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MULTIDIMENSIONAL POLARON WITHIN THE GENERALIZED GAUSSIAN REPRESENTATION

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A path-integral approach called the *Generalized Gaussian Representation* is systematically applied to the polaron problem in arbitrary spatial dimensions ($d \geq 1$). This method represents a generalized Gaussian approximation, whose leading order represents the best variational estimation over Gaussian fluctuations. Main quasi-particle characteristics of the Fröhlich and Dirac polaron, namely, the ground-state energy and the effective mass are derived within and beyond the generalized Gaussian approximation. Explicit analytical results are obtained in the weak- and strong-coupling limit.

Метод обобщенного гауссовского представления для интегралов по траекториям систематично применен к проблеме полярона в пространстве произвольной размерности. Подход является, по сути, обобщенным гауссовским представлением, ведущее приближение которого воспроизводит лучшую вариационную оценку для гауссовских флуктуаций в системе. Основные квазичастичные характеристики поляронов Фрелиха и Дирака, такие как энергия основного состояния и эффективная масса, получены в рамках и вне пределов обобщенного гауссовского приближения. Явные аналитические результаты получены в пределах слабой и сильной связи.

1. INTRODUCTION

The polaron concept introduced by Landau [1] describes a nonrelativistic conduction electron placed in an ionic crystal. The Coulomb field of the electron causes distortion of the surrounding ions which reacts back on the electron, changing its energy and mass. A slowly moving electron followed by accompanying perturbation of the lattice forms a quasi-particle which is called a *polaron*.

The polaron problem in condensed-matter physics has been attracting much attention over the last decades, including the general field-theoretic formulation as well as particular experiment on cyclotron-resonances and transport properties [2, 3]. As a simplified model of a particle interacting with surrounding medium the polaron can serve as a testing ground of various nonperturbative methods developed for systems where conventional perturbative approaches do not work.

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The physical properties of the polaron are different from those of the band electron and depend on the electron-lattice interaction strength α. Quantities of interest are the ground-state energy $E(\alpha)$, the effective mass $m^*(\alpha)$ and some other quasi-particle characteristics of the polaron such as the effective radius, average phonon number, the mobility, the impedance, etc. Further developments of the standard polaron concept spread into a large area considering the effect of the external fields, the piezo-, acoustic-, bound-, small- and spin-polaron, bipolarons and polaronic excitons, etc. Experimentally, the polaron effects have been observed in various physical systems [4, 5].

A great number of studies has been devoted to the ground-state energy (GSE) and the effective mass (EM) of the polaron. The problem of deriving the GSE and the EM simultaneously by one method is of considerable significance because one can suppose that in comparing two approximate methods the one giving the better $E(\alpha)$ will likely give the better $m^*(\alpha)$ that can be measured directly [6]. Second, experiments on the ionization energy of bound polarons [7] require accurate estimation of the free-polaron GSE.

Different approaches and methods have been developed to investigate the polaron in the weak [8], intermediate [9] and strong coupling regime [10].

Typically, exact results are available only in the limiting cases of weak coupling ($\alpha \to 0$) and strong coupling ($\alpha \to \infty$). While the weak-coupling results may be obtained by conventional perturbation expansions, rigorous proofs of the strong-coupling behaviour require more advanced techniques [11, 12], reflecting the qualitative difference between the polaron states in the two limits.

The first studies on the polaron self-energy and effective mass were performed in three dimensions within a «Produkt-Ansatz» [10]. In fact Pekar's method corresponds to the adiabatic *strong-coupling* regime of the polaron theory. In the pioneer works [13, 14], a canonical-transformation method was applied to this problem.

A systematic field-theoretic formulation of the polaron theory suitable for the *weak-coupling* was proposed by Fröhlich [8] to describe the interaction between the band electron (or hole) and phonons, quanta associated with the long-wave optical branch of lattice vibrations. In his original paper, Fröhlich obtained the first weak-coupling perturbation results for the GSE and EM. A method based on two successive canonical transformations by introducing the polaron total momentum and a set of adjustable functions opens a variational weak-coupling approach to the polaron problem [9].

The first attempt to built the *all-coupling* polaron theory, valid for arbitrary values of coupling, was made by Feynman [2] within the path integral (PI) formalism. The Feynman approach for the polaron has an advantage because the phonon coordinates are adequately eliminated and as a consequence, the polaron problem is reduced to an effective one-particle problem with a retarded interaction. Thus, the solution of the polaron problem amounts to the technical mathematical problem how to calculate the non-Gaussian PI. As far as the PI formalism allows to build a class of exactly solvable models corresponding to quadratic functionals, one can use these functionals as bases for variational estimations of the polaron problem. As a result, Feynman's PI approach gives a good upper bound to the GSE in the whole range of the coupling constant. Later Feynman's variational approach was generalized to two [15], more than two [16, 17], and even to a continuum of such oscillators [18, 19] within the variational ansatz.

The question arises, can the Feynman's variational estimations of the polaron PI be improved by a more general approach? Although there exists small hope to calculate this PI exactly, we can realize the following programme. The idea is to get the representation

$$\mathrm{e}^{-F} = \int \frac{\delta r}{\sqrt{\det D_0}} \mathrm{e}^{-\frac{1}{2}(rD_0^{-1}r)+W[r]} = \mathrm{e}^{-F_0} \int \frac{\delta \rho}{\sqrt{\det D}} \mathrm{e}^{-\frac{1}{2}(\rho D^{-1}\rho)+W_1[\rho]}$$

by some transformations of the functional variables $r \to \rho$ in order to rewrite the initial integral on the left side in the form on the right side, where the zeroth approximation F_0 is the best variational Gaussian estimation of the initial integral. Calculations of the perturbation corrections over W_1 give subsequent contributions to the zeroth approximation

$$F = F_0 + F_1 + F_2 + \dots .$$

The method which realizes this programme was called the *Gaussian Equivalent Representation* (GER) and was formulated in [20, 21]. It is based on the observation that the normal-ordering quantum field technique means in reality the main contributions to functional integrals (the so-called tadpole diagrams) to be taken into account. In other words, our approach gives prescription how to find the most optimal Gaussian functional measure for the polaron path-integral. Within this approach the Gaussian leading term takes care of all Gaussian fluctuations around the ground state and remaining higher orders for non-Gaussian contributions can be calculated systematically. Our approach does not require the smallness of the coupling constant. This method is applicable to a huge number of physical problems which admit a path-integral formulation of the problem and where a ground-state exists. Some details can be found also in [22, 23].

In the present paper we purpose to give a systematic description of the *Gaussian Equivalent Representation*, suitable to derive accurately the polaron properties for whole range of coupling in different spatial dimensions. We concern neither the bound polaron, the bi-polaron nor other polaron excitations. Originally, the term polaron is only referred to the electron in an interaction with longitudinal-optical modes of lattice vibrations. In this paper, we do not concern ourselves with the acoustic modes in a piezo-electric crystal. A series of reviews devoted to these and other related themes can be found, in particular, in [24–29].

The paper is organized as follows. In Sections 2 and 3, we extend the conventional Fröhlich polaron model into $d \geq 1$ dimensions within the path integral approach. A short review of some known variational and nonvariational perturbation methods is given in Section 4. The polaron main quasi-particle properties, namely, its ground-state energy and effective mass are considered in Section 5. Hereby, we give an extended set of definitions of the polaron effective mass and compare them. The basic idea and short description of the GGR method as well as its particular application to the d-dimensional polaron are described in Section 6. Section 7 is devoted to the generalized Gaussian approximation of the d-dimensional polaron GSE and EM in the entire range of the coupling constant. The necessary non-Gaussian corrections to the GGR results are discussed in Section 8. Here, we restrict ourselves to evaluating the next-to-leading non-Gaussian corrections and find them to be rather small. Exact analytical (for the weak- and strong-coupling regimes) and some numerical results obtained in the intermediate-coupling range are represented in Section 9.

2. FRÖHLICH–FEYNMAN POLARON

The Fröhlich theory [8] of the polaron serves as an idealized construction modeling the real electron behaviour in ionic and polar crystals. Admitting several simplifying assumptions, the model Hamiltonian (three-dimensional) reads as follows [8]:

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(A_{\mathbf{k}} a_{\mathbf{k}} \mathrm{e}^{\imath \mathbf{k}\mathbf{r}} + A^{*}_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} \mathrm{e}^{-\imath \mathbf{k}\mathbf{r}} \right), \tag{1}$$

where $\mathbf{p}$, $\mathbf{r}$, and m denote the momentum, position operator and the bare mass of the electron; $a_{\mathbf{k}}$ and $a^{\dagger}_{\mathbf{k}}$ are the phonon annihilation and creation operators, whereas $\mathbf{k}$ and $\omega_{\mathbf{k}}$ are the wave vector and the frequency at which the phonons couple to the electron. For the longitudinal-optical branch of the lattice vibrations (optical polaron), $\omega_{\mathbf{k}} = \omega$ does not depend on $\mathbf{k}$. Here and in the following we set units such that $m = \omega = 1$. The electron-phonon coupling for $d = 3$ is given by

$$A_{\mathbf{k}} = -i 2^{3/4} \sqrt{\frac{\alpha\pi}{\Omega}} \frac{1}{|\mathbf{k}|}, \tag{2}$$

where Ω is the quantization volume and α is the Fröhlich dimensionless constant.

As is known, the exact solution to (1) has not been obtained yet. The Fröhlich Hamiltonian is self-adjoint and half-bounded from below [30]. Besides, $\mathcal{H}$ is invariant with respect to the Abelian group of translation: $a_{\mathbf{k}} \to a_{\mathbf{k}} \exp(-i\mathbf{a}\mathbf{k})$

and $\mathbf{r} \to \mathbf{r} + \mathbf{a}$. The total momentum

$$\mathbf{P} = \mathbf{p} + \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \tag{3}$$

commutes to the Hamiltonian $[\mathcal{H}, \mathbf{P}] = 0$ which results in the strict translational symmetry of the system, so that the momentum $\mathbf{P}$ is the good quantum number.

The conservation of the total momentum allows one to use a canonical transformation

$$\mathcal{U} = \exp\left\{ -i\mathbf{r} \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \right\}$$

and to go to the following representation of the Hamiltonian

$$\begin{aligned} \mathcal{H} \to \mathcal{U}\mathcal{H}\mathcal{U}^{\dagger} \quad &= \quad \mathcal{H}(\mathbf{P}) = \frac{1}{2m} \left(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \right)^2 + \\ &+ \quad \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + g \sum_{\mathbf{k}} \left(A_{\mathbf{k}} a_{\mathbf{k}} + A_{\mathbf{k}}^{*} a_{\mathbf{k}}^{\dagger} \right), \end{aligned} \tag{4}$$

where $\mathbf{P}$ is a c-number.

Due to the linear electron-phonon coupling in (1) the phonon variables can be analytically eliminated explicitly by either solving the operator equations of motion or by integrating out within a path-integral approach. The polaron problem can be re-formulated within different path-integral techniques [31, 32]. Among these methods Feynman's PI approach [2] stands out due to the elegance and all-coupling nature, within it one obtains a one-particle model.

The density matrix looks like

$$\rho_{\beta}(\mathbf{r}_1, \mathbf{r}_2) = \left\langle 0 \left| \mathrm{e}^{-\beta\mathcal{H}} \delta(\mathbf{r}_1 - \mathbf{r}_2) \right| 0 \right\rangle = N \int\limits_{\mathbf{r}(0)=\mathbf{r}_2}^{\mathbf{r}(\beta)=\mathbf{r}_1} \delta\mathbf{r}\, \mathrm{e}^{-S[\mathbf{r}]}, \tag{5}$$

where the normalization constant N provides with the normalization for $\alpha = 0$

$$\rho_{\beta}(\mathbf{r}_1, \mathbf{r}_2)\big|_{\alpha=0} = \exp\left\{ -\beta \frac{m}{2} \left(\frac{\mathbf{r}_1 - \mathbf{r}_2}{\beta} \right)^2 \right\}. \tag{6}$$

The effective action is introduced as follows

$$S[\mathbf{r}] \quad = \quad S_0[\mathbf{r}] + S_{\mathrm{int}}[\mathbf{r}],$$

where

$$S_0[\mathbf{r}] = \frac{m}{2}\int\limits_0^\beta dt\, \dot{\mathbf{r}}^2(t) = \frac{m}{2}\iint\limits_0^\beta dtds\, \big(\mathbf{r}(t)\, \mathbf{D}_0^{-1}(t,s)\, \mathbf{r}(s)\big) = \frac{m}{2}(\mathbf{r}\, \mathbf{D}_0^{-1}\, \mathbf{r}), \quad (7)$$

$$(\mathbf{D}_0^{-1}(t,s))_{ij} = \delta_{ij} D_0^{-1}(t,s), \qquad D_0^{-1}(t,s) = -\frac{d^2}{dt^2}\,\delta(t-s).$$

The Green function satisfying the equation

$$\left(D_0^{-1}\, D_0\right)(t,s) = \int\limits_0^\beta du\, D_0^{-1}(t,u)\, D_0(u,s) = \delta(t-s)$$

and obeying the zero boundary condition reads

$$\begin{aligned} &D_0(t,s) = -\frac{1}{2}|t-s| + \frac{1}{2}(t+s) - \frac{ts}{\beta}, \\ &(\mathbf{D}_0(t,s))_{ij} = \delta_{ij}\, D_0(t,s)\,. \end{aligned} \quad (8)$$

The interaction functional looks like

$$S_{\rm int}[\mathbf{r}] = -\frac{\alpha}{\sqrt{8}}\iint\limits_0^\beta dtds\, \frac{\mathrm{e}^{-|t-s|}}{|\mathbf{r}(t)-\mathbf{r}(s)|}\,. \quad (9)$$

The partition function reads

$$\begin{aligned} Z_\beta(\alpha) &= \mathrm{e}^{-\beta E(\alpha)} = \int d\mathbf{r}\ \rho_\beta(\mathbf{r},\mathbf{r}) = N \int\limits_{\mathbf{r}(0)=\mathbf{0}}^{\mathbf{r}(\beta)=\mathbf{0}} \delta\mathbf{r}\, \mathrm{e}^{-S[\mathbf{r}]} = \quad (10) \\ &= \int d\sigma_0[\mathbf{r}]\ \mathrm{e}^{-S_{\rm int}[\mathbf{r}]}, \qquad d\sigma_0[\mathbf{r}] = \sqrt{\det \mathbf{D}_0^{-1}}\ \delta\mathbf{r}\ \mathrm{e}^{-S_0[\mathbf{r}]}. \end{aligned}$$

where $E(\alpha)$ is the ground-state energy.

The functional integral in (10) will be the basic object of our investigation.

The advantage of the PI formulation is obvious: the original many-body problem has been transformed into an effective one-particle model, just with the electron coordinate $\mathbf{r}(t)$. On the other hand, effective action $S_{\rm int}[\mathbf{r}]$ is nonlocal and has either Coulombic (for $d \geq 2$) or δ-function (for $d = 1$) singularity. This — up to now — has prevented any further exact analytic treatment except in the limits $\alpha \to 0$ and $\alpha \to \infty$. For arbitrary couplings, an approximation method should be applied.

3. POLARON IN d DIMENSIONS

The study of the polaron properties in reduced dimensionality ($d < 3$) is currently attracting much attention. Traditionally, the polaron problem has been investigated in three dimensions. In recent years, however, polaron effects have been observed in low-dimensional systems [33]. The growing interest in low-dimensional polarons can be attributed to several factors. In particular, advanced semiconductor technology [34–37] makes it possible to confine electrons in quasi-low-dimensional structures. Another reason is due to inevitable theoretical enhancement of the conventional ($d = 3$) polaron model in lowering the spatial dimensions [31], [38–41]. Certain physical problems have been mapped into a two-dimensional ($d = 2$) polaron theory [42–44], and the possibility that an electron may be trapped on the surface of a dielectric material has attracted much interest [45]. The properties of the polaron confined to one dimension ($d = 1$) have attracted considerable attention [38, 41, 46, 47].

Considering a polaron confined in any dimensions different from three ($d \neq 3$), we assume that the electron-phonon interaction keeps its «standard» Coulomb-like ($1/|\mathbf{r}|$) behaviour [39]. Note, for $d = 1$ the Dirac «delta»-function is commonly implied rather than the nonintegrable $1/r$ form [38]. In other words, we assume that for arbitrary dimension the polaron interaction functional looks like

$$U(\mathbf{r}) = \frac{1}{\Omega}\sum_{\mathbf{k}} \widetilde{U}(\mathbf{k})\,\mathrm{e}^{i\mathbf{k}\mathbf{r}} = \begin{cases} 2\,\delta(r)\,, & d = 1\,, \\ |\mathbf{r}|^{-1}\,, & d \geq 2\,, \end{cases} \qquad \frac{\alpha}{\Omega}\,\widetilde{U}(\mathbf{k}) = \sqrt{2}\,|A_{\mathbf{k}}|^2\,. \quad (11)$$

The numerical prefactor 2 for δ function is chosen to fit the conventional weak-coupling limit $E(\alpha) = -\alpha + O(\alpha^2)$ for $d = 1$.

Assumption (11) leads to certain k-dependence of the *generalized multidimensional* coupling $A_{\mathbf{k}}$. Going to the continuous limit as $\Omega \to \infty$

$$\frac{1}{\Omega}\sum_{\mathbf{k}} \mapsto \int \frac{d\mathbf{k}}{(2\pi)^d}$$

we redefine the electron-phonon coupling factor in arbitrary dimensions ($d \geq 1$) as follows:

$$|A_{\mathbf{k}}|^2 = \frac{\alpha}{\sqrt{2}\,\Omega}\,\widetilde{U}(\mathbf{k}) = \frac{\alpha}{\sqrt{2}\,\Omega}\int d\mathbf{r}\,\mathrm{e}^{-i\mathbf{k}\mathbf{r}}\,U(\mathbf{r}) = \frac{\alpha(2\pi)^d B_d}{\sqrt{2}\,\Omega\,|\mathbf{k}|^{d-1}}\,. \qquad (12)$$

In particular,

$$B_d = \begin{cases} \pi^{-1}\,, & d = 1\,, \\ (2\pi)^{-1}\,, & d = 2\,, \\ (2\pi^2)^{-1}\,, & d = 3\,. \end{cases}$$

We see that the conventional value (2) for $d = 3$ can be reproduced from (12).

Accordingly, we redefine the interaction functional of the multidimensional polaron as follows:

$$S_{\rm int}[\mathbf{r}] = -\frac{\alpha}{\sqrt{8}} \iint\limits_0^\beta dt\, ds\; \mathrm{e}^{-|t-s|}\; U(\mathbf{r}(t) - \mathbf{r}(s)) = -\int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{k}\mathbf{R}(\mathbf{t},\mathbf{s})}\,, \quad (13)$$

where

$$d\Omega_{ts\mathbf{k}} = \frac{\alpha B_d}{\sqrt{8}}\, \mathrm{e}^{-|t-s|}\, dt\, ds\, \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}}\,, \qquad \mathbf{R}(t,s) = \mathbf{r}(t) - \mathbf{r}(s)\,.$$

4. SHORT REVIEW OF METHODS

Owing to its important practical and theoretical implications, a great number of investigations utilizing various methods have been devoted to the Fröhlich polaron. Below, we shortly survey a few original techniques.

Operator methods

• Fröhlich [8] has shown that the first studies on the polaron [1, 10] had been, in fact, devoted to the strong-coupling regime. The main idea of the Pekar «Produkt-Ansatz» is that the electron excitations are governed by a potential adopted to the ground state. The Landau-Pekar theory leads to quantum states localized around fixed space points which can be chosen arbitrary. According to this approach, the polaron wave function $|\Psi\rangle$ is written as a direct product of the electron $|\psi\rangle$ and field $|\varphi\rangle$ wave functions. Hereby, $|\varphi\rangle$ parametrically depends on $|\psi\rangle$. Further development of this method can be found, in particular, in [13, 14]. The most rigorous results for the strong-coupling limits of the GSE and EM have been reported in [11, 12, 48]. Following this Ansatz, the GSE can be found (for $d \geq 2$) by performing the following variational task:

$$-\lim_{\alpha\to\infty} E(\alpha)/\alpha^2 = \min_{\psi} \left\{ -\int d\mathbf{x} (\nabla\psi(\mathbf{x}))^2 + \iint d\mathbf{x} d\mathbf{y}\, \frac{\psi^2(\mathbf{x})\, \psi^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} \right\}$$

with respect to the trial function $\psi(\mathbf{x})$ obeying the normalization $\int d\mathbf{x}\, |\psi(\mathbf{x})|^2 = 1$.

Giving the exact GSE for the polaron, this method allows one to test other «all-coupling» methods in the limit $\alpha \to \infty$. However, the «Produkt-Ansatz» fails in describing actual polar crystals with $\alpha \propto 1$.

• Besides the conventional weak-coupling perturbation expansion in a series of α, the polaron model admits one to use also an alternate strong-coupling expansion in inverse powers of α. This unique property of the polaron model was utilized to obtain asymptotic behaviours of the polaron GSE. A systematic perturbation theory in powers of α^{-1} gives an adiabatic result in the lowest order (which is proportional to α^2) and a correction (proportional to α) which is the perturbation-theory result [49]. However, the accuracy of this method is not sufficient in comparison with the complexity of the technique.

• A weak-coupling method was proposed in [50] taking into account a few phonon correction to the Davydov phonon coherent state. Within this approach the Lee–Low–Pines canonical transformation [9] is applied to the polaron Hamiltonian. Then, a coherent-state wave function is constructed to satisfy the Schrödinger equation. Gradually improving the trial wave function to diagonalize the Hamiltonian and involving more and more phonon degrees, one obtains an iterative procedure to calculate the GSE and EM of the optical polaron. It results in smooth data for the GSE of the one-dimensional polaron for $\alpha < 2.5$. However, the complexity of the iteration scheme increases rapidly and in fact only a two- and three-phonon correlation is utilized in [38]. The obtained result is neither an upper nor a lower bound to the energy. Besides, this method belongs to the class of weak-coupling approaches and, therefore, the valid range of this technique is very restricted. Higher phonon numbers are required to extend this restricted region of α. By increasing (even theoretically) the number of involved phonons one obtains only a polynomial in powers of α. This will contradict the correct strong-coupling behaviour with expansion in powers of $1/\alpha^2$ instead of $1/\alpha$ [49].

Path-integral methods

Up to now all known analytic investigations of a two-time action (9) describing the retarded, or nonlocal Coulomb interaction are reduced to the problem how to estimate PIs like (10) by using a Gaussian-type measure. The first attempt was done in [51]. Since many approximation methods have been developed to combine the solvability of the Gaussian approach with the simplicity of the variational principle, especially to estimate the polaron ground-state characteristics. All variational approaches are based on the well-known Jensen (or, Bogoliubov) inequalities

$$\begin{aligned} e^{-F} &= N\int \delta\mathbf{r}\, e^{-S_0[\mathbf{r}]-S_{\text{int}}[\mathbf{r}]} = N\int \delta\mathbf{r}\, e^{-S_0[\mathbf{r}]-S_\mu[\mathbf{r}]+S_\mu[\mathbf{r}]-S_{\text{int}}[\mathbf{r}]} \geqslant \\ &\geqslant \exp\left\{-F_\mu + \langle S_\mu - S_{\text{int}}\rangle_\mu\right\}, \\ e^{-F_\mu} &= N\int \delta\mathbf{r}\, e^{-S_0[\mathbf{r}]-S_\mu[\mathbf{r}]}, \qquad \langle(*)\rangle_\mu = e^{F_\mu}\int \delta\mathbf{r}\,(*)e^{-S_\mu[\mathbf{r}]}, \\ F &\leqslant F_0 = \min_\mu \left[F_\mu - \langle S_\mu - S_{\text{int}}\rangle_\mu\right]. \end{aligned}$$

Here $S[\mathbf{r}]$ is a quadratic over r functional depending on a set of variational parameters μ. The choice of $S_\mu[\mathbf{r}]$ defines different variational approaches.

Now we give a short survey of a few known approaches. Note, however, that this short list does not at all cover the whole area of enormous ideas, methods and techniques developed and utilized to the polaron problem.

• The simplest variational Ansatz is to choose a one-parameter (say, μ) quadratic trial action instead of the exact one

$$S_{\rm osc}[\mathbf{r}] = S_0[\mathbf{r}] - \frac{\mu^2}{2}\int\limits_0^\beta dt\,\mathbf{r}^2(t) = \frac{1}{2}\int\limits_0^\beta dt[m\dot{\mathbf{r}}^2(t) - \mu^2\mathbf{r}^2(t)]\,.$$

This simplest version of Gaussian PI is, of course, explicitly solvable and by optimizing the obtained self-energy with respect to μ, one obtains the simplest variational approximations to the GSE (see, e.g., [19] for $d = 3$). The «simple oscillator» approach results in a discontinuous function for the self-energy that may mislead to the wrong prediction of the nature of the polaron ground state. Besides, by construction it serves as a weak-coupling approach and, therefore, it does not fit the correct strong-coupling behaviours for the GSE and EM.

• Among the approximations which are believed to describe the polaron characteristics reasonably well for all values of α, Feynman's celebrated variational method [2] stands out in that it smoothly interpolates between the weak- and the strong-coupling regime. This technique uses a two-parameter trial action and can be considered as a natural successor of the simple oscillator model. It uses the Jensen–Peierls inequality and is based on an exactly solvable quadratic action

$$S_{\rm Feyn}[\mathbf{r}] = S_0[\mathbf{r}] - \frac{C}{2}\iint\limits_0^\beta dtds\,{\rm e}^{-w\,|t-s|}\,(\mathbf{r}(t) - \mathbf{r}(s))^2\,.$$

It represents a retarded oscillator-potential model and the corresponding free energy results in a continuous upper bound to the GSE valid throughout the whole range of α.

To define the polaron EM, Feynman has introduced an imaginary-time «velocity» and replaced the polaron action with the following trial action [2]

$$S_F[\mathbf{r},\mathbf{v}] = S_0[\mathbf{r}] - \frac{C}{2}\iint\limits_0^\beta dtds\,{\rm e}^{-w\,|t-s|}\,|\mathbf{r}(t) - \mathbf{r}(s) - i\mathbf{v}\,(t-s)|^2.$$

Due to the quadratic nature of $S_F[\mathbf{r},\mathbf{v}]$, the partition function at zero temperature

$${\rm e}^{-\beta E_F(\alpha,\mathbf{v})} \propto \lim_{\beta\to\infty}\int\delta\mathbf{r}\,{\rm e}^{-S_F[\mathbf{r},\mathbf{v}]}$$

has been evaluated explicitly. A variational optimization over $E_F(\alpha,\mathbf{0})$ may define the parameters C, w. Then, by using the expansion $E_F(\alpha,\mathbf{v}) = E_F(\alpha)+$

$+\frac{1}{2}m_F^*\mathbf{v}^2 + O(\mathbf{v}^4)$ Feynman has found an approximation m_F^* to the polaron EM. In the limiting cases of $\alpha \to 0$ and $\alpha \to \infty$, the Feynman mass differs slightly from the known exact value of the EM and, for general α it gives a reasonable approximation. However, the Feynman definition of the EM is not well established. First, a reasonable set of parameters C, w optimized for the GSE may not necessarily be good for the EM. Second, Feynman's trial action does not reflect the preservation law of the total momentum $\mathbf{P}$, when the potential well seizing the particle moves. Therefore, a functional variational method modifying the Feynman approach to the case of preserving $\mathbf{P} \neq 0$ was suggested in [52]. Here, a polaron path integral in respect to the fluctuation $\mathbf{r}'(t) = \mathbf{r}(t) - i\mathbf{P}t/M$ is considered, where $i\mathbf{P}/M$ is average transportational velocity of the system. The parameter M is defined from the constrained minimum of the excited energy for fixed $\mathbf{P}$. The final result of [52] was in full agreement with corresponding Feynman estimate.

In contrast with the simplest oscillator model, the Feynman approach results in the correct behaviour of the GSE even for the strong-coupling regime, deviating from the exact value within a few per cent. Nevertheless, it remains a variational model adapted to optimize the GSE and, therefore, a more strict technique should be developed especially to define and estimate the EM.

A scaling relation connecting the Feynman estimates performed in different numbers of spatial dimension has been reported in [53, 54].

• A straightforward extension of the Feynman method for the polaron problem has been developed particularly by increasing the number of oscillators in describing the trial action as follows:

$$S_N[\mathbf{r}] = S_0[\mathbf{r}] - \sum_{n=1}^{N} \frac{C_n}{2} \iint_0^\beta dtds\, \mathrm{e}^{-\omega_n |t-s|} \left(\mathbf{r}(t) - \mathbf{r}(s)\right)^2 .$$

The estimation has been performed with $N = 2$ and $N = 3$ in [15] and [16], respectively. Later, a sum of up to 32 nonlocal oscillators has been considered and a particular estimation has been obtained for $N = 8$ [17].

• An essential generalization of the Feynman method has been proposed in [19] and [18] independently. Within this approach the polaron approximate action is given by [19]

$$S_{\mathrm{AGLS}}[\mathbf{r}] = S_0[\mathbf{r}] - \lambda \iint_0^\beta dtds\, f(t-s) \left(\mathbf{r}(t) - \mathbf{r}(s)\right)^2 \qquad (14)$$

with an isotropic trial function $f(t-s) \geq 0$. In fact, this general two-time isotropic action essentially extends the Feynman choice and corresponds to the limiting case $N \to \infty$ for the multioscillator model. The AGL–Saitoh method gives the best upper bound to the GSE for $d = 3$. Note the specific factorization of time-damping in (14).

• An original path-integral approximation scheme to the Pekar–Fröhlich polaron problem in multidimensions has been developed in [55] by using an expansion in the inverse powers of spatial dimension number d. The first step of this model is to redefine the electron-phonon coupling constant as $\alpha_d = \alpha\sqrt{8}\, d^{3/2}$ which allows one to expand the polaron GSE and EM as follows:

$$E(\alpha) = dE_0(\alpha) + E_1(\alpha) + O(1/d)\,, \qquad m^*(\alpha) = dm_0^*(\alpha) + m_1^*(\alpha) + O(1/d)\,.$$

The next key point in [55] is the stationary point calculations for $d \to \infty$. The stationary point requirement leads to the master equations that coincide with the results of the AGL–Saitoh method. The numerical results obtained for the leading terms are very close to the data due to the AGL–Saitoh method, but next corrections are distinct that stresses the different origin of the original ideas. It has been shown that the AGL–Saitoh variational method becomes asymptotically exact in the limit of $d \to \infty$. The specific factorization of the leading term resulted in a scaling relation connecting $E(\alpha)$ (and $m^*(\alpha)$) calculated in different numbers d.

5. POLARON QUASI-PARTICLE CHARACTERISTICS

The main quasi-particle characteristics of the polaron are the GSE and EM. To evaluate correctly these quantities one should first give the proper definition and then to choose an appropriate method of estimation. Hereby, the definition should not depend on an estimation method. From this point of view, some of earlier investigations devoted to the problem (see, e.g., [2, 18]) are method-dependent, i.e., they lack the clear differentiation between the proper definition and the estimation method.

Our aim is to define the ground state energy $E(\alpha)$ and the effective mass $m^*(\alpha)$ of the d-dimensional polaron self-consistently in terms of the following functional integral

$$Z_\beta(\alpha, \mathbf{u}^2) = \mathrm{e}^{-\beta\Phi(\alpha,\mathbf{u}^2)} = N \int\limits_{\mathbf{r}(0)=\mathbf{0}}^{\mathbf{r}(\beta)=\mathbf{0}} \delta\mathbf{r}\, \exp\left\{ -\frac{m}{2} \int\limits_0^\beta dt\, \dot{\mathbf{r}}^2(t) - S_{\rm int}[\mathbf{r}+\mathbf{u}] \right\} =$$

$$= \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}+\mathbf{u}]}, \tag{15}$$

where $S_{\rm int}[\mathbf{r}]$ is given in (13) and $\mathbf{u}(t) = \mathbf{u}\, t$.

Within the path-integral formalism the definition of the GSE is well established and unique — it is the zero temperature limit of free energy of the polaron system.

$$E(\alpha) = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln Z_\beta(\alpha, 0) = \Phi(\alpha, 0) = \Phi(\alpha).$$

However, there exist several ways to determine the EM by using different physical principles. Some of them are self-consistent, i.e., they involve only polaron internal dynamic variables, while others are based on the response of the polaron system to an external source like electric and magnetic field, etc. In particular, the *total momentum*- [52], *Feynman-type*- [2], or *small momentum*- [56, 57] masses are self-consistent, while the *inertial*- [18], *magnetic*- [58, 59], or *string*- [60] ones belong to the second group. Below we consider some examples of these definitions of the EM and find out how they are related to each other and to our scheme. Then, we define the GSE and EM by using expansion of the real part of the self-energy with respect to small momentum.

In any case we need to calculate the quantity

$$\Phi_\xi(\alpha) = \frac{d}{d\xi}\Phi(\alpha, \xi)\bigg|_{\xi=0}, \qquad \xi = \mathbf{u}^2\,. \tag{16}$$

To evaluate (16), it is convenient to extract the explicit dependence in (15) for infinitesimal $\mathbf{u}^2$. For this purpose, we expand functional W over small $\mathbf{u}$ as follows:

$$-S_{\rm int}[\mathbf{r}+\mathbf{u}] = \int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{k}\mathbf{R}(t,s)+i\mathbf{k}\mathbf{u}(t-s)} =$$

$$= \int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{k}\mathbf{R}(t,s)} \left\{1 + i\mathbf{k}\mathbf{u}(t-s) - \frac{1}{2}(\mathbf{k}\mathbf{u})^2\,(t-s)^2 \,+\, O(|\mathbf{u}|^3)\right\}$$

$$= -S_{\rm int}[\mathbf{r}] + iu_i W_i^{(1)}[\mathbf{r}] - \frac{1}{2}u_i u_j W_{ij}^{(2)}[\mathbf{r}] + O(|\mathbf{u}|^3),$$

where

$$\begin{aligned} W_i^{(1)}[\mathbf{r}] &= \int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{k}\mathbf{R}(t,s)}\; k_i(t-s), \\ W_{ij}^{(2)}[\mathbf{r}] &= \int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{k}\mathbf{R}(t,s)}\; k_i\, k_j\, (t-s)^2. \end{aligned} \tag{17}$$

Then,

$$\begin{aligned} Z_\beta(\alpha,\mathbf{u}^2) &= \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}]} \, \Big\{ 1 + iu_i W_i^{(1)}[\mathbf{r}] - \\ &- \frac{1}{2} u_i u_j \left(W_i^{(1)}[\mathbf{r}]\, W_j^{(1)}[\mathbf{r}] + W_{ij}^{(2)}[\mathbf{r}] \right) + O(|\mathbf{u}|^4) \Big\} = \\ &= Z_\beta(\alpha)\ \exp\left\{ -\mathbf{u}^2 \frac{Y_\beta(\alpha)}{Z_\beta(\alpha)} + O(\mathbf{u}^4) \right\}, \qquad (18) \\ Y_\beta(\alpha) &= \frac{1}{2d} \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}]} \, \left(W_j^{(1)}[\mathbf{r}]\, W_j^{(1)}[\mathbf{r}] + W_{jj}^{(2)}[\mathbf{r}] \right), \end{aligned}$$

where $Z_\beta(\alpha) = Z_\beta(\alpha, 0)$.

Finally, we have

$$\Phi_\xi(\alpha) = \lim_{\beta\to\infty} \frac{Y_\beta(\alpha)}{Z_\beta(\alpha)}\,.$$

5.1. The Effective Mass and Momentum. The most direct definition of the EM is the following. As was mentioned above, the total momentum $\mathbf{P}$ (3) of the *electron + phonon* system commutes with the total Hamiltonian $\mathcal{H}$, therefore, it is conserved and we can calculate the GSE for given $\mathbf{P}$. The energy spectrum is continuous and for infinitesimal $\mathbf{P}$ the following expansion takes place:

$$\left\langle 0 \left| \mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})} \right| 0 \right\rangle = \mathrm{e}^{-\beta E(\alpha,\mathbf{P})} = \exp\left\{ -\beta \left[E(\alpha) + \frac{\mathbf{P}^2}{2m^*(\alpha)} + O(\mathbf{P}^4) \right] \right\}, \quad (19)$$

where $E(\alpha) = E(\alpha, \mathbf{0})$ is the ground-state energy and $m^*(\alpha)$ can be considered as the effective mass of the polaron (see, for example, [52]). The next point is to express $E(\alpha)$ and $m^*(\alpha)$ in terms of the function $\Phi(\alpha, \xi)$ (15). This can be done as follows. Using the conception of T-product and the Gaussian path integral representation we can rewrite formula (19) with the Hamiltonian (4) and fixed $\mathbf{P}$ in the form

$$\begin{aligned} \mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})} &= N \int \delta\mathbf{q}\ \mathrm{T_t} \exp\Bigg\{ - \int\limits_0^\beta dt \Bigg[\frac{m}{2}\, \mathbf{q}^2(t) + i\mathbf{q}(t)\mathbf{P} - \\ &- \sum_{\mathbf{k}} (1 - i(\mathbf{k}\mathbf{q}(t)))\, a^\dagger_{\mathbf{k},t} a_{\mathbf{k},t} \Bigg] - g \int\limits_0^\beta dt \sum_{\mathbf{k}} \left(A_{\mathbf{k}} a_{\mathbf{k},t} + A^*_{\mathbf{k}} a^\dagger_{\mathbf{k},t} \right) \Bigg\}. \end{aligned}$$

Thus, the quadratic term $\left(\mathbf{P}-\sum_{\mathbf{k}}\mathbf{k}a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}\right)^2$ in $\mathcal{H}(\mathbf{P})$ is «linearized»The standard calculation gives in the continuous limit (see Section 3)

$$\left\langle 0\left|\mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})}\right|0\right\rangle = N\int\delta\,\mathbf{q}\,\exp\left\{-\frac{1}{2}\int\limits_0^\beta dt\left(m\mathbf{q}^2(t)+2i\mathbf{P}\mathbf{q}(t)\right)+\right.$$

$$\left.+\frac{\alpha}{\sqrt{8}}\iint\limits_0^\beta dtds\;\mathrm{e}^{-|t-s|}U\left(\mathbf{Q}(t,s)\right)\right\},\quad \mathbf{Q}(t,s)=\int\limits_s^t dt'\mathbf{q}(t'). \tag{20}$$

Let us introduce the new integration variable as follows:

$$\mathbf{q}(t)=\mathbf{u}+\dot{\mathbf{r}}(t)\,,\qquad \mathbf{r}(0)=\mathbf{r}(\beta)=\mathbf{0}\,.$$

Then, $\delta\mathbf{q}=d\mathbf{u}\delta\mathbf{r}$ and formula (20) with definition (15) reads

$$\left\langle 0\left|\mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})}\right|0\right\rangle = \int d\mathbf{u}\;\exp\left\{-i\beta\mathbf{P}\mathbf{u}-\frac{\beta m}{2}\mathbf{u}^2-\beta\Phi\left(\alpha,\mathbf{u}^2\right)\right\}, \tag{21}$$

where function $\Phi\left(\alpha,\mathbf{u}^2\right)$ is given by (15) and normalization in (21) is chosen such that

$$\left.\left\langle 0\left|\mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})}\right|0\right\rangle\right|_{\alpha=0} = \exp\left(-\beta\frac{\mathbf{P}^2}{2m}\right)\,.$$

Since we deal with $\beta\to\infty$, integral (21) can be derived by using the saddle point method. The extremum condition

$$\frac{\partial}{\partial\mathbf{u}}\left.\left\{-i\mathbf{P}\mathbf{u}-\frac{m\mathbf{u}^2}{2}-\Phi\left(\alpha,\mathbf{u}^2\right)\right\}\right|_{\mathbf{u}=\mathbf{u}_0}=0$$

results in the solution for infinitesimal $\mathbf{P}$

$$\mathbf{u}_0=\frac{-i\mathbf{P}}{m+2\Phi_\xi(\alpha)}+O(\mathbf{P}^4)\,,$$

and hence,

$$\begin{aligned} -\frac{1}{\beta}\ln\left\langle 0\left|\mathrm{e}^{-\beta\mathcal{H}(\mathbf{P})}\right|0\right\rangle &= i\mathbf{P}\mathbf{u}_0+\frac{m\mathbf{u}_0^2}{2}+\Phi\left(\alpha,\mathbf{u}_0^2\right)= \\ &= \Phi(\alpha)+\frac{\mathbf{P}^2}{2\left[m+2\Phi_\xi(\alpha)\right]}+O(\mathbf{P}^4)\,. \end{aligned} \tag{22}$$

Comparing (19) with (22) we define the GSE and EM as follows

$$E(\alpha)=\Phi(\alpha)\,,\qquad m^*_{\mathrm{canon}}(\alpha)=m+2\Phi_\xi(\alpha)\,. \tag{23}$$

5.2. The Effective Mass and Velocity. Another definition of the EM coinciding with (23) and connected with polaron velocity was done by Feynman [2]. The argumentation is based on the remark that the density matrix under the condition $\alpha = 0$ looks like (6), where $\mathbf{u} = (\mathbf{r}_1 - \mathbf{r}_2)/\beta$ can be considered as «the Euclidian velocity» which is related to the real velocity as $\mathbf{v} = -i\mathbf{u}$. Therefore, we define

$$\rho_\beta(\mathbf{u}\beta, \mathbf{0}) = \mathrm{e}^{-\beta E(\alpha,\mathbf{u})} = \int\limits_{\mathbf{q}(0)=\mathbf{0}}^{\mathbf{q}(\beta)=\beta\mathbf{u}} \delta\mathbf{q}\ \mathrm{e}^{-S[\mathbf{q}]}\,. \tag{24}$$

Going to the new variable $\mathbf{q}(t) = \mathbf{r}(t) + \mathbf{u}t$, we obtain

$$\begin{aligned} \mathrm{e}^{-\beta E(\alpha,\mathbf{u})} &= \mathrm{e}^{-\beta\frac{m\mathbf{u}^2}{2}} \int\limits_{\mathbf{r}(0)=\mathbf{0}}^{\mathbf{r}(\beta)=\mathbf{0}} \delta\mathbf{r} \exp\left\{-S_0[\mathbf{r}] - S_{\mathrm{int}}[\mathbf{r}+\mathbf{u}]\right\} = \\ &= \exp\left\{-\beta\frac{m\mathbf{u}^2}{2} - \beta\Phi(\alpha,\mathbf{u}^2)\right\}\,. \end{aligned} \tag{25}$$

If $\mathbf{u}$ is infinitesimal, we have

$$E(\alpha,\mathbf{u}) = \frac{m\mathbf{u}^2}{2} + \Phi(\alpha,\mathbf{u}^2) = \frac{\mathbf{u}^2}{2}\left[m + 2\Phi_\xi(\alpha)\right] + O(\mathbf{u}^4)\,.$$

Thus, we obtain the *velocity* definition of the GSE and EM as follows:

$$E(\alpha) = \Phi(\alpha)\,, \qquad m^*_{\mathrm{vel}}(\alpha) = m + 2\Phi_\xi(\alpha)\,. \tag{26}$$

We see that definitions (26) coincide with (23).

5.3. The Effective Mass and the Fourier Transform of the Density Matrix. Now we will show that definitions of the EM in (23) and (26) can be obtained by considering the Fourier transform of the density matrix. Let us follow the standard definition by using expansion of the self-energy with respect to small momentum (see, e.g., [56, 57]). To define the GSE and EM simultaneously, we consider a generalized form of (10) by involving the projected partition function at finite $\mathbf{p}$ as follows:

$$\mathrm{e}^{-\beta E(\alpha,\,\mathbf{p})} = \int d\mathbf{x}\ \mathrm{e}^{-i\mathbf{p}\mathbf{x}} \rho_\beta(\mathbf{x},\mathbf{0}) = \int d\mathbf{x}\ \mathrm{e}^{-i\mathbf{p}\mathbf{x}} \cdot N \int\limits_{\mathbf{q}(0)=\mathbf{0}}^{\mathbf{q}(\beta)=\mathbf{x}} \delta\mathbf{q}\,\mathrm{e}^{-S[\mathbf{q}]}\,. \tag{27}$$

Since the polaron action is translationally invariant, the energy spectrum of the polaron is continuous and for small $\mathbf{p}$ the following expansion takes place:

$$E(\alpha,\mathbf{p}) = E(\alpha) + \frac{\mathbf{p}^2}{2\,m^*(\alpha)} + O(\mathbf{p}^4)\,. \tag{28}$$

To arrive at the conventional zero-end-point boundary conditions, we shift the path variables by a classical straight-line reference path $\mathbf{z}(t)$

$$\mathbf{q}(\mathbf{t}) = \mathbf{r}(t) + \mathbf{z}(t)\,, \qquad \mathbf{z}(t) = \frac{\mathbf{x}}{\beta}\, t = \mathbf{y}\, t \qquad \Rightarrow \qquad \mathbf{r}(0) = \mathbf{r}(\beta) = 0\,.$$

Then, we rewrite (27)

$$\mathrm{e}^{-\beta E(\alpha,\, \mathbf{p})} = \beta^d \int d\mathbf{y}\, \mathrm{e}^{-\beta\left(i\mathbf{p}\mathbf{y} + \frac{m\mathbf{y}^2}{2} + \Phi(\alpha,\, \mathbf{y}^2)\right)}\,. \tag{29}$$

For large $\beta \to \infty$ this integral can be computed by the saddle point method. The extremal point for small $\mathbf{p}$ can be calculated

$$i\mathbf{p} + m\mathbf{y}_0 + 2\,\mathbf{y}_0 \Phi_\xi(\alpha,\, \mathbf{y}_0^2) = 0, \qquad \mathbf{y}_0 = \frac{-i\mathbf{p}}{m + 2\Phi_\xi(\alpha)} + O(\mathbf{p}^3)\,.$$

Substituting it into (29) we obtain

$$\begin{aligned} E(\alpha,\, \mathbf{p}) &= \left(i\mathbf{p}\mathbf{y}_0 + \frac{m\mathbf{y}_0^2}{2} + \Phi(\alpha, \mathbf{y}_0^2)\right) = \\ &= \Phi(\alpha, 0) + \frac{\mathbf{p}^2}{2(m + 2\Phi_\xi(\alpha))} + O(\mathbf{p}^4). \end{aligned} \tag{30}$$

Comparing (28) and (30) term by term, we define the GSE and EM as follows:

$$E(\alpha) = \Phi(\alpha), \qquad m^*_F(\alpha) = m + 2\Phi_\xi(\alpha). \tag{31}$$

We can see that definitions (23), (26) and (31) coincide explicitly.

5.4. The «Statistical» Effective Mass. A «statistical» definition of the EM was given in [60]. It was shown that the polaron functional integral was equivalent to the statistical mechanics of an anharmonic string. The variable $\mathbf{q}(t)$ in (24) can be regarded as a weighted random walk. The effective polaron mass m^* can be identified with the effective diffusion coefficient κ of the Brownian motion. In our notation, for free motion ($\alpha = 0$) it looks like

$$\left\langle \mathbf{q}^2(T) \right\rangle_0 = \int\limits_{\mathbf{q}(0)=0}^{\mathbf{q}(\beta)=0} \delta\mathbf{q}\, \mathbf{q}^2(T)\, \mathrm{e}^{-S_0[\mathbf{q}]} = \frac{3T}{m}\left(1 - \frac{T}{\beta}\right) \xrightarrow[\beta\to\infty]{} \frac{3T}{m}$$

and

$$\frac{1}{\kappa} = \lim_{T\to\infty} \frac{1}{3T} \left\langle [\mathbf{q}(T) - \mathbf{q}(0)]^2 \right\rangle_0 = \frac{1}{m}\,.$$

Naturally, for $\alpha \neq 0$, the effective polaron mass should be defined as

$$\frac{1}{m^*_{\rm stat}(\alpha)} = \lim_{T\to\infty} \frac{1}{3T} \left\langle [\mathbf{q}(T) - \mathbf{q}(0)]^2 \right\rangle ,$$
$$\left\langle \mathbf{q}^2(T) \right\rangle = \frac{1}{Z_\beta(\alpha)} \int d\sigma_0[q] \; \mathbf{q}^2(T) \; {\rm e}^{-S_{\rm int}[\mathbf{q}]} .$$

One can write

$$\left\langle [\mathbf{q}(T) - \mathbf{q}(0)]^2 \right\rangle = \frac{\partial^2}{\partial y_j \partial y_j} \ln Z_\beta\left(\alpha, \mathbf{y}_T^2\right)\Big|_{\mathbf{y}=\mathbf{0}} ,$$
$$Z_\beta\left(\alpha, \mathbf{y}_T^2\right) = \int d\sigma[\mathbf{q}] \; {\rm e}^{-S_{\rm int}[\mathbf{q}] + \int_0^\beta dt \; \mathbf{q}(t)\mathbf{y}_T(t)}, \quad \mathbf{y}_T(t) = \mathbf{y}\delta(T-t).$$

Here $\mathbf{y}$ is infinitesimally small and $1 \ll T \ll \beta \to \infty$.

By introducing a new variable

$$\mathbf{q}(t) = \mathbf{r}(t) + \mathbf{y}(t) , \qquad \mathbf{y}(t) = \frac{\mathbf{y}}{m} D_0(T,t) ,$$

where $D_0(T,t)$ is given by (8), one can obtain for $1 \ll T \ll \beta \to \infty$

$$Z_\beta(\alpha, \mathbf{y}_T^2) = {\rm e}^{\frac{\mathbf{y}^2}{2m}T} \int d\sigma_0[\mathbf{r}] \; {\rm e}^{-S_{\rm int}[\mathbf{r}+\mathbf{y}]} .$$

Then, for infinitesimal $\mathbf{y}$ one can show that (for details see *Appendix B*)

$$Z_\beta(\alpha, \mathbf{y}_T^2) = Z_\beta(\alpha) \; \exp\left\{ T\frac{\mathbf{y}^2}{2m} - T\Phi\left(\alpha, \frac{\mathbf{y}^2}{m}\right) + O(\mathbf{y}^4) \right\}$$

and hence,

$$\frac{1}{m^*_{\rm stat}(\alpha)} = \frac{1}{m} - \frac{2}{m^2}\Phi_\xi(\alpha) \quad \Rightarrow \quad m^*_{\rm stat}(\alpha) = \frac{m^2}{m - 2\Phi_\xi(\alpha)} . \qquad (32)$$

5.5. The «Inertial» Effective Mass. There exist other ways to define the effective mass. One of them is the idea to determine the «inertial» mass of the polaron which has been suggested in [18]. Remember, that Feynman-type variational estimates possess the same perturbation nature, the only difference is that the variational optimization allows one to optimize the perturbation answer getting reasonable results even for large α. Namely, this strategy has been fulfilled by Saitoh [18] by considering the acceleration rate against the fictitious constant driving field (a static electric field $\mathbf{E}$) incorporated in the generalized Feynman-type action. Now we follow this idea. Consider an electron in the presence of external electric field $\mathbf{E}$. The Lagrangian is

$$\mathcal{L}_{cl} = m\dot{\mathbf{x}}^2/2 - \mathbf{E}\mathbf{x}.$$

The solution of the classical equation of motion with boundary conditions $\mathbf{x}(0) = \mathbf{x}(\beta) = 0$ is

$$\mathbf{x}_{cl}(t) = \frac{\mathbf{E}\beta}{2m}\, a(t)\,, \qquad a(t) = t\left(1 - \frac{t}{\beta}\right),$$

and the classical action becomes

$$\mathcal{S}_{cl}[\mathbf{x}] = \int\limits_0^\beta dt\ \mathcal{L}_{cl} = -\frac{(\beta\mathbf{E})^2}{24m}\beta\,.$$

Therefore, the value $(\beta\mathbf{E})^2$ we consider to be infinitesimally small for $\beta \to \infty$. In the presence of interaction, the «inertial» EM of the multidimensional polaron can be defined as follows

$$\begin{aligned} \mathrm{e}^{-\beta E(\alpha,\mathbf{E})} &= \int d\sigma_0[\mathbf{q}]\ \exp\left\{-S_{\mathrm{int}}[\mathbf{q}] - \mathbf{E}\int\limits_0^\beta dt\ \mathbf{q}(t)\right\} = \\ &= \exp\left\{-\beta\left[E(\alpha) - \frac{(\beta\mathbf{E})^2}{24m^*_{\mathrm{iner}}} + O((\beta\mathbf{E})^4)\right]\right\}, \end{aligned} \tag{33}$$

where the external field is infinitesimally weak $|\mathbf{E}| \to 0$. Let us show the connection between this definition and the functional integral (15). Going to the new integration variable

$$\mathbf{q}(t) = \mathbf{r}(t) - \mathbf{x}_{cl}(t),$$

which satisfies the same zeroth boundary conditions. Then (33) reads

$$\mathrm{e}^{-\beta E(\alpha,\mathbf{E})} = \exp\left\{-\beta\left[-\frac{(\beta\mathbf{E})^2}{24m} + \Psi\left(\alpha, \frac{(\beta\mathbf{E})^2}{4m^2}\right)\right]\right\},$$

$$\exp\left\{-\beta\Psi\left(\alpha, \frac{(\beta\mathbf{E})^2}{4m^2}\right)\right\} = \int d\sigma_0[\mathbf{r}]\ \mathrm{e}^{-S_{\mathrm{int}}[\mathbf{r}-\mathbf{x}_{cl}]}.$$

Thus, we get

$$\begin{aligned} E(\alpha,\mathbf{E}) &= -\frac{(\beta\mathbf{E})^2}{24m} + \Psi\left(\alpha, \frac{(\beta\mathbf{E})^2}{4m^2}\right) = \\ &= -\frac{(\beta\mathbf{E})^2}{24m} + \Psi(\alpha) + \frac{(\beta\mathbf{E})^2}{4m^2}\Psi_\xi(\alpha) + O((\beta\mathbf{E})^4), \end{aligned}$$

where

$$\Psi(\alpha) = \Psi(\alpha, 0), \qquad \Psi_\xi(\alpha) = \left.\frac{d}{d\xi}\Psi(\alpha,\xi)\right|_{\xi=0}.$$

One can show (see *Appendix A*) that in the limit $\beta \to \infty$

$$\Psi(\alpha) = \Phi(\alpha), \qquad \Psi_\xi(\alpha) = \frac{1}{3}\Phi_\xi(\alpha).$$

Therefore, the *inertial* version looks:

$$E(\alpha) = \Psi(\alpha) = \Phi(\alpha),$$
$$\frac{1}{m^*_{\rm iner}(\alpha)} = \frac{1}{m} - \frac{6}{m^2}\Psi_\xi(\alpha) = \frac{1}{m} - \frac{2}{m^2}\Phi_\xi(\alpha),$$

so

$$m^*_{\rm iner}(\alpha) = \frac{m^2}{m - 2\Phi_\xi(\alpha)} \underset{\alpha\to 0}{\longrightarrow} m + 2\Phi_\xi(\alpha) \approx m^*_{\rm canon}(\alpha). \qquad (34)$$

Definitions (32) and (34) turn to be identical. However, one can see that the *statistical* and *inertial* versions of the EM do not coincide with the *canonical* definition. These definitions may be equivalent only in the weak-coupling regime $\alpha \ll 1$, i.e., they may coincide with each other in the framework of the first-order of any perturbation methods (see, for example [59]).

5.6. The «Magnetic» Effective Mass. Consider the polaron in a weak magnetic field $\mathbf{H} = (H_1, H_2, H_3)$ at zero-temperature limit $\beta \to \infty$. The vector potential in the symmetric gauge is $\mathbf{B} = [\mathbf{H}\times\mathbf{q}]/2$. So, we consider the following model Hamiltonian [58, 59]

$$\mathcal{H} = \frac{1}{2m}\left(\mathbf{p} + \frac{e}{c}\mathbf{B}\right)^2 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + g\sum_{\mathbf{k}}\left(A_{\mathbf{k}} a_{\mathbf{k}} e^{\imath\mathbf{kq}} + A^*_{\mathbf{k}} a^\dagger_{\mathbf{k}} e^{-\imath\mathbf{kq}}\right).$$

For weak magnetic field $\mathbf{H}$, the free energy up to the order $|\mathbf{H}|^3$ is given in [61]. By analogy with (33) we expand the energy for $|\mathbf{H}| \ll 1$

$$Z_\beta = \mathrm{Tr}\, e^{-\beta\mathcal{H}} = e^{-\beta E(\alpha,\mathbf{H})}, \qquad E(\alpha,\mathbf{H}) = E(\alpha) + \frac{\chi}{2}\mathbf{H}^2 + O(|\mathbf{H}|^3), \quad (35)$$

where the polaron «magnetic» mass m_H is defined through the diamagnetic susceptibility

$$\chi = -\frac{e^2\beta}{12\, m_H^2 c^2}.$$

Expanding the partition function up to $\mathbf{H}^2$, one is able to calculate χ and hence, m_H.

In perturbational calculations (see [59]) up to α^2 term, it was noted that for $\beta \to \infty$, the «inertial» mass equaled the «magnetic» one defined through the Landau zero-point energy [58]. This statement has been made by considering a

Feynman-like general quadratic action, but *not* the true polaron retarded nonlocal interaction. Besides, a Jensen–Peierls inequality and a variational optimization have been used before getting the final results for both the «inertial» and «magnetic» masses in [59].

In this section we would like to connect the definition of the polaron «magnetic» mass in (35) with the function $\Phi_\xi(\alpha)$. For this purpose we rewrite the partition function in the path-integral formulation as follows

$$Z_\beta = \int d\sigma_0[\mathbf{q}]\, \mathrm{e}^{-S_{\mathrm{mag}}[\mathbf{q}]-S_{\mathrm{int}}[\mathbf{q}]} = \sqrt{\det \mathbf{D}_0^{-1}} \int\limits_{\mathbf{q}(0)=\mathbf{0}}^{\mathbf{q}(\beta)=\mathbf{0}} \delta\mathbf{q}\ \mathrm{e}^{-\frac{m}{2}(\mathbf{q}[\mathbf{D}_0^{-1}+\hat{\mathbf{H}}]\mathbf{q})-S_{\mathrm{int}}[\mathbf{q}]}, \tag{36}$$

where

$$S_{\mathrm{mag}}[\mathbf{q}] = \frac{i}{2}\int\limits_0^\beta dt\ \left(\mathbf{H}\left[\mathbf{q}(t)\times\dot{\mathbf{q}}(t)\right]\right) = \frac{m}{2}(\mathbf{q},\hat{\mathbf{H}}\mathbf{q})\,,$$

$$(\hat{\mathbf{H}}(t,s))_{ij} = \frac{i}{m}\epsilon_{ijl}H_l\delta(t-s)\frac{\partial}{\partial s}\,, \qquad \epsilon_{ijl} = \text{antisymmetric unit tensor}\,.$$

The magnetic field is supposed to be infinitesimal ($\beta\mathbf{H}^2 \ll 1$) and all subsequent calculations will be done with accuracy $O((\beta\mathbf{H}^2)^2)$.

In contrast to the «inertial» mass definition, where the external force was proportional to $\mathbf{q}$, the additional term due to the external magnetic field is now proportional to $\mathbf{q}^2$ that makes it possible to use the following trick. To evaluate (36) we go to a new path variable

$$\mathbf{r} = \mathbf{D}_0^{1/2}\left(1+\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\mathbf{D}_0^{1/2}\right)^{1/2}\mathbf{D}_0^{-1/2}\mathbf{q}$$

so that

$$(\mathbf{q},[\mathbf{D}_0^{-1}+\hat{\mathbf{H}}]\mathbf{q}) = \left(\mathbf{q},\mathbf{D}_0^{-1/2}[1+\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\mathbf{D}_0^{1/2}]\mathbf{D}_0^{-1/2}\mathbf{q}\right) = \left(\mathbf{r},\mathbf{D}_0^{-1}\mathbf{r}\right)$$

and

$$\begin{aligned}\mathbf{q} &= \mathbf{D}_0^{1/2}\left[1+\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\mathbf{D}_0^{1/2}\right]^{-1/2}\mathbf{D}_0^{-1/2}\mathbf{r} = \\ &= \left[1-\frac{1}{2}\mathbf{D}_0\hat{\mathbf{H}}+\frac{3}{8}\mathbf{D}_0\hat{\mathbf{H}}\mathbf{D}_0\hat{\mathbf{H}}+O(|\mathbf{H}|^3)\right]\mathbf{r}\end{aligned}$$

with boundary conditions $\mathbf{r}(0)=\mathbf{r}(\beta)=\mathbf{0}$.

Differential operator $\mathbf{D}_0^{-1}(t,s)$ and its Green function $D_0(t,s)$ are defined in (7) and (8). Some useful relations for $D_0(t,s)$ are given in *Appendix C*. Obviously,

$$S_0[\mathbf{q}] + S_{\rm mag}[\mathbf{q}] = S_0[\mathbf{r}]\,.$$

Further, we omit terms $\sim O(|\mathbf{H}|^3)$. Then, we rewrite the partition function in terms of the new paths as follows

$$\begin{aligned}
Z_\beta &= {\rm e}^{-\beta E(\alpha) - \frac{\beta^2 \mathbf{H}^2}{24 m_H^2}} = \det\left\{1 - \frac{1}{2}\mathbf{D}_0\hat{\mathbf{H}} + \frac{3}{8}\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\right\} \times \qquad (37)\\
&\times \int d\sigma_0[\mathbf{r}]\, \exp\left\{-S_{\rm int}\left[\left(1 - \frac{1}{2}\mathbf{D}_0\hat{\mathbf{H}} + \frac{3}{8}\mathbf{D}_0^{1/2}\hat{\mathbf{H}}\right)\mathbf{r}\right]\right\} = \\
&= \exp\left\{-\frac{1}{2}\,{\rm Tr}\left(\mathbf{D}_0\hat{\mathbf{H}}\right) + \frac{1}{4}\,{\rm Tr}\left(\mathbf{D}_0\hat{\mathbf{H}}\mathbf{D}_0\hat{\mathbf{H}}\right)\right\} \times \\
&\times \int d\sigma_0[\mathbf{r}]\,{\rm e}^{-S_{\rm int}[\mathbf{r}]}\left\{1 - \int d\Omega_{ts\mathbf{k}}{\rm e}^{i\mathbf{k}\mathbf{R}(t,s)}(\mathbf{k}\mathbf{A}(t,s)) \; + \right.\\
&+ \int d\Omega_{ts\mathbf{k}}{\rm e}^{i\mathbf{k}\mathbf{R}(t,s)}(\mathbf{k}\mathbf{B}(t,s)) + \frac{1}{2}\int d\Omega_{ts\mathbf{k}}{\rm e}^{i\mathbf{k}\mathbf{R}(t,s)}(\mathbf{k}\mathbf{A}(t,s))^2 + \\
&+ \left.\frac{1}{2}\left(\int d\Omega_{ts\mathbf{k}}{\rm e}^{i\mathbf{k}\mathbf{R}(t,s)}(\mathbf{k}\mathbf{A}(t,s))\right)^2\right\},
\end{aligned}$$

where

$$(\mathbf{k}\mathbf{A}(t,s)) = \frac{i}{2}\;k_i\int_0^\beta dz\;\left[\left(D_0\,\hat{H}\right)_{ij}(t,z) - \left(D_0\,\hat{H}\right)_{ij}(s,z)\right] r_j(z) =$$

$$= \frac{1}{2m}\;k_i\epsilon_{ijl}H_l\int_0^\beta dz\, r_j(z)\left(\frac{{\rm sign}\,(z-t) - {\rm sign}\,(z-s)}{2} + \frac{t-s}{\beta}\right),$$

$$(\mathbf{k}\mathbf{B}(t,s)) = \frac{3i}{8m^2}k_i\int_0^\beta dz\left[\left(D_0\hat{H}D_0\hat{H}\right)_{ij}(t,z) - \left(D_0\hat{H}D_0\hat{H}\right)_{ij}(s,z)\right] r_j(z) =$$

$$= \frac{3i}{8m^2}k_i\left(H^2\delta^{ij} - H_iH_j\right)\int_0^\beta dz\, r_j(z)\left\{\frac{1}{2}[a(t) - a(s)] - D_0(t,z) + D_0(s,z)\right\}.$$

It is easy to show that (see *Appendix B*)

$$\frac{1}{2}\,\mathrm{Tr}\left(\mathbf{D}_0\hat{\mathbf{H}}\right) = 0\,, \qquad \frac{1}{4}\,\mathrm{Tr}\left(\mathbf{D}_0\hat{\mathbf{H}}\mathbf{D}_0\hat{\mathbf{H}}\right) = -\frac{\beta\mathbf{H}^2}{24m^2}\beta\,.$$

To evaluate (37) we use the Wick theorem

$$\int d\sigma_0[\mathbf{r}]\,(\mathbf{k}\mathbf{M}(t,s)\mathbf{r})\;\; \mathrm{e}^{i(\mathbf{k}\mathbf{Q}(t,s)\mathbf{r})}\;\; \mathrm{e}^{-S_{\mathrm{int}}[\mathbf{r}]} =$$

$$= \mathrm{e}^{\Delta}\left\{(\mathbf{k}\mathbf{M}(t,s)\mathbf{r})\,\mathrm{e}^{i(\mathbf{k}\mathbf{Q}(t,s)\mathbf{r})}\,\mathrm{e}^{-S_{\mathrm{int}}[\mathbf{r}]}\right\}\Big|_{\mathbf{r}=\mathbf{0}} =$$

$$= i\,(\mathbf{k}\mathbf{M}(t,s)\mathbf{D_0}\mathbf{Q}(t,s)\mathbf{k})\;\; \mathrm{e}^{\Delta}\left\{\mathrm{e}^{i(\mathbf{k}\mathbf{Q}(t,s)\mathbf{r})}\,\mathrm{e}^{-S_{\mathrm{int}}[\mathbf{r}]}\right\}\Big|_{\mathbf{r}=\mathbf{0}} +$$

$$+\, i\int d\Omega_{xy\mathbf{p}}\,\mathrm{e}^{i(\mathbf{p}\mathbf{Q}(x,y)\mathbf{r})}\,(\mathbf{k}\mathbf{M}(t,s)\mathbf{D}_0\mathbf{Q}(x,y)\mathbf{p})\,\mathrm{e}^{\Delta}\left\{\mathrm{e}^{i(\mathbf{k}\mathbf{Q}(t,s)\mathbf{r})}\,\mathrm{e}^{-S_{\mathrm{int}}[\mathbf{r}]}\right\}\Bigg|_{\mathbf{r}=\mathbf{0}},$$

where

$$\Delta = \frac{1}{2}\left(\frac{\delta}{\delta\mathbf{r}}\mathbf{D}_0\frac{\delta}{\delta\mathbf{r}}\right), \qquad (\mathbf{k}\mathbf{M}(t,s)\mathbf{r}) = k_i\int_0^\beta dz\;(\mathbf{M}(t,s;z))_{ij}r_j(z)\,.$$

Then, for $\beta\to\infty$ the terms in curly brackets in (37) may be replaced by the corresponding contributions (see *Appendix B*)

$$\begin{aligned}
&(\mathbf{k}\mathbf{A}(t,s)) \to 0,\\
&(\mathbf{k}\mathbf{B}(t,s)) \to \frac{\beta\mathbf{H}^2}{48}\Bigg\{\mathbf{k}^2[a(t)-a(s)]^2 +\\
&+\int d\Omega_{xy\mathbf{p}}\,\mathrm{e}^{i\mathbf{p}\mathbf{R}_{xy}}\mathbf{k}\mathbf{p}[a(t)-a(s)][a(x)-a(y)]\Bigg\},\\
&\frac{1}{2}(\mathbf{k}\mathbf{A}(t,s))^2 \to \frac{\beta\mathbf{H}^2}{48}\mathbf{k}^2\;[a(t)-a(s)]^2,\\
&\frac{1}{2}(\mathbf{k}\mathbf{A}(t,s))(\mathbf{p}\mathbf{A}(x,y)) \to \frac{\beta\mathbf{H}^2}{48}\mathbf{k}\mathbf{p}\;[a(t)-a(s)][a(x)-a(y)].
\end{aligned}$$

We obtain for large β

$$Z_\beta = \mathrm{e}^{-\beta\frac{\beta\mathbf{H}^2}{24m^2}} \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}]} \left\{1+\frac{\beta\mathbf{H}^2}{24m^2}\left[\int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{kR}(t,s)}\, \mathbf{k}^2[a(t)-a(s)]^2 \; + \right.\right.$$

$$\left.\left. + \iint d\Omega_{ts\mathbf{k}} d\Omega_{xy\mathbf{p}}\, \mathrm{e}^{i\mathbf{kR}(t,s)+i\mathbf{pR}(x,y)}\, \mathbf{kp}\, [a(t)-a(s)][a(x)-a(y)]\right]\right\} =$$

$$= \mathrm{e}^{-\beta\frac{\beta\mathbf{H}^2}{24m^2}} \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}]} \left\{1+\frac{\beta\mathbf{H}^2}{72m^2}\left[\int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{kR}(t,s)}\, \mathbf{k}^2\, (t-s)^2 \; + \right.\right.$$

$$\left.\left. + \iint d\Omega_{ts\mathbf{k}} d\Omega_{xy\mathbf{p}}\, \mathrm{e}^{i\mathbf{kR}(t,s)+i\mathbf{pR}(x,y)}\, \mathbf{kp}(t-s)(x-y)\right]\right\}. \tag{38}$$

Comparing (38), in particular, with analogous expansion (25)

$$\mathrm{e}^{-\beta\Phi(\alpha,\mathbf{u}^2)} = \int d\sigma_0[\mathbf{r}]\, \mathrm{e}^{-S_{\rm int}[\mathbf{r}]} \left\{1-\frac{\mathbf{u}^2}{6}\left[\int d\Omega_{ts\mathbf{k}}\, \mathrm{e}^{i\mathbf{kR}(t,s)}\, \mathbf{k}^2\, (t-s)^2 \; + \right.\right.$$

$$\left.\left. + \iint d\Omega_{ts\mathbf{k}} d\Omega_{xy\mathbf{p}}\, \mathrm{e}^{i\mathbf{kR}(t,s)+i\mathbf{pR}(x,y)}\, \mathbf{kp}\, (t-s)(x-y)\right]\right\}$$

we deduct that

$$\frac{1}{m_H^2} = \frac{1}{m^2} - \frac{2}{m^3}\Phi_\xi(\alpha)\,. \tag{39}$$

This definition does not coincide with the definitions of the «statistical» and «inertial» masses, the obvious difference is the squared mass power in (39) instead of a linear one.

One the other hand, there is a statement [62] that in the expansion of the GSE of a polaron in a weak magnetic field, the first-order (not the second!) term is inversely proportional to the polaron «magnetic» mass. The EM obtained so is exactly equivalent to the free polaron EM as defined by Fröhlich. In [58] the Landau zero-point EM at zero temperature has been found exactly the same as the «inertial» one. This EM was also found as the inverse coefficient of the first order of the magnetic field. Obviously, our definition of the polaron «magnetic» mass does not coincide with that given in [58] because (39) is proportional to the second-order term $\propto |\mathbf{H}|^2$ by the very construction.

Below we tabulate a comparison of various definition schemes for the polaron GSE and EM obtained in this Section.

In this Section, we have given several definitions of the polaron EM based on different physical principles, but independent of the specific approximate method. We have shown that definitions based on the polaron internal dynamics do not coincide, in general, with those obtained by using a responce principle to external sources (forces). They are equivalent either in the weak-coupling regime or, in case of some variational optimizations having in fact, the same perturbation nature.

Schemes	Definition of the EM	Effective mass
«Momentum's»	$E_{\rm eff}(\mathbf{P}) = E_{\rm eff}(\mathbf{0}) + \frac{\mathbf{P}^2}{2m^*}$	$m^* = m + 2\Phi_\xi(\alpha)$
«Velocity's»	$E_{\rm eff}(\mathbf{v}) = E_{\rm eff}(\mathbf{0}) + \frac{m^*\mathbf{v}^2}{2}$	$m^* = m + 2\Phi_\xi(\alpha)$
«Density matrix's»	$E_{\rm eff}(\mathbf{p}) = E_{\rm eff}(\mathbf{0}) + \frac{\mathbf{p}^2}{2m^*}$	$m^* = m + 2\Phi_\xi(\alpha)$
«Statistical»	$\frac{1}{m^*} = \lim\limits_{T\to\infty} \frac{1}{3T}\langle \mathbf{q}^2(T)\rangle$	$\frac{1}{m^*} = \frac{1}{m} - \frac{2}{m^2}\Phi_\xi(\alpha)$
«Inertial»	$E_{\rm eff}(\mathbf{E}) = E_{\rm eff}(\mathbf{0}) - \frac{(\beta\mathbf{E})^2}{24m^*}$	$\frac{1}{m^*} = \frac{1}{m} - \frac{2}{m^2}\Phi_\xi(\alpha)$
«Magnetic»	$E_{\rm eff}(\mathbf{H}) = E_{\rm eff}(\mathbf{0}) - \frac{e^2\beta\mathbf{H}^2}{24c^2(m^*)^2}$	$\frac{1}{(m^*)^2} = \frac{1}{m^2} - \frac{2}{m^3}\Phi_\xi(\alpha)$

Below, we follow the «density matrix» definition of the polaron EM.

6. GENERALIZED GAUSSIAN REPRESENTATION

Path integrals $Z_\beta(\alpha)$ and $Y_\beta(\alpha)$ in (18) are the central quantities of the present paper. To evaluate them, we use the Generalized Gaussian Representation method developed partly in [20, 63, 64] and successfully applied earlier to some problems in quantum physics [21, 65].

The key idea of our approach comes from quantum field theory and consists in the following. In QFT the main ultraviolet contributions estimated by the perturbation theory come from the so-called tadpole Feynman diagrams and they can be taken into account effectively if the interaction Lagrangian is chosen in the normal-ordered form with respect to the free Lagrangian, which realizes the Gaussian measure in the functional integral approach.

Thus, if a PI over a Gaussian measure is given, it should be rewritten in the representation where the interaction functional is given in the normal form, according to the new Gaussian measure, and does not contain any linear and quadratic terms over the fields – variables of the functional integration. As a result, we obtain a representation which isolates the main contribution to the PI, and the high-order corrections can be calculated by using a perturbation expansion over the new interaction term.

6.1. Basic Formulae. To demonstrate our idea, we consider a d-component vector $\mathbf{q}(t) = \{q_j(t)\} \in \Re^d$, $(j = 1, ..., d)$ in the Euclidean imaginary time $t \in [0, \beta]$ and a PI in the following general form

$$I_\beta = \int d\sigma_0[\mathbf{q}]\, \mathrm{e}^{S_I[\mathbf{q}]} = \langle \mathrm{e}^{S_I[\mathbf{q}]}\rangle_0\,, \qquad \langle 1\rangle_0 = 1\,, \tag{40}$$

where the initial Gaussian measure $d\sigma_0[\mathbf{q}]$ is given in (10).

The following items characterize shortly the basic idea of our method.

1. Without loss of generality the interaction functional may be given by

$$S_I[\mathbf{q}] = \int d\Omega_{\mathbf{a}}\, \mathrm{e}^{i(\mathbf{qa})}\,, \quad (\mathbf{qa}) = \int\limits_0^\beta dt\; q_j(t) a_j(t)\,.$$

For theories possessing a central symmetry (like the polaron) we specify

$$\int d\Omega_{\mathbf{a}}\; a_j(t) = 0\,, \qquad \text{or} \qquad \frac{\delta}{\delta q_j(t)} S_I[\mathbf{q}]\Big|_{\mathbf{q}=0} = 0\,.$$

2. By introducing a new operator $\mathbf{D}^{-1} = \delta_{ij} D^{-1}(t,s)$ we rewrite (40) as follows:

$$I_\beta = \sqrt{\det\left(\frac{\mathbf{D}}{\mathbf{D}_0}\right)} \int d\sigma[\mathbf{q}]\; \mathrm{e}^{-\frac{1}{2}(\mathbf{q}[\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{q}) + S_I[\mathbf{q}]} \tag{41}$$

$$= \sqrt{\det\left(\frac{\mathbf{D}}{\mathbf{D}_0}\right)} \cdot \left\langle \mathrm{e}^{-\frac{1}{2}(\mathbf{q}[\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{q}) + S_I[\mathbf{q}]} \right\rangle\,,$$

where a general Gaussian measure is introduced

$$d\sigma[\mathbf{q}] = \frac{\delta\mathbf{q}}{\sqrt{\det\mathbf{D}}}\; \mathrm{e}^{-\frac{1}{2}(\mathbf{q}\mathbf{D}^{-1}\mathbf{q})}, \qquad \langle(*)\rangle = \int d\sigma\; (*)\,, \tag{42}$$

The following relation takes place:

$$\langle \mathrm{e}^{i(\mathbf{qa})} \rangle = \int d\sigma\; \mathrm{e}^{i(\mathbf{qa})} = \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})} \qquad \forall a_j(t) \in \Re^d\,.$$

3. Now we introduce the conception of the *normal-ordered form* with respect to the general measure $d\sigma$. In particular, we use the following normal forms:

$$\begin{aligned} :\mathrm{e}^{i(\mathbf{qa})}: \quad &= \quad \mathrm{e}^{i(\mathbf{qa})} \cdot \mathrm{e}^{\frac{1}{2}(\mathbf{aDa})} \\ :(\mathbf{q}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{q}): \quad &= \quad (\mathbf{q}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{q}) - ([\mathbf{D}_0^{-1} - \mathbf{D}^{-1}], \mathbf{D})\,, \end{aligned}$$

so that

$$\langle :\mathrm{e}^{i(\mathbf{qa})}: \rangle = 1\,, \qquad \langle :\mathbf{q}(t_1) \cdot \ldots \cdot \mathbf{q}(t_n): \rangle = 0\,, \quad n \geq 1\,.$$

4. Functional $W[\phi]$ should be represented in the normal ordered form as follows:

$$S_I[\mathbf{q}] = \int d\Lambda_{\mathbf{a}} \ :\mathrm{e}^{i(\mathbf{qa})}: = :W[\mathbf{0}]: + :W_1[\mathbf{q}]: + :W_2[\mathbf{q}]: + :W_{\mathrm{int}}[\mathbf{q}]:, \quad (43)$$

$$:W[\mathbf{0}] := \int d\Lambda_{\mathbf{a}} = \int d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})},$$

$$:W_1[\mathbf{q}] := \int d\Lambda_{\mathbf{a}} \ (\mathbf{qa}) = \int d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})} \ (\mathbf{qa}),$$

$$:W_2[\mathbf{q}] := \int d\Lambda_{\mathbf{a}} \ :(\mathbf{qa})(\mathbf{qa}) := \int d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})} \ :(\mathbf{qa})(\mathbf{qa}):,$$

$$:W_{\mathrm{int}}[\mathbf{q}] := \int d\Lambda_{\mathbf{a}} \ :e_2^{i(\mathbf{qa})} := \int d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})} \ :e_2^{i(\mathbf{qa})}:,$$

where

$$d\Lambda_{\mathbf{a}} = d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})}, \qquad \mathrm{e}_2^S = \mathrm{e}^S - 1 - S - \frac{S^2}{2}.$$

5. The requirement that all Gaussian terms over $\mathbf{q}$ are concentrated in the measure $d\sigma$ corresponds to the complete elimination of any quadratic parts from the interaction and it leads to the constraint equation

$$:(\mathbf{q}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{q}): + \int d\Lambda_{\mathbf{a}} \ :(\mathbf{qa})(\mathbf{qa}):= 0, \qquad \forall \mathbf{q}(t) \qquad (44)$$

which results in

$$\delta_{ij}[D_0^{-1}(t,s) - D^{-1}(t,s)] + \int d\Lambda_{\mathbf{a}} \, a_i(t) \, a_j(s) = 0$$

or

$$D_0^{-1}(t,s) - D^{-1}(t,s) + \frac{1}{d}\int d\Omega_{\mathbf{a}} \ \mathrm{e}^{-\frac{1}{2}(\mathbf{aDa})} \ (\mathbf{a}(t)\mathbf{a}(s)) = 0$$

defining the adjustable Green function $\mathbf{D}(t,s) = \delta_{ij} D(t,s)$.

6. Substituting formulae (43) and (44) into the representation (41), we obtain the new representation of the initial PI (40) as follows:

$$I_\beta = \mathrm{e}^{-F_\beta} J_\beta, \qquad (45)$$

$$F_\beta = -\frac{1}{2}\mathrm{Tr}\left\{\ln(\mathbf{D}_0^{-1}\mathbf{D}) + \mathbf{D}_0^{-1}\mathbf{D} - \mathbf{1}\right\} - :W[\mathbf{0}]:,$$

$$J_\beta = \int d\sigma[\mathbf{q}] \, \mathrm{e}^{:W_{\mathrm{int}}[\mathbf{q}]:} = \left\langle \mathrm{e}^{:W_{\mathrm{int}}[\mathbf{q}]:} \right\rangle.$$

Thus, the original PI is rewritten as a product of a prefactor e^{-F_β} and a new PI J_β based on the new Gaussian measure $d\sigma$. Hereby, F_β describes the leading-order General Gaussian Representation and the remaining non-Gaussian contributions can be systematically computed by evaluating J_β into a perturbation series over the interaction term $:W_{\mathrm{int}}[\mathbf{q}]:$.

Note that the suggested scheme has a general structure and can be easily adapted for different physical problems, including the polaron in statistical physics.

6.2. Application to the Polaron. Below we apply the GGR method to the d-dimensional polaron problem in statistical mechanics. We deal with the path-integration variable $\mathbf{r}(t)$ with closed ends $\mathbf{r}(0) = \mathbf{r}(\beta) = \mathbf{0}$ in the Euclidean imaginary time $t \in [0, \beta]$. Our purpose is to derive the GSE and EM in (31) by evaluating PIs in (18) in the limit $\beta \to \infty$.

First, we evaluate $Z_\beta(\alpha)$ by using the representation (45). For this purpose, we should use $-S_{\rm int}[\mathbf{r}]$ defined in (13) instead of $W[\phi]$. Also, measure $d\Omega_a$ should be changed to $d\Omega(t, s, \mathbf{k})$ given in (13). In doing so, we remark the following correspondence:

$$(\phi, a) \Rightarrow (\mathbf{kR})(t,s) = \int\limits_0^\beta d\tau\, \mathbf{r}(\tau)\, \mathbf{a}(\tau, t, s)\,, \qquad \mathbf{a}(\tau,t,s) = \mathbf{k}\cdot[\delta(\tau - t) - \delta(\tau - s)]\,.$$

The initial functional measure in the polaron problem is given by $d\sigma_0[\mathbf{r}]$, where the differential operator $\mathbf{D}_0^{-1}(t,s)$ and its Green function $\mathbf{D}_0(t,s) = \delta_{ij} D_0(t,s)$ are given in (7) and (8).

Note, as $\beta \to \infty$ the Green function $D_0(t,s)$ becomes translationally invariant. To trace it, we make a shift $\{t, s\} \to \{t + \beta/2, s + \beta/2\}$ in «time» and go to the symmetrical region $\{t, s\} \in [-\beta/2, \beta/2]$. The boundary conditions for paths remain: $\mathbf{r}(-\beta/2) = \mathbf{r}(\beta/2) = 0$. Then,

$$D_0(t,s) = -\frac{|t-s|}{2} + \frac{\beta}{4} - \frac{ts}{\beta} \underset{\beta\to\infty}{\longrightarrow} -\frac{|t-s|}{2} + \frac{\beta}{4} = D_0(t-s)$$

and its Fourier transform reads

$$\widetilde{D}_0(p) = \int\limits_{-\beta/2}^{\beta/2} dt\, \mathrm{e}^{ipt} \left(-\frac{|t|}{2} + \frac{\beta}{4}\right) = \frac{1 - \cos(\beta p/2)}{p^2} \underset{\beta\to\infty}{\longrightarrow} \frac{1}{p^2}\,. \tag{46}$$

Now the application of the GGR method to $Z_\beta(\alpha)$ is straightforward. Following (42), we introduce a new Gaussian measure $d\sigma[\mathbf{r}]$.

By analogy with (41), we go to another functional averaging scheme based on the measure $d\sigma[\mathbf{r}]$ and rewrite the partition function as follows:

$$Z_\beta(\alpha) = \sqrt{\det\left(\frac{\mathbf{D}}{\mathbf{D}_0}\right)} \int d\sigma[\mathbf{r}] \exp\left\{-\frac{1}{2}\left(\mathbf{r}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\mathbf{r}\right) + W[\mathbf{r}]\right\}\,.$$

The normal-ordering procedure with respect to $d\sigma[\mathbf{r}]$ implies

$$\begin{aligned} \mathrm{e}^{i\mathbf{kR}(t,s)} &= :\mathrm{e}^{i\mathbf{kR}(t,s)}:\ \mathrm{e}^{-\mathbf{k}^2 F(t-s)}\,, \\ (\mathbf{r}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\,\mathbf{r}) &= :(\mathbf{r}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\,\mathbf{r}): + ([\mathbf{D}_0^{-1} - \mathbf{D}^{-1}], \mathbf{D})\,, \end{aligned}$$

where a shifted Green function has been introduced

$$F(t-s) = D(0) - D(t-s)\,. \tag{47}$$

According to (44), we remove all quadratic path configurations from the interaction as follows:

$$:(\mathbf{r}, [\mathbf{D}_0^{-1} - \mathbf{D}^{-1}]\,\mathbf{r}): + \int d\Lambda(t,s,\mathbf{k})\ :(\mathbf{kR})^2 := 0\,, \tag{48}$$

where

$$d\Lambda_{ts\mathbf{k}} = d\Omega_{ts\mathbf{k}}\ \mathrm{e}^{-\mathbf{k}^2 F(t-s)} = \frac{\alpha}{\sqrt{8}}\ \mathrm{e}^{-|t-s|} dt ds\ \frac{d\mathbf{k}}{(2\pi)^d} \widetilde{U}(\mathbf{k})\ \mathrm{e}^{-\mathbf{k}^2 F(t-s)}\,.$$

Requirement (48) results in the following set of constraint equations (for details see *Appendix C*):

$$\begin{aligned} F(t) &= \frac{1}{\pi}\int_0^\infty dk\,[1-\cos(kt)]\,\widetilde{D}(k)\,, \\ \widetilde{D}(k) &= \frac{1}{k^2 + \alpha_d\cdot\widetilde{\Sigma}(k)}\,, \\ \widetilde{\Sigma}(k) &= \frac{1}{3\sqrt{2\pi}}\int_0^\infty dt\,[1-\cos(kt)]\,\frac{\exp(-t)}{F^{3/2}(t)} \end{aligned} \tag{49}$$

which self-consistently define adjustable functions $F(t)$ and $\widetilde{D}(k)$.

Then, following (45) we rewrite

$$Z_\beta(\alpha) = \mathrm{e}^{-\beta E_0(\alpha)} J_\beta(\alpha)\,, \tag{50}$$

where the zeroth Gaussian approximation to the polaron exact GSE is

$$\begin{aligned} E_0(\alpha) = &-\frac{d}{2\pi}\int_0^\infty dk\left[\ln(k^2\widetilde{D}(k)) - k^2\widetilde{D}(k) + 1\right] - \\ &-\frac{\alpha B_d}{\sqrt{8}\,\beta}\iint_{-\beta/2}^{-\beta/2} dt\,ds\,\mathrm{e}^{-|t-s|}\int\frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}}\,\mathrm{e}^{-\mathbf{k}^2F(t-s)} = \\ = &-d\left\{\frac{1}{2\pi}\int_0^\infty dk\left[\ln\left(k^2\widetilde{D}(k)\right) - k^2\widetilde{D}(k) + 1\right] + \frac{\alpha_d}{3\sqrt{2\pi}}\int_0^\infty dt\frac{\exp(-t)}{F^{1/2}(t)}\right\}. \end{aligned} \tag{51}$$

The remaining non-Gaussian contributions should be evaluated systematically by considering a new PI

$$J_\beta(\alpha) = \langle \exp\{:W_{\text{int}}[\mathbf{r}]:\}\rangle = \int d\sigma \exp\{:W_{\text{int}}[\mathbf{r}]:\}\,, \tag{52}$$

where

$$:W_{\text{int}}[\mathbf{r}]:= \int d\Lambda_{ts\mathbf{k}}\, :e_2^{i\mathbf{k}\mathbf{R}(t,s)}: \,.$$

Substituting (50) into (31) we obtain the polaron GSE as follows

$$E(\alpha) = E_0(\alpha) - \lim_{\beta\to\infty} \frac{1}{\beta} \ln J_\beta(\alpha)\,.$$

Obviously, $\langle : W_{\text{int}}[\mathbf{r}] :\rangle = 0$ due to normal ordering. Then, applying the Jensen–Peierls inequality we arrive at a lower bound to the non-Gaussian correction

$$J_\beta(\alpha) \geq \mathrm{e}^{\langle :W_{\text{int}}[\mathbf{r}]:\rangle} = 1\,.$$

Therefore, our leading-order Gaussian term $E_0(\alpha)$ represents an *upper bound* to the polaron exact ground-state energy

$$E_0(\alpha) \geq E(\alpha)\,. \tag{53}$$

Note also that inequality (53) turns to an equation as $d \to \infty$ because $\alpha_d \propto O(1/d^{3/2}) \to 0$ and so $J_\beta(\alpha) \to 1$. Therefore,

$$\lim_{d\to\infty} E(\alpha) = E_0(\alpha)\,.$$

A similar property has earlier been observed [55] by considering the leading term for the GSE within the $1/d$ expansion method applied to the multidimensional Fröhlich polaron.

The next point is to evaluate $Y_\beta(\alpha)$ within the GGR technique by analogy with $Z_\beta(\alpha)$. The only difference between these two PIs is an additional factor $W_i^{(1)}[\mathbf{r}]\,W_i^{(1)}[\mathbf{r}] + W_{ii}^{(2)}[\mathbf{r}]$ entering into $Y_\beta(\alpha)$. This factor does not influence the exponential $\mathrm{e}^{W[\mathbf{r}]}$ in (18) as $\beta \to \infty$. Therefore, the normal ordering for $W[\mathbf{r}]$ as well as the elimination of the quadratic parts from the interaction remains the same as for $Z_\beta(\alpha)$. In other words, a constraint equation for $Y_\beta(\alpha)$ in the limit $\beta \to \infty$ is given by (49), too. Repeating all the steps made in the previous subsection we obtain

$$Y_\beta(\alpha) = \mathrm{e}^{-\beta\, E_0(\alpha)}\, \langle \mathrm{e}^{:W_{\text{int}}[\mathbf{r}]:}\{W_i^{(1)}[\mathbf{r}]\,W_i^{(1)}[\mathbf{r}] + W_{ii}^{(2)}[\mathbf{r}]\}\rangle\,. \tag{54}$$

Now we represent functionals (17) in the normal-ordered form with respect to the measure $d\sigma[\mathbf{r}]$ as follows:

$$\begin{aligned}
W_i^{(1)}[\mathbf{r}] &= \int d\Lambda_{ts\mathbf{k}} \, :\mathrm{e}^{i\mathbf{kR}(t,s)}: \, k_i(t-s) = \\
&= \int d\Lambda_{ts\mathbf{k}} \, :e_0^{i\mathbf{kR}(t,s)}: \, k_i(t-s)\,, \\
W_{ij}^{(2)}[\mathbf{r}] &= \int d\Lambda_{ts\mathbf{k}} \, :\mathrm{e}^{i\mathbf{kR}(t,s)}: \, k_i\, k_j\,(t-s)^2 = \\
&= \int d\Lambda_{ts\mathbf{k}}\, k_i\, k_j\,(t-s)^2 + \\
&+ \int d\Lambda_{ts\mathbf{k}} \, :\mathrm{e}_2^{i\mathbf{kR}(t,s)}: \, k_i\, k_j\,(t-s)^2\,.
\end{aligned}$$

Therefore,

$$W_i^{(1)}[\mathbf{r}]\; W_i^{(1)}[\mathbf{r}] + W_{ii}^{(2)}[\mathbf{r}] = \int d\Lambda_{ts\mathbf{k}}\; \mathbf{k}^2\;(t-s)^2 + \,:Q[\mathbf{r}]:\,, \tag{55}$$

where

$$\begin{aligned}
:Q[\mathbf{r}]: &= \int d\Lambda_{ts\mathbf{k}} \int d\Lambda_{uv\mathbf{q}}\, \mathbf{kq}\,(t-s)\,(u-v)\; :\mathrm{e}_0^{i\mathbf{kR}(t,s)}::\mathrm{e}_0^{i\mathbf{qR}(u,v)}: \\
&+ \int d\Lambda_{ts\mathbf{k}}\; \mathbf{k}^2\,(t-s)^2\; :\mathrm{e}_2^{i\mathbf{kR}(t,s)}: \;.
\end{aligned}$$

Substituting (54) and (55) into (31) we obtain

$$\Phi_\xi(\alpha) = \Phi_\xi^0(\alpha) + \Delta\Phi_\xi(\alpha)\,,$$

where the Gaussian approximation is

$$\begin{aligned}
\Phi_\xi^0(\alpha) &= \frac{\alpha B_d}{\sqrt{8}\,\beta\, d} \iint\limits_{-\beta/2}^{\beta/2} dt\, ds\, \mathrm{e}^{-|t-s|} \int \frac{d\mathbf{k}}{|\mathbf{k}|^{d-1}}\, \mathrm{e}^{-\mathbf{k}^2 F(t-s)}\, \mathbf{k}^2\,(t-s)^2 = \\
&= \frac{\alpha_d}{6\sqrt{2\pi}} \int\limits_0^\infty dt\, \frac{t^2\; \mathrm{e}^{-t}}{F^{3/2}(t)}
\end{aligned} \tag{56}$$

so

$$m_0^*(\alpha) = m + \frac{\alpha_d}{3\sqrt{2\pi}} \int\limits_0^\infty dt\, \frac{t^2\; \mathrm{e}^{-t}}{F^{3/2}(t)}\,. \tag{57}$$

The remaining non-Gaussian correction is given by

$$\Delta\Phi_\xi(\alpha) = \lim_{\beta\to\infty} \frac{1}{\beta\, d} \frac{\mathcal{J}_\beta(\alpha)}{J_\beta(\alpha)}\,,$$

where a new PI is defined as follows

$$\mathcal{J}_\beta(\alpha) = \langle \mathrm{e}^{:W_{\rm int}[\mathbf{r}]:} :Q[\mathbf{r}]:\rangle\,. \tag{58}$$

Note, for a weak coupling $J_\beta(\alpha) \propto 1 + O(\alpha^2)$ while $\mathcal{J}_\beta(\alpha) \propto O(\alpha)$.

7. GAUSSIAN LEADING-ORDER ENERGY AND MASS

Now we consider only the Gaussian leading terms for the self-energy and effective mass of the polaron. In doing so, we take the following approximations:

$$J_\beta(\alpha) = 1\,, \qquad \mathcal{J}_\beta(\alpha) = 0\,.$$

Thus, we obtain $E(\alpha) = E_0(\alpha)$ and $m^*(\alpha) = m_0^*(\alpha)$, where $E_0(\alpha)$ and $m_0^*(\alpha)$ have been defined in (51) and (57), respectively.

The following remarks are in order to conclude the Gaussian approximation.

i. According to (53), the Gaussian approximation $E_o(\alpha)$ gives an upper bound to the exact polaron GSE, which slightly improves Feynman's celebrated estimate.

ii. As $d \to \infty$ our $E_0(\alpha)$ and $m_0^*(\alpha)$ tend to the exact GSE and EM, respectively, because $\alpha_d \propto O(d^{-3/2})$ suppresses any non-Gaussian correction.

iii. To our knowledge, equivalent forms of integral equations (49) have been previously obtained, e.g., in [19] for $d = 3$, by considering the stationarity condition for extension of Feynman's variational approach to general quadratic trial actions. This idea was independently utilized also in [18]. Note, that the same equations govern the leading term of the $1/d$-expansion scheme applied to the polaron model [55]. We derive exact analytic solutions to (49) in the weak- and strong-coupling limits as follows:

$$F(t) = \begin{cases} t/2 - \alpha_d\, f_1(t) + \alpha_d^2\, f_2(t) + O(\alpha_d)\,, & \alpha \to 0\,, \\ \left[1 - \exp\left(-v_\infty t\right)\right]/2v_\infty\,, \qquad v_\infty = 4\alpha_d^2/9\pi\,, & \alpha \to \infty\,. \end{cases} \tag{59}$$

Therefore, both the Gaussian leading-order term and the second-order non-Gaussian correction may be derived analytically for the weak- and strong-coupling limits. The resulting GSE and EM are in complete agreement with the exact data for $\alpha \ll 1$ and differ very slightly for $\alpha \gg 1$.

iv. For intermediate-coupling ($\alpha \propto 1$) equations (49) seem to admit no analytic solutions. Nevertheless, any strictly positive function can be used instead of $F(t)$ to derive an approximation to the GSE and EM, following the lines of the Gaussian approximation. The result, however, will in general be inferior to $E_0(\alpha)$. For example, Feynman's celebrated variational model can be recovered if one chooses a convex combination

$$F_2(t) = w_0 \frac{t}{2} + (1 - w_0) \frac{1 - \exp(-vt)}{2v}, \qquad 0 \le w_0 \le 1 \tag{60}$$

of the two known asymptotic solutions (59) instead of $F(t)$. The parameter w_0 corresponds to the contribution of the pure weak-coupling solution in this combination. The second term in the r.h.s of (60) corresponds to the strong-coupling contribution. Therefore, the stronger the interaction, the smaller the weight factor $w_0 = (w/v)^2$ should be. Substituting (60) into (51) and optimizing the result with respect to parameters $\{w, v\}$ one reproduces Feynman's upper

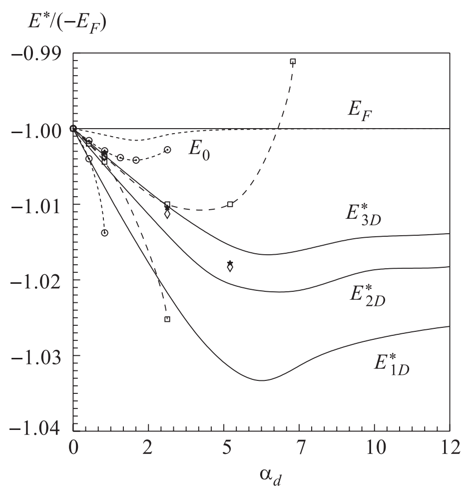

Fig. 1. Ground-state energy of the one-, two- and three-dimensional polaron normalized to the Feynman variational result as a function of the re-scaled electron-phonon coupling constant α_d. Due to the scaling feature, all Gaussian approximations to the GSE estimated in different spatial dimensions ($d = 1, 2, 3$) are represented by one curve versus the effective coupling α_d. The abscissa stands for all d-dimensional Feynman estimates. Taking into account the next-order non-Gaussian contribution splits this junction into separate curves in different dimensions. The marked solid curves depict our corrected result $E_2(\alpha)$ for $d = 1$, $d = 2$, and $d = 3$, respectively. For comparison some three-dimensional results are shown: circles correspond to the upper and lower bounds reported in [75], boxes — analogous bounds due to the Páde scheme [73], stars — result from [75], asterisks — the Monte-Carlo calculation [71], and rhombuses depict results due to the two-phonon perturbation method [50]

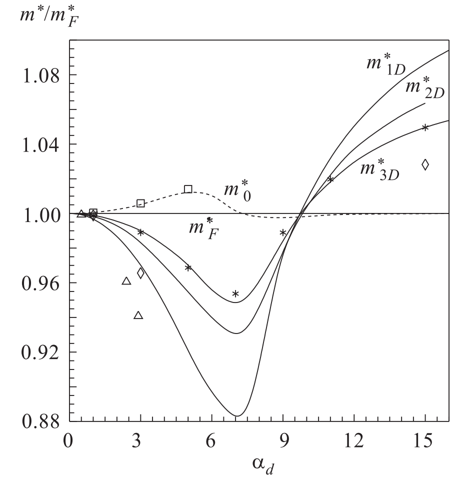

Fig. 2. Effective mass of the one-, two- and three-dimensional polaron normalized to the Feynman variational result as a function of the re-scaled electron-phonon coupling constant α_d. The notation is the same as for Figure 1. For comparison some three-dimensional results are shown: rhombuses and boxes denote the Monte Carlo data from [71] and [56]; stars correspond to the result from [75]; asterisks show the corrected Feynman result from [57]; and up (down) triangles depict lower (upper) bounds due to the Páde scheme [73]

bound to the GSE as follows:

$$E_{\rm Feyn}(\alpha) = \min_{v,w} \left\{ \frac{3\,(v-w)^2}{4\,v} - \right.$$

$$\left. - \frac{\alpha}{\sqrt{\pi}} \int\limits_0^\infty dt \frac{{\rm e}^{-t}}{\sqrt{tw^2/v^2 + (v^2-w^2)\,(1-\exp{(-vt)})/v^3}} \right\}.$$

The corresponding substitution of the optimized $F_2(t)$ into (57) results in Feynman's mass $m^*_F(\alpha)$. Note, however, that (60) is *not* a solution of equations (49).

v. An obvious improvement of the Feynman approximation can be obtained by increasing the number of strong-coupling components in (60)

$$F_N(t) = w_0 \frac{t}{2} + \sum_{i=1}^{N} w_i \frac{1-\exp{(-v_i t)}}{2v_i}, \qquad N \geq 2.$$

Optimization with $N = 2$, $N = 3$ and $N = 8$ reproduces the data obtained in [15], [16] and [17], respectively. The limiting case $N \to \infty$ leads, obviously, to the results of the general quadratic action [19].

vi. Exact analytic solutions to (49) feature the following scaling properties:

$$F^{[n]}(\alpha_m, t) = F^{[m]}(\alpha_n, t)\,, \qquad \widetilde{\Sigma}^{[n]}(\alpha_m, k) = \widetilde{\Sigma}^{[m]}(\alpha_n, k), \qquad n, m > 1\,,$$

where different spatial-dimension numbers are given in the square brackets. This results in the scaling relations for the GSE and EM, too. In particular,

$$E_0^{[1]}(\alpha) = \frac{1}{3}\,E_0^{[3]}(3\alpha), \qquad m_0^{*\,[1]}(\alpha) = m_0^{*\,[3]}(3\alpha). \tag{61}$$

Note, this has been observed earlier in [66] for the special case of Feynman's approximation. The scaling feature allows us to depict all one-, two- and three-dimensional Gaussian leading-order terms by only one curve in Figs. 1 and 2. To show the deviation of all results from Feynman's more clearly, we have plotted them normalized with respect to the corresponding Feynman results. Stress also that taking into account non-Gaussian corrections to the GSE and EM breaks the scaling feature.

8. NEXT-TO-GAUSSIAN APPROXIMATION

The Gaussian leading-order terms $E_0(\alpha)$ and $m_0^*(\alpha)$ approximate well the exact GSE and EM of the polaron. The higher the spatial dimensions, the better the approximations. Nevertheless, according to (50), the contribution of the multiplicators $J_\beta(\alpha)$ and $\mathcal{J}_\beta(\alpha)$ should be estimated more precisely to check the accuracy of the obtained Gaussian approximations in the physically meaningful dimensions $1 \le d \leqslant 3$.

To evaluate (52) and (58), we use the following expansion schemes:

$$\begin{aligned} J_\beta(\alpha) &= \langle \mathrm{e}^{:W_{\rm int}[\mathbf{r}]:} \rangle = \sum_{n=2}^{\infty} V_n\,, \qquad (62)\\ \mathcal{J}_\beta(\alpha) &= \langle \mathrm{e}^{:W_{\rm int}[\mathbf{r}]:}\ :Q[\mathbf{r}]:\rangle = \sum_{j=0}^{\infty} \mathcal{V}_j\,, \end{aligned}$$

where the higher-order non-Gaussian terms are

$$V_n = \frac{1}{n!}\langle :W_{\rm int}[\mathbf{r}]:^n\rangle\,, \qquad \mathcal{V}_j = \frac{1}{j!}\langle :W_{\rm int}[\mathbf{r}]:^j :Q[\mathbf{r}]:\rangle\,, \qquad n \ge 2\,, \quad j \ge 0\,.$$

Note, $V_1 = 0$ due to normal ordering. Besides, (62) are not the conventional perturbation series in the coupling constant because α enters into each term in a more complicated way by involving the function $F(t)$ which depends on α, too.

We restrict ourselves to estimating only the second-order (over $:W_{\rm int}[\mathbf{r}]:$) non-Gaussian corrections to the GSE and EM as follows

$$\Delta E_2(\alpha) = -\lim_{\beta\to\infty}\frac{1}{\beta}\,V_2(\alpha)\,, \qquad \Delta m_2^*(\alpha) = \lim_{\beta\to\infty}\frac{1}{\beta\, d}\,\{\mathcal{V}_0(\alpha)+\mathcal{V}_1(\alpha)\}\ .$$

Appropriate analyses performed for the weak- and strong-coupling regimes have indicated that taking into account higher-order corrections ($n \geqslant 3$) results in only slight improvement over the obtained estimate. We suppose that this picture remains valid in the intermediate region of α, too.

Omitting the details of calculations we write the final results for the second-order non-Gaussian contributions to the GSE and EM as follows:

$$\Delta E_2(\alpha) = -\frac{\alpha_d^2\, d^2\,\Gamma[d/2]}{9\pi^{d/2+2}\,B_d}\int\limits_0^1 d\eta(1-\eta^2)^{\frac{d-3}{2}}\int\limits_0^\infty dz_1\int\limits_{z_1}^\infty dz_2\int\limits_{z_2}^\infty dz_3\left\{\mathrm{e}^{-z_3-|z_1-z_2|}\times\right.$$
$$\times\left(\frac{1}{[4F(z_1)F(z_2-z_3)-\eta^2\Xi^2]^{1/2}}-\frac{1}{[4F(z_1)F(z_2-z_3)]^{1/2}}-\right.$$
$$\left.\left.-\frac{\eta^2}{2}\frac{\Xi^2(z_1,z_2,z_3,0)}{[4F(z_1)F(z_2-z_3)]^{3/2}}\right)+(z_1\leftrightarrow z_2)+(z_1\leftrightarrow z_3)\right\},$$

$$\Delta m_2^*(\alpha) = \frac{2\,\alpha_d^2\, d\,\Gamma[d/2]}{9\pi^{d/2+2}\,B_d}\int\limits_0^1 d\eta(1-\eta^2)^{\frac{d-3}{2}}\int\limits_0^\infty dz_1\int\limits_{z_1}^\infty dz_2\int\limits_{z_2}^\infty dz_3\left\{\mathrm{e}^{-z_3-|z_1-z_2|}\times\right.$$
$$\times\Bigg[\ [F(z_2-z_3)z_1^2+F(z_1)(z_2-z_3)^2]\left(\frac{1}{[4F(z_1)F(z_2-z_3)-\eta^2\Xi^2]^{3/2}}-\right.$$
$$\left.-\frac{1}{[4F(z_1)F(z_2-z_3)]^{3/2}}-\frac{3\eta^2}{2}\frac{\Xi^2(z_1,z_2,z_3,0)}{[4F(z_1)F(z_2-z_3)]^{5/2}}\right)+$$
$$+\eta^2\, z_1\,(z_2-z_3)\,\Xi(z_1,z_2,z_3,0)\left(\frac{1}{[4F(z_1)F(z_2-z_3)-\eta^2\Xi^2]^{3/2}}-\right.$$
$$\left.\left.-\frac{1}{[4F(z_1)F(z_2-z_3)]^{3/2}}\right)\Bigg]+(z_1\leftrightarrow z_2)+(z_1\leftrightarrow z_3)\right\},$$

where a four-point correlation function Ξ has been introduced:

$$\Xi(t,s,u,v)\ =\ F(t-u)+F(s-v)-F(s-u)-F(t-v)\,.$$

Finally, combining both the Gaussian leading-order and the second-order non-Gaussian contribution, we estimate the polaron GSE and EM as follows:

$$\begin{aligned} E_2(\alpha) &= E_0(\alpha) + \Delta E_2(\alpha)\,, \\ m_2^*(\alpha) &= m_0^*(\alpha) + \Delta m_2^*(\alpha)\,. \end{aligned} \tag{63}$$

9. EXACT AND NUMERICAL RESULTS

The Gaussian (leading-order) and the next-to-Gaussian contributions to the GSE and EM have been derived analytically for the weak- and strong-coupling limits. For intermediate coupling, we have calculated these quantities numerically. The obtained intermediate-coupling results for the polaron GSE and EM $d = 1, 2$ and $d = 3$ are represented in Figures 1 and 2, respectively, in comparison with several known data.

Weak-Coupling Limit

The exact results by fourth-order perturbation theory are as follows:

$$E_{4th-PT}(\alpha) = \begin{cases} -\alpha - 0.06066\,\alpha^2 - O(\alpha^3)\,, & d = 1\,, \\ -\alpha - 0.06397\,\alpha^2 - O(\alpha^3)\,, & d = 2\,, \\ -\alpha - 0.01592\,\alpha^2 - O(\alpha^3)\,, & d = 3 \end{cases}$$

for the GSE [38, 39, 67] and

$$m^*_{4th-PT}(\alpha) = \begin{cases} 1 + (1/2)\,\alpha + 0.1919417\,\alpha^2 + O(\alpha^3)\,, & d = 1\,, \\ 1 + (\pi/8)\,\alpha + 0.1272348\,\alpha^2 + O(\alpha^3)\,, & d = 2\,, \\ 1 + (1/6)\,\alpha + 0.0236276\,\alpha^2 + O(\alpha^3)\,, & d = 3 \end{cases}$$

for the EM [38, 59, 66, 68].

The coefficient of the α^2 term of the Feynman polaron mass overestimates the exact value by 7.8 and 4.5 per cent for $d = 2$ and $d = 3$. The next correction to the Feynman result [57] for $d = 3$ fits the correct behaviour.

Knowing explicitly the weak-coupling behaviour of $F(t)$ we derive the leading-order Gaussian contributions. Considering the next-to-Gaussian corrections, it is sufficient to use the asymptotic solution $F(t) = t/2 - \alpha_d f_1(t)$ because the neglected terms $O(\alpha_d^2)$ will generate corrections proportional to $O(\alpha_d^3)$. We obtain

$$\begin{aligned} E_2(\alpha) &= \begin{cases} -\alpha - 0.060660\,\alpha^2 + O(\alpha^3)\,, & d = 1\,, \\ -\alpha - 0.063974\,\alpha^2 + O(\alpha^3)\,, & d = 2\,, \\ -\alpha - 0.015919\,\alpha^2 + O(\alpha^3)\,, & d = 3\,, \end{cases} \\ m_2^*(\alpha) &= \begin{cases} 1 + (1/2)\,\alpha + 0.191941738\,\alpha^2 + O(\alpha^3)\,, & d = 1\,, \\ 1 + (\pi/8)\,\alpha + 0.127234835\,\alpha^2 + O(\alpha^3)\,, & d = 2\,, \\ 1 + (1/6)\,\alpha + 0.023627630\,\alpha^2 + O(\alpha^3)\,, & d = 3\,. \end{cases} \end{aligned} \tag{64}$$

Our final results for the weak-coupling polaron GSE and EM are in complete agreement with previously known data obtained within the perturbation [59,66,67] and $1/d$-expansion [69] methods.

Strong-Coupling Limit

It is known that in the strong-coupling polaron regime the polaron is described well by the Pekar Produkt-Ansatz implying that electron excitations are governed by a potential adopted to the ground state. The wave function corresponding to the ground state has rather exponential function behaviour than a Gaussian shape. Therefore, one should not expect to see exact coincidence of the GGR result and extensive numerical data obtained in [12, 48, 53, 60]:

$$
\begin{aligned}
E_{\rm Adiab}(\alpha) &= \begin{cases} -0.33203\,\alpha^2 + O(1)\,, & d=1\,,\\ -0.4047\,\alpha^2 + O(1)\,, & d=2\,,\\ -0.108513\,\alpha^2 + O(1)\,, & d=3\,,\end{cases}\\
m^*_{\rm Adiab}(\alpha) &= \begin{cases} 2.1254\,\alpha^4 + O(1)\,, & d=1\,,\\ 0.7328\,\alpha^4 + O(1)\,, & d=2\,,\\ 0.022702\,\alpha^4 + O(1)\,, & d=3\,.\end{cases}
\end{aligned}
$$

Note, the exact solution to the one-dimensional Pekar problem (strong-coupling regime) has been found in [23] which resulted in $E(\alpha) = -\alpha^2/3$ and $m^*(\alpha) = -32\alpha^4/15$.

As α becomes very large, $F(t)$ behaves like that in (59). By using this asymptotic solution, we derive

$$
\begin{aligned}
E_2(\alpha) &= \begin{cases} -0.236926\,\alpha^2 + O(1)\,, & d=1\,,\\ -0.400538\,\alpha^2 + O(1)\,, & d=2\,,\\ -0.108433\,\alpha^2 + O(1)\,, & d=3\,,\end{cases}\\
m^*_2(\alpha) &= \begin{cases} 1.858065\,\alpha^4 + O(1)\,, & d=1\,,\\ 0.681878\,\alpha^4 + O(1)\,, & d=2\,,\\ 0.021656\,\alpha^4 + O(1)\,, & d=3\,.\end{cases}
\end{aligned}
\tag{65}
$$

We observe that the leading-order Gaussian GSE and EM as $\alpha \to \infty$ behave similarly to the corresponding results obtainable within the Feynman and $1/d$-expansion methods. These results underestimate the corresponding adiabatic ones [48, 53]. This is probably due to the fact that for increasing α the nonlocal Coulomb-like polaron self-interaction is less well approximated by an oscillator-type term used for our leading-order mass. Hence, higher-order non-Gaussian corrections are required to fill this gap.

Intermediate-Coupling Range

For intermediate coupling we have solved equations (49) numerically by means of an iterative procedure accepting (60) as the first approximation. We have checked that after the fourth and fifth iteration steps with a sufficiently large integration domain the final results did not change within the given accuracy.

The obtained intermediate-coupling results for the Gaussian leading-order GSE and EM as well as for the corrected values $E_2(\alpha)$ and $m_2^*(\alpha)$ in one, two and three dimensions are presented in Figures 1 and 2, respectively, in comparison with several known data. The scaling feature (61) for $m_0^*(\alpha)$ allows us to depict one-, two- and three-dimensional Gaussian leading-order masses by only one curve in Fig. 2. In doing so, we plot, for example, our two-dimensional results scaled actually by $\alpha_d/\alpha = 3\pi/4$ times in the horizontal (α-axis) direction. Data cited as Feynman's have been re-obtained by us to cover more data sets. To show the deviation of all results from the Feynman ones more clearly, we have plotted them normalized to the Feynman data. The results of the fourth-order perturbation theory and the adiabatic strong-coupling model extrapolated to the intermediate-coupling region $1 < \alpha_d < 10$ have not been plotted due to their relative large deviations from Feynman's result. Taking into account non-Gaussian corrections breaks the scaling feature (61) and the deviations of the corrected results from Feynman's estimates (and from Gaussian, too) for $d = 1$ is larger than for $d = 3$. This is because α_d vanishes as $d \to \infty$. In lower spatial dimensions non-Gaussian corrections play more important role.

Comparing our intermediate-coupling results to that obtained within other approaches, we note that our method works well in the whole range of α for all spatial dimensions $d \geq 1$. It does not require extensive numerical calculations on supercomputers [70–72], but is able to give more reliable and consistent results rather quickly.

Comparing to another type of approaches characterized by constructing different interpolation algorithms [73, 74], our approach does not suffer any singularity and hypersensitivity intrinsic to these algorithms.

In conclusion, we have represented the generalized Gaussian representation method to evaluate a wide class of path integrals arising in various fields of modern theoretical physics. This method is a non-variational path-integral approach, whose leading order already takes care of all Gaussian fluctuations and higher orders correct systematically for non-Gaussian contributions. As a particular application of this method, we have considered the Fröhlich–Feynman polaron model at arbitrary value of the electron-phonon coupling $\alpha \geq 0$ by extending it into different ($d \geq 1$) spatial dimensions.

Considering the polaron quasi-particle characteristics, we have given several definitions of the polaron EM based on different physical principles, but independent of the specific approximate method. We have shown that definitions based on the polaron internal dynamics do not coincide, in general, with those obtained by using a responce principle to external sources (forces). They are equivalent either in the weak-coupling regime or, in case of some variational optimizations having in fact, the same perturbation nature.

Applied to the polaron problem in statistical physics, the GGR method allows one to estimate main quasi-particle characteristics of the polaron with accuracy superior to other methods, improving, e.g., the Feynman variational estimations. We have calculated the ground-state energy and the effective mass of the polaron in all the weak-, strong- and intermediate-coupling regimes. For explicit results we concentrate on the physically relevant cases of $d = 1$, $d = 2$, and $d = 3$. In the weak-coupling limit we have obtained exact analytic answers while a systematic iteration estimation has been developed to get a fast converging series to the exact results for the strong-coupling regime. By calculating the next-to-leading non-Gaussian corrections to both the GSE and EM, we have found that these corrections are rather small for an arbitrary value of α in $d = 1$, $d = 2$, and $d = 3$, and higher orders can result only in a tiny improvement. Therefore, we believe that the obtained results are sufficiently close to the exact polaronic characteristics. This can be verified also by comparing our results with the recent numerical data due to extensive Monte Carlo calculations for the polaron GSE ($d = 3$) performed in [71, 72]. Our results lie very close to Monte Carlo estimates wherever the latter is available.

Besides, we have shown that the GGR can serve as a source of various approximation techniques. In particular, the Feynman variational method is readily obtained when a simple trial function is substituted by the exact solution derived from the integral equation governing the GGR method. Other generalizations of the Feynman methods are also obtainable as particular cases of the general Gaussian approximation. The estimated Gaussian self-energy improves, as it can be expected by the very construction, the Feynman estimate through the entire range of α and belongs to the lowest *upper bounds* available at present. The corresponding estimation of the Gaussian effective mass has also been performed for arbitrary coupling in one, two and three dimensions. Quantitatively, the Gaussian GSE improves the corresponding Feynman estimate not too much; the deviation is slightly higher for the effective mass. This difference disappears as strong coupling tends to infinity, which proves once again the common nature of both the methods.

Discussing on our method we would like to point out that still there is room for diversification and improvement. Being a nonvariational approach, the GGR method can deal with non-Hermitean functionals and, therefore, may be successfully applied to other related problems such as the magneto-polaron, the bi-polaron or the spin-polaron. Another interesting item is to reformulate the method by using Wiener-type stochastic integration «measure» rather than Feynman «paths». This may allow one to use a powerful mathematical technique developed in this area. And, specially for $\alpha \gg 1$ our method can be modified to take into account more efficiently higher-order non-Gaussian terms.

Acknowledgments. We are indebted to H. Leschke, N.M. Plakida and V.B. Priezzhev for several useful discussions.

APPENDIX A

Consider a general functional

$$\mathrm{e}^{-\beta\widetilde{\Phi}(\alpha,\mathbf{u}^2,\lambda)} = N\int_{\mathbf{r}(0)=\mathbf{0}}^{\mathbf{r}(\beta)=\mathbf{0}}\delta\mathbf{r}\exp\Bigg\{-S_0[\mathbf{r}] + \iint_0^\beta dtds\, V\left[\mathbf{r}(t)-\mathbf{r}(s)-\mathbf{u}(t-s)\left(1-\lambda\frac{t+s}{\beta}\right)\right]\Bigg\}.$$

Obviously, function $\widetilde{\Phi}(\alpha,\mathbf{u}^2,\lambda)$ is related to $\Phi(\alpha,\xi)$ and $\Psi(\alpha,\xi)$ as follows

$$\begin{aligned}\Phi(\alpha,\xi) &= \widetilde{\Phi}(\alpha,\xi,0)\,, \qquad \Psi(\alpha,\xi)=\widetilde{\Phi}(\alpha,\xi,1)\,, \qquad \xi=\mathbf{u}^2\,,\\ \Phi_\xi(\alpha,\xi) &= \widetilde{\Phi}'(\alpha,\xi,0)\,, \qquad \Psi_\xi(\alpha,\xi)=\widetilde{\Phi}'(\alpha,\xi,1)\,.\end{aligned}$$

By the very definition it takes place

$$\Phi(\alpha,0)=\Psi(\alpha,0)\,.$$

The first part of $\widetilde{\Phi}'(\alpha,0,\lambda)$ is proportional to

$$\iint_0^\beta dtds\, V_1(t-s)(t-s)^2\left(1-\lambda\frac{t+s}{\beta}\right)^2 = 2\int_0^\beta ds\, s^2\, V_1(s)\int_s^\beta dt\left(1-\lambda\frac{2t-s}{\beta}\right)^2. \tag{66}$$

For $\beta\to\infty$ (66) becomes

$$2\beta\int_0^\beta ds\, s^2\, V_1(s)\cdot\int_0^1 dx\,(1-2\lambda x)^2 = 2\beta\left((1-\lambda)^2+\frac{\lambda^2}{3}\right)\int_0^\beta ds\, s^2\, V_1(s)\,.$$

An analogous calculation takes place for the second part of $\widetilde{\Phi}'(\alpha,\mathbf{u}^2,\lambda)$ and it results in

$$\iiiint_0^\beta dtdsdxdy\, V_2(t,s,x,y)(t-s)(x-y)\left(1-\lambda\frac{t+s}{\beta}\right)\left(1-\lambda\frac{x+y}{\beta}\right) =$$

$$= 2\beta\left((1-\lambda)^2+\frac{\lambda^2}{3}\right)\frac{1}{\beta}\iiiint_0^\beta dtdsdxdy\, V_2(t,s,x,y)(t-s)(x-y). \tag{67}$$

In (66) and (67) we have taken into account that functions $V_1(t,s)$ and $V_2(t,s,x,y)$ depend only on the absolute differences of their arguments. Therefore, we find for $\beta \to \infty$

$$\widetilde{\Phi}_\xi(\alpha,\lambda) = \widetilde{\Phi}'(\alpha,0,\lambda) = \beta\left((1-\lambda)^2 + \frac{\lambda^2}{3}\right) C(\alpha) + O(1)\,.$$

Note, function $C(\alpha)$ is finite and behaves $C(\alpha) \sim \alpha$ as $\alpha \to 0$. In particular,

$$\widetilde{\Phi}'(\alpha,0,0) = \beta C(\alpha)\,, \qquad \widetilde{\Phi}'(\alpha,0,1) = \frac{1}{3}\beta C(\alpha)\,.$$

In other words,

$$\Phi_\xi(\alpha,0) = 3\,\Psi_\xi(\alpha,0)\,.$$

APPENDIX B

According to (8), for large β we have

$$D_0(T,t) - D_0(T,s) = \begin{cases} 0 & \text{if} \quad T < t,s\,, \\ t-s & \text{if} \quad t,s < T\,, \\ T-s & \text{if} \quad s < T < t\,, \\ -T+t & \text{if} \quad t < T < s\,. \end{cases}$$

The following relations take place

$$\frac{d}{dt}D_0(t,s) = \frac{1}{2} - \frac{1}{2}\,\mathrm{sign}\,(t-s) - \frac{s}{\beta}, \quad \frac{d}{ds}D_0(t,s) = \frac{1}{2} + \frac{1}{2}\,\mathrm{sign}\,(t-s) - \frac{t}{\beta},$$

$$\frac{d^2}{dsdt}D_0(t,s) = \delta(t-s) - \frac{1}{\beta},$$

$$\int\limits_0^z ds\,D_0(t,s) = \frac{1}{2}(z-t)D_0(z,t) + \frac{z}{2}\,a(t), \quad a(t) = t\left(1 - \frac{t}{\beta}\right),$$

$$\int\limits_0^\beta dz\,a(z) = \frac{\beta^2}{6}, \quad \int\limits_0^\beta dz\,D_0(z,t) = \frac{\beta}{2}\,a(t), \quad \iint\limits_0^\beta dtds\,D_0(t,s) = \frac{\beta^3}{12},$$

$$\int\limits_0^\beta dz[D_0(t,z) - D_0(s,z)]^2 = \frac{\beta}{3}[a(t)-a(s)]^2 + O(1),$$

$$\int_0^\beta dz[D_0(t,z)-D_0(s,z)][D_0(x,z)-D_0(y,z)] =$$

$$= \frac{\beta}{3}[a(t)-a(s)][a(x)-a(y)] + O(1),$$

$$\int_t^s dz\, a(z) = \frac{s}{2}\, a(s) - \frac{t}{2}\, a(t) + \frac{s^3-t^3}{6\beta}.$$

APPENDIX C

First, we note that

$$\int d\Lambda_{ts\mathbf{k}} :(\mathbf{kR})^2 := \frac{\lambda_d}{2} \iint_{-\beta/2}^{\beta/2} dt\, ds\, \Phi(t-s) \; :[\mathbf{r}(t)-\mathbf{r}(s)]^2:,$$

where

$$\Phi(t) = \frac{\exp(-|t|)}{F^{3/2}(t)}, \qquad \lambda_d = \frac{\alpha_d}{6\sqrt{2\pi}}, \qquad \alpha_d = \alpha\, \frac{3\pi^{d/2+1}}{d\,\Gamma(d/2)}\, B_d\,.$$

Then, in the limit $\beta \to \infty$ the constraint equation in (48) becomes

$$\iint_{-\infty}^{\infty} dt\, ds\, \left\{ :\mathbf{r}(t)\,[\mathbf{D}_0^{-1}(t-s) - \mathbf{D}^{-1}(t-s)]\,\mathbf{r}(s): + \right. \tag{68}$$
$$\left. + \lambda_d\, \Phi(t-s) \; :\mathbf{r}^2(t) - \mathbf{r}(t)\,\mathbf{r}(s): \right\} = 0\,.$$

Substituting the identity

$$\mathbf{r}^2(t) = \mathbf{r}(t) \int_{-\infty}^{\infty} dz\, \delta(z-t)\, \mathbf{r}(z)$$

into (68) and interchanging the variables $s \leftrightarrow z$ we obtain

$$\iint_{-\infty}^{\infty} dt\, ds \; :\mathbf{r}(t) \left\{ \mathbf{D}_0^{-1}(t-s) - \mathbf{D}^{-1}(t-s) + \right.$$
$$\left. + \lambda_d \left[\delta(t-s) \int_{-\infty}^{\infty} dz\, \Phi(z-t) - \Phi(t-s) \right] \right\} \mathbf{r}(s) := 0\,.$$

In other words,

$$D_0^{-1}(t-s) - D^{-1}(t-s) + \lambda_d \left[\delta(t-s) \int\limits_{-\infty}^{\infty} dz\, \Phi(z) - \Phi(t-s) \right] = 0\,. \qquad (69)$$

Going to the Fourier transform for (69) and taking into account (46) we obtain

$$k^2 - \widetilde{D}^{-1}(k) + \lambda_d \left[\widetilde{\Phi}(0) - \widetilde{\Phi}(k) \right] = 0 \quad \text{or} \quad \widetilde{D}(k) = \frac{1}{k^2 + \lambda_d \left[\widetilde{\Phi}(0) - \widetilde{\Phi}(k) \right]},$$

where

$$\widetilde{\Phi}(k) = \int\limits_{-\infty}^{\infty} dz\, \mathrm{e}^{ikz}\, \Phi(z) = 2 \int\limits_{0}^{\infty} dz\, \cos(kz)\, \frac{\exp(-z)}{F^{3/2}(z)}\,.$$

Introducing an auxiliary function

$$\widetilde{\Sigma}(k) = \frac{\lambda_d}{\alpha_d} \left[\widetilde{\Phi}(0) - \widetilde{\Phi}(k) \right] = \frac{1}{6\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} dz \left[1 - \mathrm{e}^{ikz} \right] \frac{\exp(-z)}{F^{3/2}(z)}$$

and performing the Fourier transform for (47) we obtain

$$F(t) = \frac{1}{2\,\pi} \int\limits_{-\infty}^{\infty} dk \left[1 - \mathrm{e}^{ikt} \right] \widetilde{D}(k)\,.$$

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