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ON APPLICATION OF GENERALIZED NONLINEAR MODELS IN POLARON THEORY

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The polaron theory is the simplest example of the nonrelativistic quantum field theory where the sequential research computational methods of physical parameters are developed both for the case of strong interactions of a particle and a field /1/ and for weak interactions /2/ . The best results in the framework of the intermediate coupling theory have been obtained in ref. /3/ . The solutions of the equations for the strong coupling polaron

$$\Delta_r \Psi + \phi(r)\, \Psi(r) + W\Psi(r) = 0,$$
$$\Delta_r \phi(r) + c\Psi^2(r) = 0 \qquad /1/$$

have been found numerically in ref. /4/ . The solutions /1/ correspond to a discrete set of different self-consistent states of a particle and a field, each possessing its own effective mass. The way to generalize the results was proposed in ref. /5/ for the case of arbitrary electron-phonon coupling constant. The generalized polaron model of Luttinger - Lu /6/ has been taken as a starting point in ref. /5/ . The model with the arbitrary electron-phonon coupling constant leades to the infinite system of nonlinear differential equations.

$$-\frac{1}{2\mu}\nabla^2\Psi(r) - \frac{4\pi\sqrt{2}\,a}{\mu}\Psi(r)\,(V_{10}(r) - V_{20}(r)) -$$
$$-\frac{a4\pi}{\sqrt{2\mu}}\sum_{n=1}^{\infty} u_n^*(r)(V_{1n}(r) - V_{2n}(r)) + \epsilon_0\Psi(r) = 0,$$
$$\nabla^2 V_{10}(r) + \Psi^2(r) = 0, \qquad /2/$$
$$\nabla^2 V_{20}(r) - c^2 V_{20}(r) + \Psi^2(r) = 0,$$
$$\nabla^2 V_{1n}(r) + \frac{\Psi^*(r)\, u_n(r)}{1+\Delta\epsilon_n} = 0,$$

$$\nabla^2 V_{2n}(r) - c^2(1+\Delta\epsilon_n)\, V_{2n}(r) + \frac{\Psi^*(r)\, u_n(r)}{1+\Delta\epsilon_n} = 0,$$
$$[-\frac{1}{2\mu}\nabla^2 - v(r)]\,\Psi(r) = \epsilon_0\Psi(r), \qquad /2/$$
$$[-\frac{1}{2\mu}\nabla^2 - v(r)]\,u_n(r) = \epsilon_n u_n(r),$$
$$\Delta\epsilon_n = \epsilon_0 - \epsilon_n, \quad c = \mu\sqrt{2}/\sqrt{1-\mu}, \quad \mu \in (0,1).$$

It is to be noted that the strong and weak coupling limiting cases are both correctly described by eqs. /2/.

Some results of the numerical solution of the system /2/ for "zero approximation" represented by the first three equations (see 3, 1) have been obtained in /7/ . In the framework of the simplest zero approximation the system /2/ leads to the system of nonlinear differential equations /7/ :

$$-\frac{1}{2\mu}\Delta\phi(r) - \frac{a}{\sqrt{2\mu}}\phi(r)\,(\Pi_1(r) - \Pi_2(r)) + \epsilon_0\phi(r) = 0,$$
$$\Delta\Pi_1(r) + 4\pi\phi^2(r) = 0, \qquad /3/$$
$$\Delta\Pi_2(r) - 4c^2\Pi_2(r) + 4\pi\phi^2(r) = 0.$$

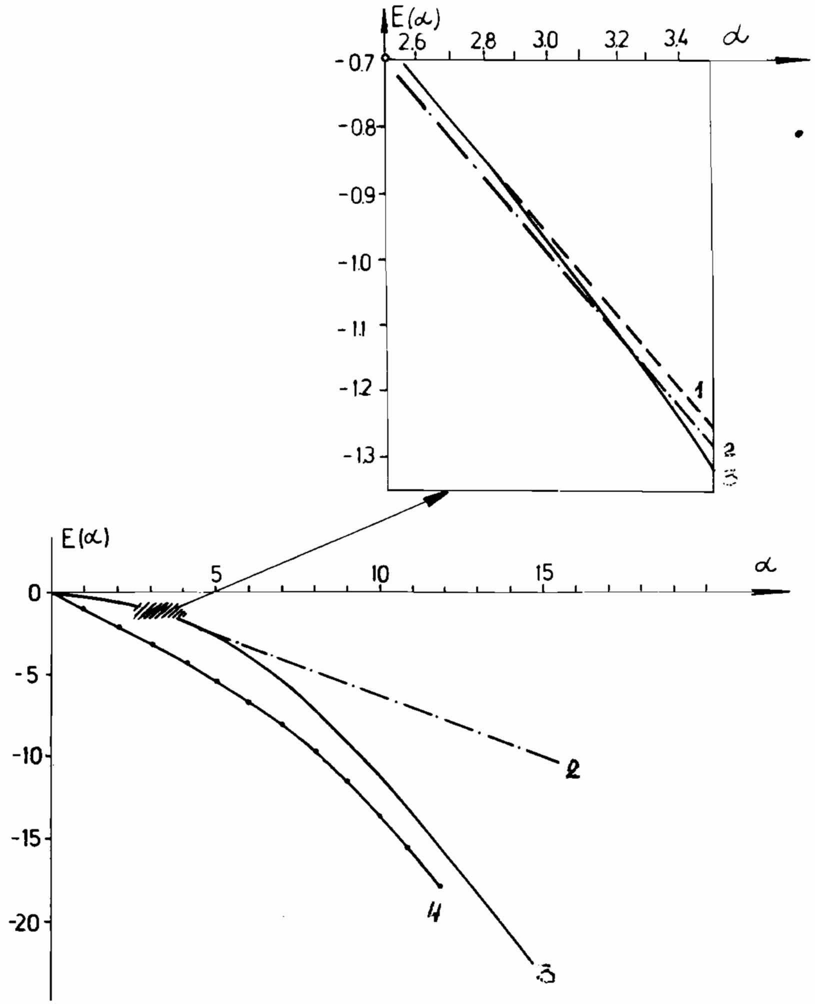
The solution of eqs. /3/ determines polaron wave function and arbitrary coupling energy; $\Pi_1(r)$, $\Pi_2(r)$ mean the polarization potentials induced by electron in polaron state, ϵ_0 is electron energy; a , a coupling constant.

The parameter $\mu \in (0,1)$ is determined by the extremum condition

$$\delta\Phi/\delta\mu = 0 \qquad /4/$$

of the corresponding variational functional. From eqs. /2/ it follows that as $\mu \to 1$ the system /2/ is transformed into the polaron equations /1/ of a strong coupling limit.

The attempt to solve the variational problem for eqs. /3/ by means of the direct Ritz method has failed (see. ref. /8/). This point was considered in detail in ref. /5/ . In particular, it was pointed out that the problem for eqs. /3/, /4/ has an exact solution when $\mu = 1$ for all the values of the



coupling constant α. The dissimilar result can be obtained only by direct solution of the problem /3/.

The detailed description of the numerical methods used for integration of the system /3/ is presented in ref. /7/ . Below we shall consider only the results obtained. In the figure the curve corresponds to the dependence $E(\alpha)$ of the polaron ground state energy obtained from the numerical solution of eqs. /3/. The line 1 goes everywhere above the line 3 that corresponds to the solution of eqs./2/ in the strong coupling limit (eq./1/ /9/)

$$E_0(\alpha) = -0.1085\alpha^2. \qquad /5/$$

Reasoning from this fact the curve 1 could not be found by the method /8/ . The curve 2 corresponds to the solution of the equation which is the first order approximation to the self-consistent equations /3/. To this end, the corresponding eigenvalue problem has been solved

$$[-\frac{1}{2\mu}\Delta + v(r)]\, u_n(r) = \epsilon_n u_n(r) ,$$

$$v(r) = -\frac{\alpha\sqrt{2}}{\mu} \int d^3r \frac{|\phi(r')|^2}{|\vec{r}-\vec{r}'|}(1 - e^{-2c|\vec{r}-\vec{r}'|}) . \qquad /6/$$

The solution was used for more accurate definition of the functional $\Phi_0 = E_0$ value. As can be seen from the figure, there exists a small region of values of α, where the results appear to be better than the strong coupling model results. Finally, the curve 4 (see the figure) represents the Feinman result /3/ that is the best one for not large α.

The results obtained show that the assumption in ref./6/ is questionable. It was stated that the zero approximation of eqs./3/ leads to the correct limiting transition $E_0 = -\alpha$ for $\alpha \to 0$. As is shown in our analysis the minimal value of the coupling constant (the figure) is $\alpha \approx 2.5$ in that case. There are no solutions for $\alpha < 2.5$ if $\mu \neq 1$.

Thus, the detailed study of the zero approximation of eqs./3/ gives higher ground-state energies than ref./9/ for all the values of α. Therefore, it is essential to proceed to more complicated self-consistent equations which follow from eqs./2/. The preliminary estimation of the first order approximation /6/ makes one to believe that at a resonable decoupling stage /2/ one can obtain differential equations describing the state at intermediate α with sufficient accuracy. Solution of the equations thus obtained yields a regular means for studying the full discrete set of solutions/4/ as $\alpha < \infty$. In particular, one hopes to understand in more detail a strong coupling polaron transition that has a complicated internal structure within this limit into structureless weak coupling polarons.

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Амирханов И.В. и др. E17-88-257
К использованию обобщенных нелинейных моделей в теории полярона

В работе обсуждаются некоторые результаты численного решения системы трех нелинейных дифференциальных уравнений в обобщенной поляронной модели Латинжера-Лу. Приведено сравнение с ранее известными данными. Полученный результат свидетельствует о необходимости перехода к более сложным самосогласованным уравнениям для более точного описания зависимости $E(\alpha)$.

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Amirchanov I.V. et al. E17-88-257
On Application of Generalized Nonlinear Models in Polaron Theory

Some results of the numerical solutions to the system of three nonlinear differential equations in the framework of the generalized Luttinger-Lu polaron model are discussed. The comparison with the known data is presented. For the more accurate description of the $E(\alpha)$ dependence a processing to the more complicated self-consistent equations should be done.

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

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