c r_c} \frac{1}{r_0} = \frac{6(\tau - \tau_c)}{\tau_c} \quad (3.25)$$

meaning that $r_0 \sim (\tau - \tau_c)^{-1}$ so that $\nu = 1$ and $\gamma = 2$

as was expected (see /3/).

The specific heat C_h is given in this approximation

by

$$C_h = - \frac{\Theta}{N} \frac{\partial^2 F(\Psi)}{\partial \Theta^2} \quad (3.26)$$

A tedious but not difficult calculation shows that the corresponding critical index $\alpha = 0$. Then, from scaling theory relations, $\delta = 5$ and $\beta = 1/2$.

4. Gaussian and Biquadratic Trial Functionals. Numerical Results for the Critical Temperature

In the particular case $P = 1$

$$\Psi = \sum_{\vec{R}} A(\vec{R}) |\eta(\vec{R})|^2 \quad (4.1)$$

we have

$$\langle |\eta(\vec{R})|^2 \rangle_{\Psi} = \frac{1}{2A(\vec{R})} \quad (4.2)$$

and $A = 1$, $C = 1$. Formula (3.7) can be directly obtained without series expansion of $Q_S(x)$ in the following way:

$$-\lim_{N \rightarrow \infty} \langle \frac{\Phi_1}{N} \rangle_{\Psi} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{f=1}^N \langle Q_S(\beta l_f) \rangle_{\Psi} = \langle Q_S(\beta l_1) \rangle_{\Psi}$$

$$\langle Q_S(\beta l_1) \rangle_{\Psi} = L \frac{\int \prod_{f=1}^N dl_f e^{-\sum_{fg=1}^N A_{fg} l_f l_g} Q_S(\beta l_1)}{\int \prod_{f=1}^N dl_f e^{-\sum_{fg=1}^N A_{fg} l_f l_g}}$$

where $A_{fg} = \frac{1}{N} \sum_{\vec{k}} A(\vec{k}) e^{i\vec{k} \cdot (\vec{r}_f - \vec{r}_g)}$

$$-\lim_{N \rightarrow \infty} \langle \frac{\Phi_1}{N} \rangle_{\Psi} = L \int_{-\infty}^{\infty} dl_1 e^{-A_{11} l_1^2} Q_S(\beta l_1) \frac{\int \prod_{f=2}^N e^{-\sum_{fg=2}^N A_{fg} l_f l_g - 2l_1 \sum_{g=2}^N A_{1g} l_g} dl_f}{\int \prod_{f=1}^N dl_f e^{-\sum_{fg=1}^N A_{fg} l_f l_g}} \quad (4.3)$$

using the well known formula

$$\int \prod_{m=1}^N dS_m e^{-\frac{1}{2} \sum_{n,m=1}^N A_{nm} S_n S_m + \sum_{m=1}^N X_m S_m} = \left[\frac{(2\pi)^N}{\det A} \right]^{1/2} \exp \left\{ \frac{1}{2} \sum_{n,m=1}^N A_{nm}^{-1} X_n X_m \right\}$$

and

$$\frac{\det A(N-1)}{\det A(N)} = (A^{-1})_{11} = \frac{1}{N} \sum_{\vec{k}} A^{-1}(\vec{k}) = \frac{2\omega^2}{\beta^2}$$

and taking into account that for $Q_S(\beta l) \equiv 1$, $\langle \frac{\Phi_1}{N} \rangle = 1$ we obtain (3.7)

$$\lim_{N \rightarrow \infty} \langle \frac{\Phi_1}{N} \rangle = - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{-\frac{t^2}{2}} Q_S(\omega t)$$

The equation for the critical temperature

$$\tau_c^{1/2} = \frac{1}{\sqrt{2\pi} g} \int_{-\infty}^{\infty} dt e^{-\frac{\tau_c}{2g} t^2} Q_S^N(t) \quad (4.4)$$

can be solved numerically. The results are presented in the table. They show that $\tau_c(s) < \tau_c^0(s)$ and that $\frac{\tau_c(s)}{\tau_c^0(s)}$ increases with S. This behaviour was expected since it is well known that the result of mean field theory is an upper bound for the critical temperature which is better for large spin.

Numerical results can also be obtained in the case $p=2$, using

$$\psi[\eta] = \frac{1}{2} \sum_{\kappa} r(\kappa) |\eta(\kappa)|^2 + A(\kappa) |\eta(\kappa)|^4 \quad (4.5)$$

with $r(\kappa)$ fixed and equal to

$$r(\kappa) = \beta \left[\bar{J}(\kappa) - \frac{\beta S(S+1)}{3} \right] \quad (4.6)$$

Then we obtain for $A(\kappa)$ the equation

$$A(\kappa) = \beta^2 \left[\frac{S(S+1)}{3} - I_S(\omega) \right] \frac{\langle |\eta(\kappa)|^2; |\eta(\kappa)|^4 \rangle_{\psi}}{\langle |\eta(\kappa)|^4; |\eta(\kappa)|^4 \rangle_{\psi}} \quad (4.7)$$

The critical temperature corresponds to $A(\kappa=0, \theta=\theta_c) = 0$ and is found to satisfy again equation (3.16).

The correlation function for $\theta=\theta_c$ and small κ is given by

$$\langle |\eta(\kappa)|^2 \rangle = \frac{1}{2 [\bar{r}(\kappa) - r(0)]} \quad (4.8)$$

Using (4.8) and (4.6) in calculating ω we obtain $\omega \approx \frac{9}{2\tau_c}$ and the explicit equation for τ_c results

$$\tau_c^{1/2} = \frac{1}{\sqrt{\pi g}} \int_{-\infty}^{\infty} e^{-\frac{\tau_c t^2}{9}} Q_3^H(t) dt \quad (4.9)$$

The numerical solution of (4.9) for $S=1/2$ is $\frac{\tau_c(1/2)}{\tau_c^0(1/2)} = 0.79110$ not far from the generally accepted value $0.75180^{15)}$.

Table 1

S	$\tau_c(s) / \tau_c^0(s)$
1/2	0.6461
1	0.7217
3/2	0.7454
2	0.7560
5/2	0.7616
3	0.7650
4	0.7686

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