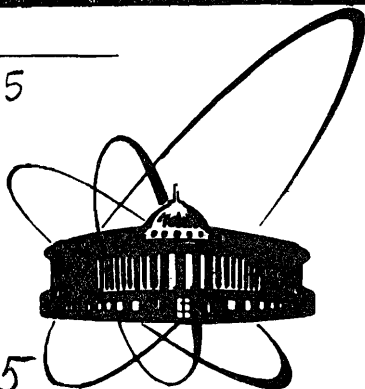


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PHASE TRANSITION  
AND PADÉ APPROXIMANTS FOR POLARON

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## I. INTRODUCTION

Discussing the optical polaron some physicists obtained indications that when the electron-phonon coupling  $\alpha$  increases then at a certain critical value  $\alpha_c$  there occurs a phase transition from a state of freely moving weak-coupling polaron to a localized state of a strong-coupling polaron. As one supposes, the ground state energy  $E(\alpha)$  seems not to be analytic in coupling constant at that point, and other physical characteristics of the polaron (e.g. average number of phonons) have discontinuities.

As far as we know, the first indication on such a phase transition has been obtained by Gross<sup>1/</sup>. He used the so-called Gaussian, or harmonic approximation which is a variant of a variational upper estimate of the polaron ground state energy. In this approximation the polaron energy takes the form

$$E_G(\alpha) = \frac{3}{4}V - \frac{\alpha}{\sqrt{V}} \frac{\Gamma(1/\sqrt{V})}{\Gamma(1/\sqrt{V} + 1/2)}, \quad V \geq 0, \quad (1.1)$$

where  $V$  is a variational parameter. On the boundary  $V = 0$  the Eq.(1.1) leads to a trivial solution  $E_G = -\alpha$ . The variational equation  $\partial E_G / \partial V = 0$  leads to a relation between the coupling constant  $\alpha$  and the variational parameter  $V$ :

$$\alpha = \frac{3}{4}V^{5/2} \frac{\Gamma(1/\sqrt{V} + 1/2)}{\Gamma(1/\sqrt{V})} \left[ \Psi(1/\sqrt{V} + 1/2) - \Psi(1/\sqrt{V}) - V/2 \right]^{-1}, \quad (1.2)$$

$$\Psi(x) = \Gamma'(x)/\Gamma(x).$$

At the point  $V = 0$  the function  $\alpha(V) = 6$ . Then  $\alpha(V)$  decreases and reaches its minimum  $\alpha_m = 5.798$  at  $V_m = 0.613$ . After that  $\alpha(V)$  increases to infinity taking the value  $\alpha = 6$  at  $V = 1.54$ . Therefore when  $\alpha < \alpha_m$  there do not exist any solutions for the energy except the trivial one. In the interval  $\alpha_m < \alpha < 6$  one has two additional solutions from which there remains only one when  $\alpha > 6$ . The latter has the proper asymptotics  $-\alpha^2/3\pi$  at infinity and

lays below the trivial solution when  $\alpha > \alpha_c = 5.842$ . So one can consider  $\alpha_c$  as the critical point of the phase transition. Evidently this phase transition manifests itself rather indistinctly: the points  $\alpha_m$ ,  $\alpha_c$  and  $\alpha = 6$  are too close to each other. The same is true while comparing the values of the first derivative of the energy  $E_G(\alpha)$  with respect to  $\alpha$  near the critical point:

$$E_G'(\alpha_c - 0) = -1, \quad E_G'(\alpha_c + 0) = -1.08. \quad (1.3)$$

The harmonic approximation has been used by a whole number of authors. Other variational approximations are very similar to the harmonic one and often lead almost to the same picture of a "phase transition" (see, e.g., papers<sup>2/</sup>). Recently a number of such papers has been increased appreciably. For the critical value  $\alpha_c$  different results from 3 to 10 have been obtained. Devreese and Peeters published the critical analysis of the problem<sup>3/</sup> and came to the conclusion that for the moment there were no any definite evidences for the phase transition in this system. One of their arguments was the existence of the well-known Feynman variational approximation which leads to the smooth function  $E_F(\alpha)$ . This function provides us with the upper bound for the polaron ground state energy and lays below other estimates indicating on the phase transition.

We also considered some of the papers published after the paper<sup>3/</sup> and devoted to the "discovery" of the phase transition, and convinced ourselves that this "phase transition" was an artefact of the approximations being made. As is known, Fröhlich model of the optical polaron treats the medium in a continuous limit. We dare say there are no physical reasons for the electron being self-trapped in this theory which does not include the structure of the lattice. But to criticize the arguments in favour of the phase transition means to do only the half of the job. Then the question arises, how to prove the smoothness of the function  $E(\alpha)$  dealing only with exact information about its properties.

The goal of the present paper is to give arguments which testify against the existence of such a phase transition. To do that we construct upper and lower bounds for the polaron characteristics using two-point nondiagonal Padé approximants.

In Sec.II of the present paper we demonstrate the power of the method taking as an example the Feynman polaron. In Sec.III the same technique is applied to evaluate the actual polaron ground state

energy and average number of phonons, and in Sec.IV - to calculate its effective mass.

## II. PADÉ APPROXIMANTS FOR THE FEYNMAN POLARON

The Feynman polaron energy<sup>/4/</sup> is as follows:

$$E_F(\alpha) = \frac{3}{4V} (V-W)^2 - \frac{\alpha V}{\sqrt{\pi}} \int_0^\infty dx \frac{e^{-x}}{[W^2x + V^2 - \frac{W^2}{V}(1-e^{-Vx})]^{1/2}}, \quad (2.1)$$

$$V \geq W \geq 0,$$

where  $V$  and  $W$  are variational parameters. On the boundary  $W=0$  the Eq.(2.1) gives us the harmonic approximation with its "phase transition" described above. But all this disappears like fata morgana when we recall the basic variational equations

$$\partial E_F / \partial V = \partial E_F / \partial W = 0, \quad (2.2)$$

which leads to the smooth function  $E_F(\alpha)$ . How can one prove this smoothness? To simulate the real situation let us imagine that we cannot minimize expression (2.1) and thus can use nothing but conventional expansions in powers of a small parameter. It is possible here to obtain the expansions about points  $\alpha = 0$  and  $\alpha = \infty$ . In the weak-coupling limit, the perturbation series takes the form:

$$E_F(\alpha) = \sum_{\kappa \geq 1} E_\kappa \alpha^\kappa. \quad (2.3)$$

In the strong-coupling limit it is possible to expand  $E_F(\alpha)$  in inverse powers of  $\alpha$ :

$$E_F(\alpha) = \sum_{\kappa \geq 0} A_\kappa \alpha^{2-\kappa}. \quad (2.4)$$

We calculated from Eqs.(2.1, 2.2) a rather large number of coefficients  $E_\kappa$  and  $A_\kappa$  (see Table 1). Now let us consider how the information collected in Table 1 can be used to approximate the Feynman solution which plays the role of the exact one in this case. For this purpose we apply the two-point nondiagonal Padé approximants<sup>/5/</sup>:

$$E(n, n-1) = -\alpha \frac{1 + a_1 \alpha + \dots + a_n \alpha^n}{1 + b_1 \alpha + \dots + b_{n-1} \alpha^{n-1}}, \quad n \geq 2. \quad (2.5)$$

Table 1. Coefficients ( $E_\kappa$ ) of the Weak- and ( $A_\kappa$ ) of the Strong-Coupling Expansions for the Feynman Polaron Energy

$E_1 = -1$	$A_{2k+1} = 0$
$E_2 = -1.234568 \cdot 10^{-2}$	$A_0 = -0.406103$
$E_3 = -0.634366 \cdot 10^{-3}$	$A_2 = -2.829442$
$E_4 = -0.464315 \cdot 10^{-4}$	$A_4 = -4.863866$
$E_5 = -0.395686 \cdot 10^{-5}$	$A_6 = -34.195252$
$E_6 = -0.363852 \cdot 10^{-6}$	$A_8 = 533.14083$
$E_7 = -0.347453 \cdot 10^{-7}$	$A_{10} = 51525.155$
$E_8 = -0.336375 \cdot 10^{-8}$	
$E_9 = -0.323953 \cdot 10^{-9}$	
$E_{10} = -0.304353 \cdot 10^{-10}$	
$E_{11} = -0.271495 \cdot 10^{-11}$	
$E_{12} = -0.218526 \cdot 10^{-12}$	

We need  $(2n-1)$  equations to find the parameters  $a_1, \dots, a_n$  and  $b_1, \dots, b_{n-1}$ . Using the information about weak- and strong-coupling expansions equivalently we have two alternative cases. In the first case we reproduce the coefficients  $E_2, \dots, E_n$  and  $A_0, \dots, A_{n-1}$  and obtain the Padé approximant denoted  $E_u(n, n-1)$ . In the second case we obtain another Padé approximant  $E_l(n, n-1)$  of the same form (2.5) which reproduces the coefficients  $E_2, \dots, E_{n+1}$  and  $A_0, \dots, A_{n-2}$ .

The data collected in Table 1 allow us to construct  $E_u(n, n-1)$  for  $n = 2, \dots, 12$  and  $E_l(n, n-1)$  for  $n = 2, \dots, 11$ . In Table 2 we give approximants  $E_u(12, 11)$  and  $E_l(11, 10)$  at some values of the coupling constant  $\alpha$  in comparison with the exact energy  $E_F$  of the Feynman polaron.

Here we do not show the estimates for lower values of  $n$ . The fact is that the value of  $E_u(n, n-1)$  at any given  $\alpha$  increases with  $n$  but remains below the exact solution  $E_F(\alpha)$ , so it provides us with lower estimates of  $E_F(\alpha)$ . On the contrary, the value of  $E_l(n, n-1)$  at any given  $\alpha$  decreases with  $n$  being above the exact solution. So approximants  $E_l(n, n-1)$  give us upper estimates of  $E_F(\alpha)$ . Therefore in Table 2 we present only the best upper and lower bounds. (Note that indices "u" and "l" in our

notations mean upper and lower bounds for the absolute value of the polaron energy).

Table 2. Upper and Lower Bounds for the Energy and the Average Number of Phonons of the Feynman Polaron

$\alpha$	1	3	5	7	9	11	20
- $E_l(11,10)$	1.0130	3.1333	5.4398	8.0969	11.413	15.619	45.272
- $E_F$	1.0130	3.1333	5.4401	8.1127	11.486	15.710	45.283
- $E_u(12,11)$	1.0130	3.1333	5.4419	8.1279	11.500	15.715	45.283
$N_l(11,10)$	0.5272	1.8104	3.7147	7.2613	13.641	22.361	81.992
$N_u(12,11)$	0.5272	1.8106	3.7567	7.6565	14.187	22.691	82.003

In the polaron theory one can derive the relation between average number of phonons and ground state energy (see our paper<sup>6/</sup>). We have for the motionless polaron

$$N(\alpha) = E(\alpha) - \frac{3}{2} \alpha E'(\alpha), \quad (2.6)$$

from which follow weak- and strong-coupling expansions similar to those of Eqs. (2.3, 2.4). Padé approximants take the same form as in Eq. (2.5) where one should replace factor  $-\alpha$  by  $\alpha/2$ . The best upper and lower bounds for the average number of phonons are given also in Table 2.

Let us discuss now the results obtained. Both the Padé approximants for the polaron energy being smooth functions reproduce the Feynman solution well enough. The accuracy of our approximations can be estimated even without  $E_F(\alpha)$ : the discrepancy between upper and lower bounds do not exceed 0.4% in the intermediate coupling region. Naturally, these bounds almost coincide in the weak- and strong-coupling limits. We should mention also that all calculated coefficients

$a_k$  and  $b_k$  are positive so no poles appear in Padé approximants (2.5) at physical values of the coupling constant  $\alpha \geq 0$ .

Besides we investigated the motion of poles of Padé approximants in the complex plane of  $\alpha$ . It occurs that the formula

$$R_n = R + \frac{a}{(n+b)^{3/2}} \quad (2.7)$$

gives the best fit for the distance  $R_n$  between the nearest pole and the origin of coordinates. For Padé approximants  $E_u(n, n-1)$  and  $E_l(n, n-1)$  we obtained closed values of  $R$ :  $R_u = 6.92$  and  $R_l = 6.90$  correspondingly. It means that  $E_F(\alpha)$  is analytic in the circle of the radius  $R \approx 6.9$ . In other words we estimated the range of convergence of the perturbation series.

The discrepancy between two smooth functions giving upper and lower bounds for the average number of phonons do not exceed 2.6%. Here again the motion of the poles indicates that the range of analyticity is near 7. Evidently one can suspect at the "critical" point  $\alpha \approx 7$  the existence of a jump  $\Delta N$  of the average number of phonons with a probable value  $\Delta N \approx (N_u - N_l)/2 \approx 0.2$ . If the jump of the first derivative of  $E_F(\alpha)$  is the same as in the case of harmonic approximation (that is  $\approx 0.1$ , see Eq. (1.3)), then it would inevitably lead to the jump  $\Delta N \approx 1$ . Thus we obtain strong arguments in favour of smoothness of the function  $E_F(\alpha)$  and its first derivative.

The range of convergence is close to "critical" values  $\alpha_c$  of the harmonic and other approximations. Thus an idea strikes that these approximations spoil the analytical properties of  $E(\alpha)$  to such an extent that the "phase transition" seems to appear. Earlier Larsen<sup>7/</sup> found the "phase transition" at  $\alpha_c = 6.25 + 6.5i$  and assumed that the range of convergence of the perturbation series for  $E(\alpha)$  should be finite. However, it is evident, that this fact should not lead for sure to the jumps of  $E(\alpha)$  and/or its derivatives in a physical region of the coupling constant  $\alpha$ . Besides, Larsen used in his arguments the asymptotics  $E(z) \approx O(z^2)$  when  $|z| \rightarrow \infty$  for any complex  $z$ , albeit it was obtained only for real positive  $z = \alpha$ .

### III. ACTUAL POLARON ENERGY AND AVERAGE NUMBER OF PHONONS

We have demonstrated that the two-point nondiagonal Padé approximants provides us with a very accurate upper and lower bounds for the Feynman polaron energy. Therefore we can hope to succeed in the case of an actual polaron with the same technique.

Unfortunately, we do not know as many expansion coefficients as for the Feynman polaron. In the weak-coupling expansion we know only three terms, the last of which has been calculated in our papers<sup>6,8/</sup>:

$$E_1 = -1, \quad E_2 = -1.591962 \cdot 10^{-2}, \quad E_3 = -0.806 \cdot 10^{-3} \quad (3.1)$$

In the strong-coupling limit we have the results obtained by Miyake<sup>9/</sup>:

$$A_0 = -0.108513, \quad A_2 = -2.336, \quad A_1 = A_3 = 0. \quad (3.2)$$

With Eqs.(3.1),(3.2) the exact results for the polaron ground state energy are exhausted. Now we can construct Padé approximants  $E_u(2,1)$ ,  $E_u(3,2)$  and  $E_l(2,1)$ . Again  $E_u(3,2)$  provides us with the better lower bound than  $E_u(2,1)$ . Such a small number of Padé approximants do not allow to estimate the range of convergence of the perturbation series. However, the location of poles does not differ too much from the location of poles in the analogous Padé approximants for the Feynman polaron. So we can hope that the estimate  $R=6.9$  of the preceding section does not decline too much from the true value.

For the actual polaron the lower bound has the form

$$\tilde{E}_u(3,2) = -\alpha \frac{1 + 0.138386\alpha + 0.013289\alpha^2 + 1.143 \cdot 10^{-3}\alpha^3}{1 + 0.122467\alpha + 0.010534\alpha^2}. \quad (3.3)$$

For the upper bounds we have the Feynman variational solution  $\tilde{E}_F(\alpha)$  and the following Padé approximant:

$$E_l(2,1) = -\alpha \frac{1 + 2.462435 \cdot 10^{-2}\alpha + 9.445759 \cdot 10^{-4}\alpha^2}{1 + 2.704726 \cdot 10^{-3}\alpha}. \quad (3.4)$$

The weak- and strong-coupling expansions for the average number of phonons can be derived from Eq.(2.6). The Padé approximants giving upper and lower bounds are as follows:

$$N_u(3,2) = \frac{\alpha}{2} \cdot \frac{1 + 0.193445\alpha + 0.056325\alpha^2 + 0.018413\alpha^3}{1 + 0.129767\alpha + 0.042420\alpha^2}, \quad (3.5)$$

$$N_l(2,1) = \frac{\alpha}{2} \cdot \frac{1 + 7.291175 \cdot 10^{-2}\alpha + 6.612032 \cdot 10^{-3}\alpha^2}{1 + 1.523327 \cdot 10^{-2}\alpha}.$$

The numerical calculations with the help of Eqs.(3.3-3.5) are presented in Table 3.

Table 3. Upper ( $\tilde{E}_l(2,1)$ ,  $\tilde{E}_F$ ,  $N_u(3,2)$ ) and Lower ( $\tilde{E}_u(3,2)$ ,  $N_l(2,1)$ ) Bounds for the Ground State Energy and the Average Number of Phonons of the Actual Polaron

$\alpha$	0.5	1	3	5	7	9	11
$-\tilde{E}_F$	0.5032	1.0130	3.1333	5.4401	8.1127	11.486	15.710
$-\tilde{E}_l(2,1)$	0.5041	1.0167	3.1645	5.4945	8.0406	10.834	13.905
$-\tilde{E}_u(3,2)$	0.5041	1.0175	3.2122	5.7767	8.8832	12.654	17.165
$N_l(2,1)$	0.2583	0.5346	1.8594	3.6236	5.9345	8.8875	12.568
$N_u(3,2)$	0.2587	0.5409	2.1888	5.2383	10.034	16.643	25.062

One can see that  $\tilde{E}_l(2,1)$  gives us better upper bound than  $\tilde{E}_F$  for  $\alpha \lesssim 6$ . In the strong-coupling limit the better upper bound is given by the Feynman solution. This is also true for the improved versions of the Feynman method (see, e.g., the paper by Adamowski, Gerlach and Leschke<sup>10/</sup>). This should not surprise us because while constructing  $E_l(2,1)$  we do not use even the equality  $A_1 = 0$ . A subsequent Padé approximant would lead to better upper bound, but to construct  $E_l(3,2)$  one has to know the coefficient  $E_4$  in the perturbation series (2.3) for the actual polaron. Nevertheless,  $\tilde{E}_F$  and  $\tilde{E}_l(2,1)$  give us independent upper bounds for the ground state energy of the actual polaron. They are both smooth and do not decline too much from each other.

The Padé approximant  $\tilde{E}_u(3,2)$  gives us the lower bound which is much more better than the only known lower bounds by Leib and Yamazaki<sup>11/</sup> and by Larsen<sup>12/</sup> (besides, the latter works only for small values of  $\alpha$ ). Evidently upper and lower bounds for the polaron energy differ less than by 10% in the whole range of the coupling constant. Padé approximants allow to estimate almost with the same accuracy the first derivative of the energy which leads to essentially

larger gap between upper and lower bounds for the average number of phonons. But even such accuracy allows us to obtain some conclusions. Thus, at the "critical" point  $\alpha \simeq 7$  one can assume the jump  $\Delta N \simeq (N_u - N_e)/2 \simeq 2$ . This excludes the phase transition with the jump  $\Delta N \simeq 14$ , the existence of which was conjectured in the paper<sup>/13/</sup>.

So, in the case of the actual polaron the exact solution lies again between two smooth functions. However, we do not see any hints of the phase transition, at least in the given numerical bounds. Of course, subsequent Padé approximants can change the whole situation, but now it seems almost incredible.

#### IV. POLARON EFFECTIVE MASS

In this section we consider the Padé approximants for the polaron effective mass. To begin with, we take the expression for the mass of the Feynman polaron:

$$m_F = 1 + \frac{\alpha V^3}{3\sqrt{\pi}} \int_0^{\infty} dx \frac{x^2 e^{-x}}{[W^2 x + \sqrt{V^2 - W^2}(1 - e^{-Vx})]^{3/2}} \quad (4.1)$$

with the same variational parameters  $V$  and  $W$  as in Eq.(2.1). In the weak coupling limit the perturbation series for  $m_F$  takes the form

$$m_F = 1 + \sum_{k \geq 1} m_k \alpha^k \quad (4.2)$$

In the strong coupling limit  $m_F$  is expanded in inverse powers of the coupling constant:

$$m_F = \sum_{k \geq 0} M_k \alpha^{4-k} \quad (4.3)$$

Coefficients  $m_k$  and  $M_k$  are collected in Table 4.

From Eqs. (4.2, 4.3) it follows that similar expansions for  $m_F^{1/4}$  are like those for the energy  $E_F$ , and we can use again the two-point nondiagonal Padé approximants. So, we have a representation

$$m(n, n-1) = \left[ \frac{1 + a_1 \alpha + \dots + a_n \alpha^n}{1 + b_1 \alpha + \dots + b_{n-1} \alpha^{n-1}} \right]^4 \quad (4.4)$$

from which two Padé approximants follow.

Table 4. Coefficients of the Weak-Coupling ( $m_k$ ) and of the Strong-Coupling ( $M_k$ ) Expansions for the Feynman Polaron Effective Mass

$m_1 = 1/6$	$M_{2k+1} = 0$
$m_2 = 2.469136 \cdot 10^{-2}$	$M_0 = 2.001406 \cdot 10^{-2}$
$m_3 = 3.566719 \cdot 10^{-3}$	$M_2 = -1.012775$
$m_4 = 5.073952 \cdot 10^{-4}$	$M_4 = 11.85579$
$m_5 = 7.117137 \cdot 10^{-5}$	$M_6 = 43.09859$
$m_6 = 9.840535 \cdot 10^{-6}$	
$m_7 = 1.340209 \cdot 10^{-6}$	
$m_8 = 1.796109 \cdot 10^{-7}$	

One of them  $m_u(n, n-1)$  reproduces coefficients  $m_1, \dots, m_{n-1}$  and  $M_0, \dots, M_{n-1}$  and gives the upper bound. The other,  $m_l(n, n-1)$ , reproduces coefficients  $m_1, \dots, m_n, M_0, \dots, M_{n-2}$  and provides us with the lower bound. With data from Table 4 it is possible to construct both Padé approximants for  $n = 2, \dots, 8$ . In Table 5 we present  $m_u(8,7)$  and  $m_l(8,7)$  for some values of the coupling constant  $\alpha$  in comparison with the exact effective mass  $m_F$  of the Feynman polaron.

Table 5. Upper and Lower Bounds for the Feynman Polaron Effective Mass

$\alpha$	1	3	5	7	9	11
$m_l(8,7)$	1.1955	1.8886	3.8077	11.336	42.755	141.073
$m_F$		1.89	3.89	14.4	62.5	185
$m_u(8,7)$	1.1955	1.9081	4.6026	18.413	67.610	186.635

One can see that the convergence of our approximations is worse than that for the polaron energy. Besides, the discrepancy grows due to the fourth power in Eq.(4.4). The upper bound works better in the strong-coupling limit and the lower bound is more suitable in the weak-coupling regime.

Again all the coefficients  $\alpha_k$ ,  $\beta_k$  in Eq. (4.4) are positive, so no poles appear at physical values of the coupling constant.

For the actual polaron we know only two terms of expansion (4.2):

$$m_1 = 1/6, \quad m_2 = 2.362763 \cdot 10^{-2}. \quad (4.5)$$

In the strong-coupling limit it is known the result by Miyake<sup>/9/</sup>:

$$M_0 = 2.27019 \cdot 10^{-2}, \quad M_1 = 0. \quad (4.6)$$

So, we can construct only  $m_u(2,1)$  and  $m_l(2,1)$  for the actual polaron:

$$m_u(2,1) = \left[ \frac{1 + 0.328164\alpha + 0.134498\alpha^2}{1 + 0.346498\alpha} \right]^4,$$

$$m_l(2,1) = \left[ \frac{1 + 5.119845 \cdot 10^{-2}\alpha + 3.699899 \cdot 10^{-3}\alpha^2}{1 + 9.531786 \cdot 10^{-3}\alpha} \right]^4. \quad (4.7)$$

The numerical results obtained with Eqs.(4.7) are collected in Table 6.

Table 6. Upper and Lower Bounds for the Effective Mass of the Actual Polaron

$\alpha$	0.5	1	3	5	7	9	11
$m_l(2,1)$	1.09	1.19	1.77	2.74	4.34	6.91	11.0
$m_u(2,1)$	1.20	1.64	7.50	28.3	82.0	195	402

The well-known trouble with the mass is that one cannot state that the variational result  $m_F$  is an upper (or lower) bound for the actual polaron mass. The results of Table 6 are the only known upper and lower bounds for the polaron mass but the gap between them is too large due to the lack of information about strong- and weak-coupling expansions.

One can hope to improve slightly the lower bound constructing Padé approximant  $m_l(3,2)$ . To do this one needs the coefficient  $m_3$  of the weak-coupling expansion (4.2). It can be obtained within the diagrammatic technique of our paper<sup>/6/</sup>, and the calculations are on march now.

To conclude, we should mention the paper by Sheng and Dow<sup>/14/</sup> devoted to Padé approximants for the polaron. In this paper the authors obtained a wrong result for the coefficient  $E_3$  in the third order of perturbation series (2.3) for the polaron energy:  $\tilde{E}_3 = -0.8765 \cdot 10^{-2}$ . This essentially exceeds our value of Eq.(3.1). The mistake is due to distinctions in diagrammatic techniques: the contribution corresponding to one of disconnected diagrams of our paper<sup>/6/</sup> is absent in their calculations. As a result, they obtained the pole in Padé approximant at  $\alpha \simeq 400$ . Besides, they considered only one of the two versions of Padé approximants.

While constructing estimates for the polaron mass they subtracted leading terms  $O(\alpha^4)$  and  $O(\alpha^2)$  of the strong-coupling expansion and used diagonal Padé approximants for the residue. Such a procedure cannot be applied to the actual polaron because one does not know coefficient  $M_2$  in Eq. (4.3). In the case of the Feynman polaron this leads to a negative mass at some values of the coupling constant  $\alpha$ . So, we consider it is more adequate to construct two-point nondiagonal Padé approximants for  $m^{1/4}$  as in our Eq.(4.4).

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#### REFERENCES

1. Gross E., Ann. Phys. 8, 78 (1959).
2. Komarov L.I., Feranchuk I.D. and Fisher S.I., J.Phys. C17, 4309 (1984); 18, 5083 (1985).
3. Devreese J.T. and Peeters F.M., phys.stat.sol. (b) 112, 219 (1982).
4. Feynman R.P., Phys.Rev. 97, 660 (1955).
5. Baker G. and Graves-Morris P., Padé Approximants. Addison-Wesley Publ. Co. (1981).

6. Smondyrev M.A., JINR preprint E17-85-222, Dubna (1985); Teor. i Mat.Fiz. 68, 29 (1986) (in Russian).
7. Larsen D., Phys.Rev. 187, 1147 (1969).
8. Seljugin O.V. and Smondyrev M.A., Comm. JINR P17-85-9, P17-85-169, Dubna (1985).
9. Miyake S., J.Phys.Soc. Jap. 38, 181 (1975); 41, 747 (1976).
10. Adamowski J., Gerlach B. and Leschke H. In: Functional Integration, Theory and Applications. Plenum Publ. Co, N.Y. (1980).
11. Leib E. and Yamazaki K., Phys.Rev. III, 728 (1958).
12. Larsen D., Phys.Rev. 172, 967 (1968).
13. Gorshkov S.N., Lakhno V.D., Rodriguez C. and Fedyanin V.K., Dokl. Akad. Nauk SSSR 278, 1343 (1984) (in Russian).
14. Sheng P. and Dow J.D., Phys.Rev. B4, 1343 (1971).

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Фазовый переход и Падде-приближение  
для полярона

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В рамках двухточечного недиагонального Падде-приближения получены нижняя и верхняя оценки на энергию и эффективную массу полярона. Обе оценки для энергии достаточно близки друг к другу, что указывает на гладкость энергии как функции константы связи. Поэтому не должно существовать фазового перехода полярона в самолокализованное состояние.

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Phase Transition and Padé Approximants  
for Polaron

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Upper and lower bounds for the polaron energy and effective mass are obtained in the framework of the two-point nondiagonal Padé method. Both Padé approximants for the polaron energy are close enough to each other indicating that the energy is a smooth function of the coupling constant. Therefore no phase transition to a self-trapped state should occur.

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

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