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# ON FEYNMAN'S VARIATIONAL PRINCIPLE FOR THE POLARON IN A MAGNETIC FIELD

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## 1. INTRODUCTION

Formulation and application of accurate inequalities in statistical physics is an important method for studying physical systems [1]. Thus, in particular, a number of concrete results was derived in [2] on the basis of the general conception of quasi-averages and inequalities for commutator Green's functions.

The well-known Bogolubov inequality

$$F(\hat{H}) \leq F(\hat{H}_0) + \langle \hat{H} - \hat{H}_0 \rangle_{H_0} \tag{1}$$

is a powerful instrument for research of quite different nontrivial models of statistical mechanics. Here $F(\hat{H})$, $F(\hat{H}_0)$ are the free energies corresponding to Hamiltonians $\hat{H}$ and $\hat{H}_0$ respectively, and $\langle \hat{H} - \hat{H}_0 \rangle_{H_0}$ means the statistical averaging with Hamiltonian $\hat{H}_0$. Let's note that it is not obligatory to choose for $\hat{H}_0$ the Hamiltonian of free particles (see in this connection [3]). As a rule, Bogolubov's inequality is used in the framework of the variational principle: the Hamiltonian $\hat{H}_0$ is assumed to be dependent on a set of variational parameters which are then to be chosen from the condition that the r.h.s. of (1) is minimum in order to give the best upper bound to $F(\hat{H})$. The subsequent calculation of physical characteristics of the system is carried out now with the use of the values of the parameters in $\hat{H}_0$ determined by means of Bogolubov's variational principle.

Bogolubov's inequality follows only from the hermiticity of $\hat{H}$, $\hat{H}_0$. Indeed, if we have a convex function $\Phi(\lambda)$ $(\Phi''(\lambda) \geq 0)$ of variable $\lambda$ $(0 \leq \lambda \leq 1)$, then $\Phi(1) \geq \Phi(0) + \Phi'(0)$. Let us consider a function $Z(\lambda) = \mathrm{Sp}\, e^{A+\lambda B}$, where $A$ and $B$ are arbitrary hermitian operators. It is easy to prove that $Z''(\lambda) > 0$. Putting then $A = -\beta\hat{H}$, $B = -\beta[\hat{H} - \hat{H}_0 - \langle \hat{H} - \hat{H}_0 \rangle_{H_0}]$, where $\beta = 1/kT$ is an inverse temperature, we come to Bogolubov's inequality.

Feynman's inequality for actions (see [4] and below) turns out to be very useful for obtaining concrete results in a variety of models (especially, in the polaron model). However, it is not so universal as Bogolubov's inequality.

Recently, in a series of works [5,6] Feynman's inequality was used for studying the properties of the Pekar-Fröhlich polaron in a constant magnetic field. It was conjectured in these works that Feynman's inequality, strictly proved in [4] only for the free polaron, turns out to be correct also for the polaron in an arbitrary magnetic field. When conducting the calculations, the authors in [5,6] used an anisotropic quadratic trial action, which takes into account an anisotropy introduced in the problem by the magnetic field. The result of the calculation in [6] showed that the introduction of this anisotropy in the trial action leads to the conclusion that at definite values of temperature T, magnetic field H and coupling constant of the electron-phonon interaction $\alpha$ the polaron undergoes a "phase" transition: its transverse and longitudinal mass, magnetization and some other characteristics become discontinuous. It seems essential to us that, when using isotropic trial quadratic action, phase transitions in [6] didn't emerge.



In the present paper a detailed discussion of the question of correctness of Feynman's variational inequality for the polaron in the magnetic field is given. It is shown that, when using an anisotropic trial quadratic action, this inequality is not true. This allows us to suppose that phase transitions predicted in [6] do not take place in reality and that they are the result of the incorrect application of Feynman's inequality. (Let's note that in the exactly solved linear model [7], which reproduced correctly the main properties of the Pekar-Fröhlich polaron, there are no any phase transitions in the magnetic field). In conclusion of the work it is shown that Feynman's inequality in the magnetic field is true for the linear polaron model if the isotropic trial quadratic action is used. The former is true for arbitrary $\alpha$, H, T and can be considered as an argument in favour of corrections of Feynman's inequality with the isotropic trial quadratic acrion also for the Pekar-Fröhlich polaron for arbitrary $\alpha$, H, T.

## 2. FORMULATION OF FEYNMAN'S VARIATIONAL INEQUALITY FOR THE FREE POLARON AND ITS GENERALIZATION TO THE MAGNETIC FIELD

The Pekar-Fröhlich polaron model is described by the Hamiltonian [8]:

$$\hat{H} = \frac{\vec{p}^{\,2}}{2} + \sum a^{+}_{\vec{k}} a_{\vec{k}} + \sum_{\vec{k}} C_{\vec{k}} (a_{\vec{k}} + a^{+}_{-\vec{k}})\, e^{i\vec{k}\vec{r}}, \quad C_{\vec{k}} = \left(\frac{2\sqrt{2}\,\pi\alpha}{V}\right)^{1/2} \frac{1}{|\vec{k}|}, \tag{2}$$

where $\vec{r}$ and $\vec{p}$ are respectively the electron radius vector and momentum operators, $a^{+}_{\vec{k}}$, $a_{\vec{k}}$ are the creation and annihilation operators for longitudinal optical phonons with quasi-momentum $\vec{k}$, and V is the volume of the system (in (1) the phonon frequency, the conduction electron mass and the Planck constant ħ are taken equal to unity).

In the framework of the path integral method, the statistical sum of the problem (2) can be written in the form [4]:

$$Z = \prod_{\vec{k}} \frac{1}{1-e^{-\beta}} \int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-S[\vec{x}]} ,$$

$$S[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) - \sum_{\vec{k}} C_{\vec{k}}^2 \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2\, e^{i\vec{k}[\vec{x}(\tau_1)-\vec{x}(\tau_2)]} \left\{ \frac{e^{\tau_1-\tau_2}}{e^{\beta}-1} + \frac{e^{-(\tau_1-\tau_2)}}{1-e^{-\beta}} \right\}, \tag{3}$$

where $\beta = 1/kT$ is the inverse temperature. The path integral in (3) can be calculated only approximately. Taking into account the reality of the "polaron" action $S[\vec{x}]$, we can write for another arbitrary real action $S'[\vec{x}]$ the following inequality:

$$\int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-S[\vec{x}]} \geq \int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-S'[\vec{x}]} \{1 - S[\vec{x}] + S'[\vec{x}]\} , \tag{4}$$

which follows from non-negativity of the second derivative in $\lambda$ from

$$Z(\lambda) = \int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-\lambda S[\vec{x}] - (1-\lambda) S'[\vec{x}]}$$

and can be used as a starting point for the approximate calculation of the statistical sum Z. Now, if the action $S'[\vec{x}]$ depends on some parameters, the values are to be chosen from the requirement that the r.h.s. of the inequality (4) is maximum. In particular, if the action $S'[\vec{x}]$ has the form $S'[\vec{x}] = A + S_0[\vec{x}]$, where A is some real number, then the determination of the maximum value of r.h.s. of (4) in parameter A will give

$$\int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-S[\vec{x}]} \geq \int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-S_0[\vec{x}]}\, e^{-\langle S[\vec{x}] - S_0[\vec{x}] \rangle_{S_0}} \tag{5}$$

This is the Feynman inequality in the polaron theory. If all the quantities in the r.h.s. of it can be calculated exactly, then it permits one to find an approximate expression for the statistical sum Z.

In [4] Feynman used the following trial action:

$$S_0[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) + C \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \{\vec{x}(\tau_1)-\vec{x}(\tau_2)\}^2 \left\{ \frac{e^{w(\tau_1-\tau_2)}}{e^{\beta w}-1} + \frac{e^{-w(\tau_1-\tau_2)}}{1-e^{-\beta w}} \right\}$$



depending on two variational parameters w and C. Limiting himself to the consideration of the low temperature case $\beta \to \infty$, he obtained on the basis of (5) the estimate for the ground state polaron energy $E = \lim_{\beta\to\infty} \{-\frac{1}{\beta}\ln Z\}$ which is very good in the whole region of coupling constant $\alpha$. In [9,10] Feynman's results were generalized also to the case of finite temperatures.

Feynman's inequality was widely used at $\beta \neq \infty$ in [11], and it followd one to obtain general formulas for the effective mass, ground state energy and radius of the polaron as well as concrete formulas for these characteristics in low and high temperature limits.

Unfortunately, till now, one didn't succeed in obtaining a valid generalization of the described above variational method to the case of the polaron in the magnetic field, when Hamiltonian $\hat{H}$ has the form

$$\hat{H} = \frac{1}{2}(\vec{p} - \frac{e}{c}\vec{A})^2 + \sum_{\vec{k}} a_{\vec{k}}^+ a_{\vec{k}} + \sum_{\vec{k}} C_{\vec{k}} (a_{\vec{k}} + a_{-\vec{k}}^+) e^{i\vec{k}\vec{r}} ,$$

where $\vec{A}$ is the vector potential of the magnetic field. The difficulty here is that the expression for the statistical sum of the polaron in the magnetic field includes now imaginary action $S[\vec{x}]$ [12]:

$$S[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) + i\omega_c \int_0^\beta d\tau\, \dot{x}_1(\tau) x_2(\tau) -$$

$$- \sum_{\vec{k}} C_{\vec{k}}^2 \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2\, e^{i\vec{k}[\vec{x}(\tau_1)-\vec{x}(\tau_2)]} \left\{ \frac{e^{(\tau_1-\tau_2)}}{e^{\beta}-1} + \frac{e^{-(\tau_1-\tau_2)}}{1-e^{-\beta}} \right\}$$

($\omega_c = eH/c$ – cyclotron frequency of the free electron) and can't affirm "a priori" the correctness of inequalities (4-5) with arbitrary enough choice of trial actions $S'[\vec{x}]$, $S_0[\vec{x}]$. Nevertheless, one can hope that Feynman's inequality will be true also in the arbitrary magnetic field for some special class of actions $S_0[\vec{x}]$.

In [6] such an assumption was made conformably to the action $S_0[\vec{x}]$ of the Feynman anisotropic oscillator model:

$$S_0[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) + i\omega_c \int_0^\beta d\tau\, \dot{x}_1(\tau) x_2(\tau) + \sum_{i=1}^{3} C_i \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \{x_i(\tau_1) - x_i(\tau_2)\}^2 \left\{ \frac{e^{w_i(\tau_1-\tau_2)}}{e^{\beta w_i}-1} + \frac{e^{-w_i(\tau_1-\tau_2)}}{1-e^{-\beta w_i}} \right\}, \tag{6}$$

where, taking into account that the magnetic field H introduces an anisotropy in the z-direction, we suppose that $C_1 = C_2 = C$ , $C_3 = C$ and $w_1 = w_2 = w$ , $w_3 = w$ (In [5] the assumption was made conformably to the most general anisotropic quadratic action

$$S_0[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) + i\omega_c \int_0^\beta d\tau\, \dot{x}_1(\tau) x_2(\tau) + \sum_{i=1}^{3}\int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2\, C_i(\tau_1 - \tau_2)\{x_i(\tau_1) - x_i(\tau_2)\}^2, \qquad (6')$$

where $C_i(\tau) = C_i(\beta - \tau)$ ; $C_1(\tau) = C_2(\tau) = C_\perp(\tau)$ , $C_3(\tau) = C_\parallel(\tau)$).
In the next section it is shown that the Feynman inequality (5) is not generally speaking correct under the choice of the trial action $S_0[\vec{x}]$ in the form (6-6').

## 3. PROOF OF THE VIOLATION OF THE FEYNMAN INEQUALITY WITH THE ANISOTROPIC TRIAL QUADRATIC ACTION IN THE MAGNETIC FIELD

Let us consider the Feynman inequality (5) in the case, when the electron-phonon coupling constant $\alpha$ is equal to zero. In this case both sides of the inequality (5) can be calculated exactly, and the question of its correctness or incorrectness can be verified by direct calculation. For the sake of definiteness let us take the trial action in (5) in the form (6) and consider only the zero temperature case $\beta \to \infty$. Then, after the calculation of the corresponding gaussian path integrals in (5) we shall obtain the following estimate for the ground state energy of an electron in a magnetic field $E = \frac{1}{2}\omega_c$ [6]:

$$E = \frac{1}{2}\sum_{i=1}^{3}|s_i| - w_\perp - \frac{1}{2}(v_\perp^2 - w_\perp^2)\sum_{i=1}^{3}\frac{|s_i| - w_\perp}{3s_i^2 - v_\perp^2 + 2\omega_c s_i} + \frac{(v_\parallel - w_\parallel)^2}{4v_\parallel}, \qquad (7)$$

where $s_i$ are three (real) roots of the equation

$$s(s^2 - v_\perp^2) + \omega_c(s^2 - w_\perp^2) = 0$$

and

$$v_\perp = \sqrt{w_\perp^2 + \frac{4C_\perp}{w_\perp}}, \quad v_\parallel^2 = \sqrt{w_\parallel + \frac{4C_\parallel}{w_\parallel}}.$$

Let us calculate E by minimization of the r.h.s. of the inequality (7) in parameters $w_\perp$ , $C_\perp$ ; $w_\parallel$, $C_\parallel$ or equivalently by minimization in parameters $w_\perp$ , $v_\perp$ ; $w_\parallel$, $v_\parallel$ ($v_\perp \geq w_\perp$, $v_\parallel \geq w_\parallel$). It is clear that the optimum value for $v_\parallel$ is simply $v_\parallel = w_\parallel$ .



Introducing the new designations for $w_\perp$ , $v_\perp$ , $s_i$ : $w_\perp \to \omega_c w_\perp$, $v_\perp \to \omega_c v_\perp$, $s_i \to \omega_c s_i$ and putting $v_\parallel = w_\parallel$ , we can rewrite inequality (7) in the form

$$E \leq \omega_c\left\{\frac{1}{2}\sum_{i=1}^{3}|s_i| - w_\perp - \frac{1}{2}(v_\perp^2 - w_\perp^2)\sum_{i=1}^{3}\frac{|s_i| - w_\perp}{3s_i^2 - v_\perp^2 + 2s_i}\right\}, \qquad (8)$$

where $s_i$ are now the three (real) roots of the equation $s(s^2 - v_\perp^2) + (s^2 - w_\perp^2) = 0$. The minimization of the r.h.s. of (8) can be performed only numerically. This numerical calculation gives that the minimum value is reached at $w_\perp = 0.08064$, $v_\perp = 0.4320$ and is equal to $0.490529\,\omega_c$. Consequently, the estimate E from the inequality (7) lies approximately 2% lower than the exact quantity $E = \frac{1}{2}\omega_c$, except the case H = 0. It means the violation of the Feynman inequality in the considered example of the polaron with $\alpha = 0$ in any, even small, magnetic field.
Let us note that the obtained conclusion concerning the violation of the Feynman variational inequality in the magnetic field will be completely true also for every trial action, including (6) as a special case, and will be true in particular for the trial action (6') used in [5].

## 4. PROOF OF THE CORRECTNESS OF THE FEYNMAN INEQUALITY WITH THE ISOTROPIC TRIAL QUADRATIC ACTION FOR THE LINEAR POLARON MODEL IN THE MAGNETIC FIELD

Let us consider the linear polaron model with the Hamiltonian:

$$\hat{H}_{lin.} = \frac{1}{2}(\vec{p} - \frac{e}{c}\vec{A})^2 + \sum_{\vec{k}} w_{\vec{k}}\, a^+_{\vec{k}} a_{\vec{k}} + i\sum_{\vec{k}} (\vec{k}\vec{r})\{\Lambda(\vec{k})\, a_{\vec{k}} - \Lambda^*(\vec{k})\, a^+_{\vec{k}}\} + \gamma r^2,$$

where $\Lambda(\vec{k})$ and $w_{\vec{k}} > 0$ are spherically symmetric functions of $\vec{k}$, and the quantity $\gamma$ is chosen from the condition, that Hamiltonian $\hat{H}_{lin.}$ is translationary invariant:

$$\gamma = \frac{1}{3}\sum_{\vec{k}}\frac{k}{w_{\vec{k}}}\Lambda^*(\vec{k})\,\Lambda(\vec{k}).$$

The statistical sum of this model can be written in terms of path integral approach in the following form [13]:

$$Z = \prod_{\vec{k}}\frac{1}{1 - e^{-\beta w_{\vec{k}}}}\int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-S_{lin.}[\vec{x}]}$$

$$S_{lin.}[\vec{x}] = \frac{1}{2}\int_0^\beta d\tau\, \dot{\vec{x}}^2(\tau) + i\omega_c\int_0^\beta d\tau\, \dot{x}_1(\tau) x_2(\tau) +$$

$$+\sum_{\vec{k}} B_{\vec{k}} \int_0^{\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \{\vec{x}(\tau_1) - \vec{x}(\tau_2)\}^2 \left\{ \frac{e^{w_{\vec{k}}(\tau_1-\tau_2)}}{e^{\beta w_{\vec{k}}} - 1} + \frac{e^{-w_{\vec{k}}(\tau_1-\tau_2)}}{1 - e^{-\beta w_{\vec{k}}}} \right\},$$

$$B_{\vec{k}} = \frac{\vec{k}^2}{3 w_{\vec{k}}^2} \Lambda^*(\vec{k}) \Lambda(\vec{k}) .$$

Let us take the trial action $S'[\vec{x}]$ in the following general enough form:

$$S'[\vec{x}] = A + S_0[\vec{x}],$$

$$S_0[\vec{x}] = \frac{1}{2} \int_0^{\beta} d\tau \dot{\vec{x}}^2(\tau) + i\omega_c \int_0^{\beta} d\tau \dot{x}_1(\tau) x_2(\tau) +$$

$$+ \sum_{i=1}^{N} C_i \int_0^{\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \{x(\tau_1) - x(\tau_2)\}^2 \left\{ \frac{e^{w_i(\tau_1-\tau_2)}}{e^{\beta w_i} - 1} + \frac{e^{w_i(\tau_1-\tau_2)}}{1 - e^{-\beta w_i}} \right\},$$

where $A$, $C_i$, $w_i$ ($i = 1,\ldots,N$) are considered as variational parameters. Let us show, that the second derivative in $\lambda$ of

$$\int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-\lambda S_{lin.}[\vec{x}] - (1-\lambda) S'[\vec{x}]}$$

is always non-negative. For this purpose it is enough to make an analogous conclusion about the expression:

$$Z(\lambda) = \frac{\int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-\lambda S_{lin.}[\vec{x}] - (1-\lambda) S'[\vec{x}]}}{\int_{\vec{x}(0)=\vec{x}(\beta)} D\vec{x}\, e^{-\frac{1}{2}\int_0^{\beta} d\tau\, \dot{\vec{x}}^2(\tau)}} . \qquad (9)$$

Performing in all integrals in (9) the substitution

$$\vec{x}(\tau) = \vec{a}_0 + \sum_{n=1}^{\infty} \vec{a}_n \cos\omega_n \tau + \sum_{n=1}^{\infty} \vec{b}_n \sin\omega_n \tau; \quad \omega_n = \frac{2\pi n}{\beta}$$

one can obtain

$$Z(\lambda) = \frac{\int \prod_{n=1}^{\infty} d\vec{a}_n d\vec{b}_n\, e^{-\sum_{n=1}^{\infty} \frac{\beta\omega_n^2}{4}\{a_n^2 + b_n^2\} Z_n + i\frac{\omega_c}{2} \sum_{n=1}^{\infty} \beta\omega_n \{a_n^{(1)} b_n^{(2)} - a_n^{(2)} b_n^{(1)}\} - (1-\lambda) A}}{\int \prod_{n=1}^{\infty} d\vec{a}_n d\vec{b}_n\, e^{-\sum_{n=1}^{\infty} \frac{\beta\omega_n^2}{4}\{\vec{a}_n^2 + \vec{b}_n^2\}}},$$



with

$$Z_n = 1 + \lambda \sum_{\vec{k}} \frac{2B_{\vec{k}}}{w_{\vec{k}} (w_{\vec{k}}^2 + \omega_n^2)} + (1-\lambda) \sum_{i=1}^{N} \frac{2C_i}{w_i (w_i^2 + \omega_n^2)} .$$

After performing integration in $\vec{a}_n$, $\vec{b}_n$ one has:

$$Z(\lambda) = \left\{ \prod_{n=1}^{\infty} \frac{1}{Z_n} \right\}^2 \prod_{n=1}^{\infty} \frac{1}{Z_n + \frac{\omega_c^2}{\omega_n^2 Z_n}}\, e^{-(1-\lambda) A},$$

or $Z(\lambda) = e^{L}$, where

$$L = -2 \sum_{n=1}^{\infty} \ln Z_n - \sum_{n=1}^{\infty} \ln\left\{Z_n + \frac{\omega_c^2}{\omega_n^2 Z_n}\right\} - (1-\lambda) A .$$

Taking into account that

$$Z''(\lambda) = \left\{\left(\frac{\partial L}{\partial \lambda}\right)^2 + \frac{\partial^2 L}{\partial \lambda^2}\right\} e^{L}$$

and verifying by direct differentiation that $\frac{\partial^2 L}{\partial \lambda^2}$ has the form of the sum over $n$ with positive terms, we see that $Z''(\lambda)$ is essentially non-negative quantity. Hence, it follows that in the example considered the two inequalities of the type (4-5) are really true:

$$\int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-S_{lin.}[\vec{x}]} \geq \int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-S'[\vec{x}]} \{1 - S_{lin.}[\vec{x}] + S'[\vec{x}]\}$$

and (after determination of the maximum value of the r.h.s. of the last inequality in $A$)

$$\int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-S_{lin.}[\vec{x}]} \geq \int_{\vec{x}(0) = \vec{x}(\beta)} D\vec{x}\, e^{-S_0[\vec{x}]} \times e^{-\langle S_{lin.}[\vec{x}] - S_0[\vec{x}] \rangle_{S_0}}$$

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Федянин В.К. и др. E17-84-351

О вариационном принципе Фейнмана для полярона в магнитном поле

В работе доказано, что для задачи о поляроне в магнитном поле с анизотропным квадратичным пробным действием несправедлив вариационный принцип Фейнмана для действия.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Fedyanin V.K. et al. E17-84-351

On Feynman's Variational Principle for the Polaron in a Magnetic Field

The paper argues that the Feynman variational principle for action is not valid for the problem of polaron in the magnetic field with anisotropic quadratic trial action.

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

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