Electron self-trapping at quantum and classical critical points

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Abstract

Using Feynman path integral technique estimations of the ground state energy have been found for a conduction electron interacting with order parameter fluctuations near quantum critical points. In some cases only *singular* perturbation theory in the coupling constant emerges for the electron ground state energy. It is shown that an autolocalized state (quantum fluctuon) can be formed and its characteristics have been calculated depending on critical exponents for both weak and strong coupling regimes. The concept of fluctuon is considered also for the classical critical point (at finite temperatures) and the difference between quantum and classical cases has been investigated. It is shown that, whereas the quantum fluctuon energy is connected with a true boundary of the energy spectrum, for classical fluctuon it is just a saddle-point solution for the chemical potential in the exponential density of states fluctuation tail.

Key words: quantum critical point, dynamical scaling, electron autolocalization, energy band tails

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1 Introduction

The physics of quantum critical point (QCP) [1,2,3,4,5] is now a subject of growing interest. There is a solid experimental evidence of relevance of the QCP and related phenomena for ferroelectrics [6], high-temperature superconductors [7,8], Bose-Einstein condensed atoms in traps [9], itinerant electron magnets [10,11,12,13], heavy fermion compounds [14,15] and many other systems. Similar to classical critical points or second-order phase transitions, a scaling concept is of crucial importance near the QCP and universal critical exponents can be introduced, which determine all anomalous properties of the systems near QCP [2]. The universality means that the basic physics depends not on the details of a microscopic Hamiltonian but rather on space dimensionality, dispersion law of low-frequency and long-wavelength fluctuations of an order parameter and symmetry properties of their effective action. In contrast with classical phase transitions at finite temperatures thermodynamics of the QCP is essentially dependent on the *dynamical* critical exponents [1].

There is an interesting issue how these critical fluctuations can effect on the state of an excess charge carrier which appears as a result of doping, injection, photoexcitation, etc. One can consider for example the electron motion in a crystal near the ferroelectric quantum phase transition in virtual ferroelectrics such as $SrTiO_3$ or $KTaO_3$ under doping or pressure [6,16], or near quantum magnetic phase transition due to competing exchange interactions [2]. To our knowledge this problem has not been considered yet. One may speculate that a specific nature of the order parameter is not very essential for this problem; due to softness and long-range character of the critical fluctuations the effects of their interaction with the conduction electrons may be very strong.

In particular, we will see that a self-trapping (autolocalization) of the carrier proves possible, similar to a polaron formation in ionic crystals [17,18] or spin polarons ("ferrons") in magnetic semiconductors [19]. A general concept of the self-trapped electronic state due to interaction with order parameter fluctuations ("fluctuon") has been proposed many years ago by Krivoglaz [20]. It appeared, however, that his phenomenological approach is not applicable near the critical point where the fluctuon radius is smaller than the correlation length [21]. We have considered this case [21,22,23] using Feynman path integral variational approach developed him for the polaron problem [24,25]. Here we apply similar technique to consider the quantum case. It will be shown that the classical and quantum fluctuons are drastically different: if the latter can be considered as a specific quasiparticle the former one represents some quasilocalized state in the density of states tail. Apart from possible applications to condensed matter physics the problem under consideration gives a nontrivial example of the interaction of a fermion with a bosonic quantum field with anomalous scaling properties.

Whereas only the case of dispersionless Einstein phonon has been considered originally by Feynman, later this method has been used also to describe the interaction of electron with acoustic phonons [26,27]. We consider here a general case of fluctuations with arbitrary dynamics which can be, in particular, of dissipative type. The answers will be written in terms of some frequency momenta of the fluctuations. One can assume that the type of the fluctuation dynamics, being relevant, e.g., for transport phenomena is not essential for static characteristics such as autolocalization radius and energy; anyway, the method used by us gives a rigorous upper limit for the ground-state energy. Another difference (which is more important) is that the phonon field is Gaus-

sian whereas the Gaussian approximation for the fluctuations which we will use can be justified only for not too large coupling constants. It leads to some restrictions which will be derived separately for all cases under consideration.

The interaction of electrons with quantum critical fluctuations are intensively studied, especially in connection with high-temperature superconductivity and heavy-fermion systems (for review, see Refs. [7,8] and [14,15], respectively). Usually it is assumed that the coupling constant is small in comparison with the Fermi energy. Here we consider the case of *single* carrier where the character of electron states is essentially different; one can say that this difference is similar to the difference between localized and extended states for the disordered systems. As a next step, it would be interesting to consider degenerate gas of fluctuons where the Fermi energy is finite but small in comparison with the autolocalization energy which might be a subject of future investigations.

The paper is organized as follows. In Section 2 we overview general formalism for solving the problem posed. In the present paper we consider the case of not too large coupling constant, where the problem can be considered in Gaussian approximation for the interaction with the fluctuations; explicit criteria are presented below. The quantum case (zero temperature) is considered in Section 3. Using the scaling properties of the fluctuation spectral density (Subsection 3.1) we construct regular perturbative expansion of the energy in the coupling constant (weak-coupling regime, Subsection 3.2) as well as singular perturbative expansion in strong coupling regime (Subsection 3.3). The very existence of the regular perturbative regime depends crucially on the value of dynamical critical exponent z and anomalous dimension d. The problem of fluctuon at classical critical point (finite temperature) is treated in Section 4. We solve the problem by both Feynman variational method (Subsection 4.1)

and using Green function technique with vertex corrections via Ward identity (Subsection 4.2). The similarity of the results as regards dependencies of the density of states on the energy and coupling constant justifies the variational approach.

2 Formulation of the problem using Feynman path integral

For simplicity, we will consider the case of a scalar order-parameter acting only on the orbital motion of the electron and not on its spin (for example it may be the QCP in ferroelectrics). Then, in continuum approximation, the Hamiltonian of the system consisting of the electron and the order-parameter field can be written in a simple form

$$\mathcal{H} = \mathcal{H}_f(\varphi) + \mathcal{H}_e(\mathbf{r},\varphi),\ \mathcal{H}_e(\mathbf{r},\varphi) = -\frac{1}{2}\nabla_{\mathbf{r}}^2 - g\varphi(\mathbf{r}) \tag{1}$$

where we have chosen the units $\hbar = m = 1$, m is the electron effective mass, $\mathbf{r}$ is the electron coordinate, $\varphi(\mathbf{r})$ is the quantum order-parameter field with its own Hamiltonian $\mathcal{H}_f(\varphi)$ and g is the coupling constant. The partition function of the whole system may be transformed to

$$Z = \mathrm{Tr} e^{-\beta\mathcal{H}_f(\varphi)-\beta\mathcal{H}_e(\mathbf{r},\varphi)} = Z_f \left\langle \mathrm{Tr}_{\mathbf{r}} T_\tau \exp\left[-\int_0^\beta \mathcal{H}_e(\mathbf{r},\varphi(\mathbf{r},\tau))\, d\tau\right]\right\rangle_f \tag{2}$$

where $Z_f = \mathrm{Tr}_\varphi e^{-\beta\mathcal{H}_f(\varphi)}$ is the partition function of the field, $\varphi(\mathbf{r},\tau) = e^{\tau\mathcal{H}_f(\varphi)}\varphi(\mathbf{r})\, e^{-\tau\mathcal{H}_f(\varphi)}$ and

$$\langle\mathcal{A}(\varphi)\rangle_f = \frac{1}{Z_f}\mathrm{Tr}_\varphi e^{-\beta\mathcal{H}_f(\varphi)}\mathcal{A}(\varphi) \tag{3}$$

is the average over the field states. Using Feynman path-integral approach [25,28,29] and taking average over φ yields for the electron-only free energy

$$\mathcal{F} = -\frac{1}{\beta}\left(\ln Z - \ln Z_f\right) = -\frac{1}{\beta}\ln\int_{\mathbf{r}(0)=\mathbf{r}(\beta)} e^{-\mathcal{S}}\mathcal{D}\left[\mathbf{r}\left(\tau\right)\right], \tag{4}$$

where $\mathcal{S}_0 + \mathcal{S}_{int}$ is the effective action,

$$\begin{aligned}\mathcal{S}_0 &= \frac{1}{2}\int_0^\beta \left[\dot{\mathbf{r}}\left(\tau\right)\right]^2 d\tau \\ \mathcal{S}_{int} &= -\sum_{m=2}^{\infty}\frac{g^m}{m!}\int_0^\beta ... \int_0^\beta \mathcal{K}_m\left(\mathbf{r}\left(\tau_1\right),\tau_1;...;\mathbf{r}\left(\tau_m\right),\tau_m\right)d\tau_1...d\tau_m\end{aligned} \tag{5}$$

and $\mathcal{K}_m\left(\mathbf{r}_1,\tau_1;...;\mathbf{r}_m,\tau_m\right)$ is the m-th cumulant correlators, defined recursively by

$$\begin{aligned}\mathcal{K}_1\left(\mathbf{r}_1,\tau_1\right) &= \left\langle\varphi\left(\mathbf{r}_1,\tau_1\right)\right\rangle_f, \\ \mathcal{K}_2\left(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2\right) &= \left\langle T_\tau\left[\varphi\left(\mathbf{r}_1,\tau_1\right)\varphi\left(\mathbf{r}_2,\tau_2\right)\right]\right\rangle_f - \mathcal{K}_1\left(\mathbf{r}_1,\tau_1\right)\mathcal{K}_1\left(\mathbf{r}_2,\tau_2\right),...\end{aligned} \tag{6}$$

etc. Further we will consider only the cases where $\mathcal{K}_1 = 0$.

To estimate $\mathcal{F}$ and electron energy $\mathcal{E} = \lim_{\beta\to\infty}\mathcal{F}$ we use the same trial action as was proposed by Feynman for the polaron problem [24] $\mathcal{S}_t = \mathcal{S}_0 + \mathcal{S}_{pot}$ where

$$\mathcal{S}_{pot} = \frac{C}{2}\int_0^\beta\int_0^\beta\left[\mathbf{r}\left(\tau\right)-\mathbf{r}\left(\sigma\right)\right]^2 e^{-w|\tau-\sigma|}d\tau d\sigma, \tag{7}$$

C and w being trial parameters. Then the Peierls-Feynman-Bogoliubov inequality reads

$$\mathcal{F} \le \mathcal{F}_t + \frac{1}{\beta}\left\langle\mathcal{S}_{int}-\mathcal{S}_{pot}\right\rangle_t \tag{8}$$

where

$$\mathcal{F}_t = -\frac{1}{\beta}\ln\int_{\mathbf{r}(0)=\mathbf{r}(\beta)} e^{-\mathcal{S}_t}\mathcal{D}\left[\mathbf{r}\left(\tau\right)\right],\ \left\langle\mathcal{A}\right\rangle_t = \int_{\mathbf{r}(0)=\mathbf{r}(\beta)}\mathcal{A}\left[\mathbf{r}\left(\tau\right)\right]e^{\beta\mathcal{F}_t-\mathcal{S}_t}\mathcal{D}\left[\mathbf{r}\left(\tau\right)\right], \tag{9}$$

which is equivalent to

$$\mathcal{F} \leq \mathcal{F}_t - \frac{C}{2\beta}\int_0^\beta \int_0^\beta \left\langle \left[\mathbf{r}\left(\tau\right)-\mathbf{r}\left(\sigma\right)\right]^2\right\rangle_t e^{-w|\tau-\sigma|}d\tau d\sigma$$
$$-\sum_{m=2}^{\infty}\frac{g^m}{m!\beta}\int_0^\beta ...\int_0^\beta \left\langle \mathcal{K}_m\left(\mathbf{r}\left(\tau_1\right),\tau_1;...;\mathbf{r}\left(\tau_m\right),\tau_m\right)\right\rangle_t \prod_{j=1}^{m} d\tau_j \qquad (10)$$

To proceed, we will pass to the Fourier transforms

$$\left\langle \mathcal{K}_m\left(\mathbf{r}\left(\tau_1\right),\tau_1;...;\mathbf{r}\left(\tau_m\right),\tau_m\right)\right\rangle_t$$
$$= \int ...\int \beta^{1-m}\sum_{\omega_1...\omega_{m-1}} \mathcal{K}_m\left(\mathbf{K}_1,i\omega_1;...;\mathbf{K}_{m-1},i\omega_{m-1}\right)\exp\left[i\sum_{j=1}^{m-1}\omega_j\left(\tau_j-\tau_m\right)\right]$$
$$\times\left\langle \exp\left[i\sum_{j=1}^{m-1}\mathbf{K}_j\cdot\left[\mathbf{r}\left(\tau_j\right)-\mathbf{r}\left(\tau_m\right)\right]\right]\right\rangle_t \prod_{j=1}^{m-1}\frac{\Omega_D d^D K_j}{\left(2\pi\right)^D}, \qquad (11)$$

where $\mathbf{K}_j$ are the wave-vectors, Ω_D is the unit lattice cell volume, and ω_j are the bosonic Matsubara frequencies. For the Gaussian trial action $\mathcal{S}_t$ one has

$$\left\langle \exp\left\{i\sum_{j=1}^{m-1}\mathbf{K}_j\cdot\left[\mathbf{r}\left(\tau_j\right)-\mathbf{r}\left(\tau_m\right)\right]\right\}\right\rangle_t = \exp\left[-\frac{1}{2}\sum_{j,k=1}^{m-1} f\left(\tau_j-\tau_m,\tau_k-\tau_m\right)\mathbf{K}_j\cdot\mathbf{K}_k\right], \qquad (12)$$

where

$$f\left(\tau_j-\tau_m,\tau_k-\tau_m\right)=\frac{1}{D}\left\langle\left[\mathbf{r}\left(\tau_j\right)-\mathbf{r}\left(\tau_m\right)\right]\cdot\left[\mathbf{r}\left(\tau_k\right)-\mathbf{r}\left(\tau_m\right)\right]\right\rangle_t =$$
$$\frac{1}{2D}\left\{\left\langle\left[\mathbf{r}\left(\tau_j\right)-\mathbf{r}\left(\tau_m\right)\right]^2\right\rangle_t+\left\langle\left[\mathbf{r}\left(\tau_k\right)-\mathbf{r}\left(\tau_m\right)\right]^2\right\rangle_t-\left\langle\left[\mathbf{r}\left(\tau_j\right)-\mathbf{r}\left(\tau_k\right)\right]^2\right\rangle_t\right\} \qquad (13)$$

Substituting Eqs.(17), (11)-(13) into Eq.(10) we find an exact upper-bound estimation for the free energy as a series in the coupling constant

$$\mathcal{F} \leq \mathcal{F}_t - \frac{1}{\beta}\left\langle \mathcal{S}_{pot}\right\rangle -$$
$$\sum_{m=2}^{\infty}\frac{g^m}{\beta^m m!}\int\int_0^\beta ....\int\int_0^\beta \sum_{\omega_1...\omega_{m-1}} \mathcal{K}_m\left(\mathbf{K}_1,i\omega_1;..;\mathbf{K}_{m-1},i\omega_{m-1}\right)\times$$
$$\exp\left\{i\sum_{j=1}^{m-1}\omega_j\left(\tau_j-\tau_m\right)-\frac{1}{2}\sum_{j,k=1}^{m-1} f\left(\tau_j-\tau_m,\tau_k-\tau_m\right)\mathbf{K}_j\cdot\mathbf{K}_k\right\}\times$$
$$\prod_{j=1}^{m-1}\frac{\Omega_D d^D K_j d\tau_j}{\left(2\pi\right)^D}d\tau_m. \qquad (14)$$

In this paper we restrict ourselves to Gaussian approximation, which will mean *ad hoc* the neglect of the cumulant terms with $m > 2$ in the series of Eq.(14). Unless $\varphi(\mathbf{r},\tau)$ is a Gaussian field indeed, the Gaussian approximation is believed valid in a range of small enough g, necessarily satisfying the condition

$$\frac{|g|}{W} \ll 1, \tag{15}$$

where W is a measure of the electron band width. Explicit criterion for applicability of the Gaussian approximation depends crucially on the critical exponents and space dimensionality, see Section 3.

3 Quantum case

It was demonstrated by Feynman [24] that at $\beta \to \infty$

$$\frac{1}{D}\left\langle [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]^2 \right\rangle_t = \frac{v^2 - w^2}{v^3}\left(1 - e^{-v|\tau-\sigma|}\right) + \frac{w^2}{v^2}|\tau - \sigma|, \; v^2 = w^2 + \frac{4C}{w} \tag{16}$$

(D is the space dimension) and so, with the notation $\lambda = v/w$, we obtain

$$\mathcal{F}_t - \frac{1}{\beta}\langle \mathcal{S}_{pot} \rangle = \frac{Dv(1-\lambda)^2}{4} \tag{17}$$

and

$$\begin{aligned} f(\tau_j - \tau_m, \tau_k - \tau_m) = {} & \frac{1-\lambda^2}{2v}\left(1 - e^{-v|\tau_j-\tau_m|} - e^{-v|\tau_k-\tau_m|} + e^{-v|\tau_j-\tau_k|}\right) \\ & + \frac{\lambda^2}{2}\left(|\tau_j - \tau_m| + |\tau_k - \tau_m| - |\tau_j - \tau_k|\right). \end{aligned} \tag{18}$$

Using Eqs.(16),(17),(18) and the Debye approximation for integration over $\mathbf{K}$, to obtain

$$\mathcal{F} \leq \frac{Dv\left(1-\lambda\right)^2}{4} - g^2 A_D \int_0^{K_{\max}} \sum_{\omega} \mathcal{K}_2\left(K, i\omega\right) \times \left[\int_0^{\beta} \cos\omega\tau \left(1-\frac{\tau}{\beta}\right) e^{-\frac{1}{2}\lambda^2 K^2 \tau - \frac{1-\lambda^2}{2v}\left(1-e^{-v\tau}\right)K^2} d\tau\right] K^{D-1} dK, \tag{19}$$

where $A_D = \frac{\Omega_D}{2^{D-1}\pi^{\frac{1}{2}D}\Gamma\left(\frac{1}{2}D\right)}$, $\Gamma\left(x\right)$ being the gamma function and $K_{\max}$ is the Debye wave-number cutoff satisfying $A_D K_{\max}^D = D$. For completing the limit $\beta \to \infty$ in Eq.(19) we use the method of residues to sum over the Bose frequencies and employ the spectral representation

$$\mathcal{K}_2\left(K, i\omega\right) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathcal{J}\left(K,u\right)}{u-i\omega} du, \tag{20}$$

with $\mathcal{J}\left(K,x\right)$ being an appropriate spectral density. So we obtain the variational upper-bound estimation $\mathcal{E} \leq \mathcal{E}_0\left(v,\lambda\right)$, where

$$\mathcal{E}_0\left(v,\lambda\right) = \frac{Dv\left(1-\lambda\right)^2}{4} - \frac{g^2 A_D}{2\pi}\int_0^{K_{\max}}\int_0^{\infty}\int_0^{\infty} \mathcal{J}_-\left(K,u\right) e^{-\left(u+\frac{\lambda^2}{2}K^2\right)t - \frac{1-\lambda^2}{2v}\left(1-e^{-vt}\right)K^2} K^{D-1} dK du dt \tag{21}$$

and $\mathcal{J}_-\left(K,u\right) = \mathcal{J}\left(K,u\right) - \mathcal{J}\left(K,-u\right)$. Note that for even-frequency spectrum fluctuations (in particular static ones) $\mathcal{J}_-\left(K,u\right) \equiv 0$, so the interaction term in Eq.(21) vanishes.

3.1 The use of scaling

Until now the statistical properties of the field $\varphi\left(\mathbf{r},\tau\right)$ have not been specified. Further we will use the dynamical scaling law near the QCP [2]

$$\mathcal{J}_-\left(K,u\right) = f^{2-\eta}\mathcal{J}_-\left(fK, f^z u\right), \ \forall f > 0 \tag{22}$$

where η and z is an "anomalous-dimension" and dynamical critical exponent, respectively. Using in Eq.(22) $f = K_{\max}/K$, we have

$$\mathcal{J}_{-}(K,u) = \left(\frac{K}{K_{\max}}\right)^{\eta-2} \mathcal{J}_{-}\left(K_{\max}, \left(\frac{K_{\max}}{K}\right)^{z} u\right). \tag{23}$$

Plugging Eq.(23) into Eq.(21) and using the substitutions for the integration variables

$$u = \left(\frac{K}{K_{\max}}\right)^{z} \varpi,\ K = K_{\max}\sqrt{x},\ t = v^{-1}s, \tag{24}$$

notations for the parameters

$$W = \frac{1}{2}K_{\max}^{2},\ q = \frac{v}{W},\ d = D - 2 + \eta, \tag{25}$$

W being just the band width in the Debye approximation, and for the function

$$\phi\left(s,\lambda^{2}\right) = \left(1-\lambda^{2}\right)\left(1-e^{-s}\right) + \lambda^{2}s, \tag{26}$$

as well as rescaling g to fix the normalization of the fluctuation spectrum

$$\int_{0}^{\infty} Q(\varpi)\, d\varpi = 1,\ Q(\varpi) = \frac{1}{\pi}\widetilde{\mathcal{J}}(K_{\max},\varpi),$$

we obtain

$$\mathcal{E}_{0}(v,\lambda) = \frac{D}{4}Wq(1-\lambda)^{2} - \frac{D}{4}\frac{g^{2}}{W}q^{-1}\left\langle \int_{0}^{1}\int_{0}^{\infty} x^{\frac{d+z}{2}-1} e^{-q^{-1}\left[\phi\left(s,\lambda^{2}\right)x + \frac{\varpi}{W}sx^{\frac{z}{2}}\right]} dxds \right\rangle_{\varpi} \tag{27}$$

where the indexed by ϖ angular brackets mean averaging with the weight $Q(\varpi)$.

3.2 Weak-coupling regime

In the weak-coupling regime $\mu = 1 - \lambda \ll 1$, while the range of the parameter q is not predetermined yet (however, the restriction $q < 1$ should be imposed

anyway, otherwise the continuum description could not be used). In this regime the electron is weakly "fluctuation-dressed". Using assumed smallness of μ we can expand the right-hand side of Eq.(27) in the Taylor series with respect to μ. This gives up to the terms of second order in μ inclusive

$$\mathcal{E}_0(v,\lambda) \simeq -\frac{D}{4}a_0(d,z)\frac{g^2}{W} - \frac{D}{2}a_1(d,z,q)\frac{g^2}{W}\mu + \frac{D}{4}\left[q + \left(\frac{g}{W}\right)^2 a_2(d,z,q)\right] W\mu^2 \tag{28}$$

where

$$a_0(d,z) = \left\langle \int_0^1 \frac{x^{\frac{d+z}{2}-1}}{x + \frac{\varpi}{W}x^{\frac{z}{2}}}dx \right\rangle_{\varpi}, \tag{29}$$

$$a_1(d,z,q) = q\left\langle \int_0^1 \frac{x^{\frac{d+z}{2}}}{\left(x + \frac{\varpi}{W}x^{\frac{z}{2}}\right)^2\left(q + x + \frac{\varpi}{W}x^{\frac{z}{2}}\right)}dx \right\rangle_{\varpi} \tag{30}$$

and

$$a_2(d,z,q) = 4q^2\left\langle \int_0^1 \frac{\left(2q + 3x + 3\frac{\varpi}{W}x^{\frac{z}{2}}\right)x^{\frac{d+z}{2}+1}}{\left(x + \frac{\varpi}{W}x^{\frac{z}{2}}\right)^3\left(q + x + \frac{\varpi}{W}x^{\frac{z}{2}}\right)^2\left(2q + x + \frac{\varpi}{W}x^{\frac{z}{2}}\right)}dx \right\rangle_{\varpi} - a_1(d,z,q) \tag{31}$$

The first term in Eq.(28) is the electron band edge shift in the lowest-order Born approximation, the second term is the potential energy and the third term is the renormalized kinetic energy.

The Eq.(28) is to be minimized with respect to μ and q. Let the optimum values of the variational parameters be μ_0 and q_0. Within the small μ regime, the correction $\propto g^2$ to the bare kinetic energy that describes the fluctuation-driven renormalization of the electron effective mass, results in a contribution $\propto g^6$ to the optimal bound $\mathcal{E}_0$. This contribution is negligible when expanding $\mathcal{E}_0$ up to terms $\propto g^4$ inclusive. The condition that allows to neglect the above

renormalization reads

$$\left(\frac{g}{W}\right)^2 \frac{|a_2(d,z,q_0)|}{q_0} \ll 1, \tag{32}$$

which is, in general, consistent with Eq.(15). Assuming the condition of Eq.(32) to hold, we minimize Eq.(28) first in μ and next in q. This gives the following expression for μ_0 and $\mathcal{E}_0$

$$\mu_0 = \left(\frac{g}{W}\right)^2 \frac{a_1(d,z,q_0)}{q_0} \tag{33}$$

and

$$\mathcal{E}_0 = -\frac{D}{4} a_0(d,z) \frac{g^2}{W} - \frac{D}{4} a_1(d,z) \frac{g^4}{W^3}, \tag{34}$$

respectively, where the positive number $a_1(d,z)$ is the maximum of the function

$$G(d,z,q) = \frac{a_1^2(d,z,q)}{q}, \tag{35}$$

viz.

$$a_1(d,z) = \max_{0<q<\infty} G(d,z,q) = G(d,z,q_0), \tag{36}$$

and q_0 is the point where this maximum is attained. Note that $\lim_{q\to\infty} G(d,z,q) = 0$ due to Eqs.(30), (35), so for existence of the above maximum it would be sufficient that $\lim_{q\to 0} G(d,z,q) = 0$. As deduced from the very structure of $\mathcal{E}_0(v,\lambda)$ (Eq.(28)), the parameter

$$l_0 = \frac{1}{K_{\max}\mu_0\sqrt{q_0}} = \left(\frac{W}{g}\right)^2 [a_1(d,z)]^{-\frac{1}{2}} K_{\max}^{-1} \tag{37}$$

is a measure of the fluctuon potential-well size, which should be much larger than the lattice constant, i.e. satisfy $l_0 K_{\max} \gg 1$.

By the virtue of Eq.(31) $|a_2(d,z,q)| > a_1(d,z,q)$. Therefore, once Eq.(32) is checked to hold, it automatically results in $\mu_0 \ll 1$, due to Eq.(33). On the other hand, inability to satisfy Eq.(32) would mean inapplicability of the

perturbational regime. After this general analysis, let us consider different cases regarding the critical exponent z.

3.2.1 The cases with $z \geq 2$

In this case we always have $\frac{\varpi}{W} x^{\frac{z}{2}} \ll x$, due to smallness of non-adiabaticity parameter $\frac{\varpi}{W}$, so Eqs.(29) - (31) reduce to the functions of the combined index $d^* = d + z - 2$

$$a_0\left(d, z\right) \simeq A_0(d^*) = \frac{2}{d^*}, \tag{38}$$

$$a_1\left(d, z, q\right) \simeq A_1(d^*, q) = q^{\frac{d^*}{2}} \Phi_{d^*}\left(q\right), \tag{39}$$

where

$$\Phi_b\left(x\right) = \int_0^{x^{-1}} \frac{t^{\frac{b}{2}-1}}{t+1} dt, \; b > 0 \tag{40}$$

and

$$a_2\left(d, z, q\right) \simeq A_2\left(d^*, q\right) \;\; = \left(11 + 2d^*\right) A_1\left(d^*, q\right) - 8A_1\left(d^*, 2q\right) - \frac{4q}{1+q}. \tag{41}$$

The necessary condition for the finiteness of the above integrals is $d^* > 0$. One can see that in this case the fluctuation spectral density shape is completely irrelevant.

To infer on existence of the maximum of $G\left(d, z, q\right) = G_{d^*}\left(q\right) = q^{d^*-1}\left[\Phi_{d^*}\left(q\right)\right]^2$ we first note that $\lim_{q\to 0} G_{d^*}\left(q\right) = 0$ at $2 > d^* > 1$, since for such d^*

$$\lim_{q\to 0} \Phi_{d^*}\left(q\right) = \Gamma\left(\frac{d^*}{2}\right)\Gamma\left(1 - \frac{d^*}{2}\right) = \frac{\pi}{\sin\left(\frac{\pi d^*}{2}\right)}. \tag{42}$$

For $d^* = 2$, $\Phi_2\left(q\right) = \ln\left(q^{-1} + 1\right)$, and $\lim_{q\to 0} G_2\left(q\right) = \lim_{q\to 0} q \ln^2\left(q^{-1} + 1\right) = 0$ also. The functions $\Phi_{d^*}\left(q\right)$ for (rather unrealistic) case $4 \geq d^* > 2$ are

reduced to those with $d^* \leq 2$ using the functional relation

$$q^{\frac{d^*}{2}} \Phi_{d^*}(q) = q\left[\frac{2}{d^*-2} - q^{\frac{d^*-2}{2}} \Phi_{d^*-2}(q)\right],\ d^* > 2 \tag{43}$$

and again we get $\lim_{q\to 0} G_{d^*}(q) = 0$. As outlined in the previous subsection, this means that at least one maximum point $0 < q_0 < \infty$ does exist at $d^* > 1$. One the other hand, the equation $\frac{d}{dq} G_{d^*}(q) = 0$ for determining q_0 is rigorously transformed to the following one:

$$(d^*-1)\,\Phi_{d^*}(q) - \frac{2q^{\frac{2-d^*}{2}}}{q+1} = 0, \tag{44}$$

which obviously has no solution if $d^* \leq 1$. Thus for $d^* \leq 1$, the weak coupling regime never applies. This exponents range will be revisited in Section 3.2.

For $1 < d^* < 2$, the assumption of small q_0 would allow one, by the virture of Eq.(42), to solve approximately Eq.(44) in a closed form. However, compared with numerics for specific d^*, this approximation seems to be too inaccurate. An approximate equation, which results from inclusion of the next-to-leading terms of that asymptotic, can not be solved analytically anymore. So given d^*, a reliable calculation of q_0 requires numerical approach. For some cases of rational d^*, one of them is considered below, $\Phi_{d^*}(q)$ is expressed in elementary functions.

Let us put $d^* = \frac{3}{2}$. This case is a representative for fractional-rational d^*. We have

$$A_1\left(\frac{3}{2}, q\right) = \sqrt{2} q^{\frac{3}{4}} \left[\ln \frac{(1+q^{-1})^{\frac{1}{2}}}{q^{-\frac{1}{2}} + \sqrt{2} q^{-\frac{1}{4}} + 1} + \arctan\left(\sqrt{2} q^{-\frac{1}{4}} + 1\right) + \arctan\left(\sqrt{2} q^{-\frac{1}{4}} - 1\right)\right],$$

$$G_{\frac{3}{2}}(q) = 2q^{\frac{1}{2}} \left[\ln \frac{(1+q^{-1})^{\frac{1}{2}}}{q^{-\frac{1}{2}} + \sqrt{2} q^{-\frac{1}{4}} + 1} + \arctan\left(\sqrt{2} q^{-\frac{1}{4}} + 1\right) + \arctan\left(\sqrt{2} q^{-\frac{1}{4}} - 1\right)\right]^2.$$

The graph of $G_{\frac{3}{2}}(q)$ is shown in Fig.1. Eq.(44) for $d^* = \frac{3}{2}$ has unique solution

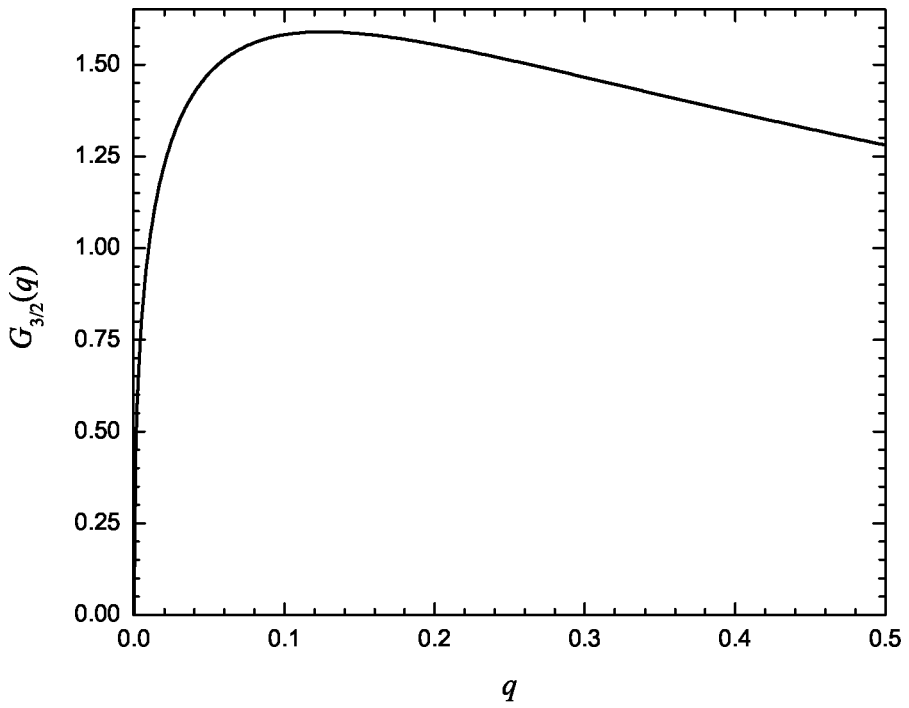

Fig. 1. Graph of the function $G_{\frac{3}{2}}(q)$

$q_0 \simeq 0.126$, for which $G_{\frac{3}{2}}(q_0) = a_1\left(\frac{3}{2}\right) \simeq 1.589$. Checking Eq.(32) yields after cumbersome calculations

$$\frac{|g|}{W} \ll 0.378\,, \tag{45}$$

Provided that Eq.(45) holds, we obtain from Eq.(34)

$$\mathcal{E}_0 \simeq -\frac{D}{3}\frac{g^2}{W}\left(1 + 1.19\frac{g^2}{W^2}\right), \tag{46}$$

and from Eq.(37)

$$l_0 K_{\max} \simeq 0.793\left(\frac{W}{g}\right)^2. \tag{47}$$

The numerical results obtained for different values of $d^* > 1$ show that within the weak copling regime the smaller d^* the larger numerical factor of the fourth-order correction in $\mathcal{E}_0$, and the narrower the range of g where that

approximation works.

3.2.2 The cases with $0 \leq z < 2$

For $0 \leq z < 2$, Eqs.(29) - (31) are transformed quite specifically. Let ϖ_0 scales fluctuation frequencies, so that $Q(\varpi)$ be a function of the reduced frequency $\nu = \frac{\varpi}{\varpi_0}$. Then, omitting from now on the index of the averaging over ϖ (or ν), we have

$$a_0(d,z) = \left(\frac{W}{\varpi_0}\right)^{1-\frac{d}{2-z}} \frac{2}{2-z} \left\langle \nu^{\frac{d+z-2}{2-z}} \Phi_{\frac{2d}{2-z}}\left(\nu\frac{\varpi_0}{W}\right)\right\rangle \tag{48}$$

and $\Phi_b(x)$ is defined by Eq.(40). It is seen that in the present case the weak coupling regime has a sense only at $d > 0$.

The asymptotic of $a_0(d,z)$ at $\frac{\varpi_0}{W} \ll 1$ depends critically upon the sign of $d+z-2$, yielding

$$a_0(d,z) \simeq \begin{cases} \frac{2}{2-z}\frac{\pi\left\langle \nu^{\frac{d}{2-z}-1}\right\rangle}{\sin\left(\pi\frac{d}{2-z}\right)}\left(\frac{W}{\varpi_0}\right)^{1-\frac{d}{2-z}}, & d+z-2<0 \\ \frac{2}{d}\ln\left(\frac{W}{\varpi_0\overline{\nu}}\right), & d+z-2=0 \\ \frac{2}{d+z-2}, & d+z-2>0 \end{cases}, \tag{49}$$

where $\ln\overline{\nu} = \langle\ln\nu\rangle$ and Eq.(42) is taken into account. Thus, the Born energy scale depends on the fluctuation dynamics: (i) drastically in the first subcase, including in particular original Feynman's polaron [24]; (ii) weakly in the second subcase; (iii) negligibly in the last subcase.

Next two integrals (30),(31) are transformed and asymptotically represented at $\frac{W}{\varpi_0} \gg 1$ as follows

$$a_i(d,z,q) \simeq \left(\frac{W}{\varpi_0}\right)^{1-\frac{d}{2-z}} A_i(d,z,\varkappa), \; i = 1,2, \tag{50}$$

where $\varkappa = q\left(\frac{W}{\varpi_0}\right)^{\frac{2}{2-z}}$ is a new variable to optimize over, and

$$A_1(d,z,\varkappa) = \frac{2\varkappa}{2-z}\left\langle \int_0^\infty \frac{u^{\frac{d}{2-z}}du}{(u+\nu)^2\left(\varkappa + u^{\frac{2}{2-z}} + \nu u^{\frac{z}{2-z}}\right)}\right\rangle, \tag{51}$$

$$A_2(d,z,\varkappa) = \frac{8\varkappa^2}{2-z}\left\langle \int_0^\infty \frac{\left(2\varkappa + 3u^{\frac{2}{2-z}} + 3\nu u^{\frac{z}{2-z}}\right)u^{\frac{d}{2-z}+1}du}{(u+\nu)^3\left(\varkappa + u^{\frac{2}{2-z}} + \nu u^{\frac{z}{2-z}}\right)^2\left(2\varkappa + u^{\frac{2}{2-z}} + \nu u^{\frac{z}{2-z}}\right)}\right\rangle$$
$$- A_1(d,z,\varkappa). \tag{52}$$

Note that for any reasonable d the integrands in Eqs.(51) and (52) fall off at $u \to \infty$ faster than u^{-2}. Therefore, in the both integrals, unlike that in Eq.(48), the upper limit $\frac{W}{\varpi_0} \gg 1$ has been safely replaced by ∞.

In the case considered the expression (35) is parametrized as follows

$$G(d,z,q) = \left(\frac{W}{\varpi_0}\right)^{2\frac{3-z-d}{2-z}} \overline{G}(d,z,\varkappa),\ \overline{G}(d,z,\varkappa) = \frac{A_1^2(d,z,\varkappa)}{\varkappa}. \tag{53}$$

Accordingly, the energy asymptotic in weak coupling regime at $z < 2$ is given by

$$\mathcal{E}_0 = -\frac{D}{4}\frac{g^2}{W}\left(\frac{W}{\varpi_0}\right)^{\frac{2-z-d}{2-z}}\left[\frac{2}{2-z}\frac{\pi\left\langle \nu^{\frac{d}{2-z}-1}\right\rangle}{\sin\left(\frac{\pi d}{2-z}\right)} + \left(\frac{g}{W}\right)^2\left(\frac{W}{\varpi_0}\right)^{\frac{4-z-d}{2-z}} A_1(d,z)\right] \tag{54}$$

for $z < 2-d$,

$$\mathcal{E}_0 = -\frac{D}{4}\frac{g^2}{W}\left[\frac{2}{d}\ln\left(\frac{W}{\varpi_0\overline{\nu}}\right) + \left(\frac{g}{W}\right)^2\left(\frac{W}{\varpi_0}\right)^{\frac{2}{d}} A_1(d,z)\right] \tag{55}$$

for $z = 2-d$, and

$$\mathcal{E}_0 = -\frac{D}{4}\frac{g^2}{W}\left[\frac{2}{d+z-2} + \left(\frac{g}{W}\right)^2\left(\frac{W}{\varpi_0}\right)^{2\frac{3-z-d}{2-z}} A_1(d,z)\right], \tag{56}$$

for $z > 2-d$, where

$$A_1(d,z) = \max_{0<\varkappa<\infty} \overline{G}(d,z,\varkappa) \tag{57}$$

Finally, Eq.(37) yields for the fluctuon size in the present case

$$l_0 K_{\max} \simeq \left(\frac{W}{g}\right)^2 \left(\frac{\varpi_0}{W}\right)^{\frac{3-z-d}{2-z}} \left[A_1\left(d,z\right)\right]^{-\frac{1}{2}}. \tag{58}$$

For a given g, the fluctuon size at $z<2$ proves parametrically much smaller than that at $z\geq 2$ unless $d+z\geq 3$.

The sufficient condition for the perturbational regime to hold is provided by Eq.(32), which reads in the present case

$$\frac{\left|A_2\left(d,z,\varkappa_0\right)\right|}{\varkappa_0}\left(\frac{g}{W}\right)^2\left(\frac{W}{\varpi_0}\right)^{\frac{4-z-d}{2-z}} \ll 1, \tag{59}$$

where the numerical factor requires a numerical calculation for specific d and z. This condition proves much more stringent than Eq.(15), but assures that $l_0 K_{\max} \gg 1$ in any case.

Now the key question is that of existing the optimal $\varkappa_0$, to answer which exploring the behavior of $A_1\left(d,z,\varkappa\right)$ at $\varkappa\to 0$ is crucial. Let us assume that $\langle\nu^{-\alpha}\rangle<\infty$ for all $\alpha>0$. Then at $z<1+\frac{1}{2}d$

$$\lim_{\varkappa\to 0}\frac{A_1\left(d,z,\varkappa\right)}{\varkappa} = \frac{2-d}{\left(2-z\right)^2}\left\langle\nu^{-\frac{4-d-z}{2-z}}\right\rangle\frac{\left(\pi\frac{d-z}{2-z}\right)}{\sin\left(\pi\frac{d-z}{2-z}\right)}<\infty,$$

so $\lim_{\varkappa\to 0}\overline{G}\left(d,z,\varkappa\right)=0$. At $z=1+\frac{1}{2}d$ we obtain the asymptotic at $\varkappa\to 0$

$$A_1\left(d,z,\varkappa\right)\approx\frac{4}{2+d}\left\langle\nu^{-3}\right\rangle\varkappa\ln\frac{\overline{\nu}^{\frac{4}{2+d}}\exp\left(-\frac{3}{2}\frac{2-d}{2+d}\right)}{\varkappa},\ \ln\overline{\nu}=\frac{\langle\nu^{-3}\ln\nu\rangle}{\langle\nu^{-3}\rangle},$$

so we have $\lim_{\varkappa\to 0}\overline{G}\left(d,z,\varkappa\right)=0$ also in this case. Hence at $z\leq 1+\frac{1}{2}d$ the maximum point $\varkappa_0$ surely exists. At $z>1+\frac{1}{2}d$, making use of the replacement $u=\left(\varkappa\nu^{-1}\right)^{\frac{2-z}{z}}t^{\frac{2-z}{z}}$ and of Eq.(42), we obtain the following asymptotic

$$A_1\left(d,z,\varkappa\right)\simeq\frac{2}{z}\varkappa^{\frac{d+2-z}{z}}\left\langle\nu^{-\frac{d+2+z}{z}}\right\rangle\frac{\pi}{\sin\left(\pi\frac{d+2-z}{z}\right)},\ \varkappa\to 0,$$

from which we infer that $\varkappa_0$ exists, since $\lim_{\varkappa\to 0}\overline{G}\left(d,z,\varkappa\right)=0$, if $z<\frac{2}{3}\left(d+2\right)$ (that holds authomatically for $d\geq 1$). If $z\geq\frac{2}{3}\left(d+2\right)$, which may occur for $0<d<1$, the above limit is either a finite number or ∞ that makes weak coupling regime nonexistent.

For completeness, it is instructive to consider numerical examples. We consider two important cases $z=0$ and $z=1$ falling into the class $z<1+\frac{1}{2}d$, for which the existence of $\varkappa_0$ has been proved above. In the both cases the relevant formulas, before the ν averaging, are expessed in elementary functions. Due to persisting ν averaging and arbitrary d, however, the formulas yet remain too comlex for illustrative numerics. To make things simpler, in the subsequent two examples we assume that $d=1$ and the ν distribution is strongly peaked at $\nu=1$. We do not expose the corresponding graphs of $\overline{G}\left(1,z,\varkappa\right)$ since they are pretty much similar in shape to the graph shown in Fig.1, apart of appreciable difference in scales of variables $\varkappa$ and q.

Example: $d=1$, $z=0$. With the above assumption this is actually the Feynman polaron problem [24,25]. We obtain

$$\overline{G}\left(1,0,\varkappa\right)=\frac{\pi^2}{\varkappa}\left(\frac{1}{2}+\frac{1-\sqrt{1+\varkappa}}{\varkappa}\right)^2. \tag{60}$$

This function achieves its maximum at $\varkappa_0=3$ in accordance with Feynman, which gives $A_1\left(1,0\right)=\frac{\pi^2}{108}$. Then Eq.(54) reproduces the Feynman result for the energy bound

$$\mathcal{E}_0=-\varpi_0\left(\alpha+\frac{\alpha^2}{81}\right),\ \alpha=\frac{3\pi}{4}\left(\frac{g}{\varpi_0}\right)^2\left(\frac{\varpi_0}{W}\right)^{\frac{1}{2}}, \tag{61}$$

while Eq.(58) yields the fluctuon (polaron) size parameter in terms of Feynman's α constant

$$l_0 \simeq \frac{1}{6\sqrt{6}} \frac{\hbar}{\sqrt{m\varpi_0}} \left(\frac{\alpha}{81}\right)^{-1}. \tag{62}$$

These results have a sense upon satisfaction of Eq.(59), which now reads

$$\frac{|A_2(1,0,3)|}{3} \left(\frac{g}{\varpi_0}\right)^2 \left(\frac{\varpi_0}{W}\right)^{\frac{1}{2}} = 8\left(7\sqrt{7}-18\right)\frac{\alpha}{81} \ll 1. \tag{63}$$

Example: $d = 1$, $z = 1$ This case corresponds to the interaction with acoustic-like critical mode. Now, one should maximize the function

$$\overline{G}(1,1,\varkappa) = \frac{4}{\varkappa}\left(\frac{3\varkappa-1}{\varkappa}\frac{\arctan\sqrt{4\varkappa-1}}{\sqrt{4\varkappa-1}} + \frac{\varkappa-1}{2\varkappa}\ln\varkappa - 1\right)^2. \tag{64}$$

We find numerically that the unique maximum point is $\varkappa_0 \simeq 3.81$ and $A_1(1,1) \simeq 0.208$. Then, Eqs.(55) and (58) yield

$$\mathcal{E}_0 \simeq -\frac{3}{2}\frac{g^2}{W}\left[\ln\left(\frac{W}{\varpi_0}\right) + 0.104\left(\frac{g}{\varpi_0}\right)^2\right] \tag{65}$$

and

$$l_0 K_{\max} \simeq 2.19\frac{W\varpi_0}{g^2}, \tag{66}$$

respectively. In the present case the condition for the perturbational regime, which doesn't contain W at all, reads

$$\frac{|A_2(1,1,\varkappa_0)|}{\varkappa_0}\left(\frac{g}{\varpi_0}\right)^2 \simeq 0.112\left(\frac{g}{\varpi_0}\right)^2 \ll 1, \tag{67}$$

or $|g| \ll 3\varpi_0$.

To conclude this section, for $0 \leq z < 2$ weak coupling regime is realized at much smaller g than for $z \geq 2$. For the latter, g should fit Eq.(15) while the characteristic fluctuation frequency ϖ_0 plays no role. For the former, however, the upper bound of $|g|/\varpi_0$, is crucial.

3.3 Strong coupling regime

3.3.1 General Consideration

In strong-coupling regime the electron is heavily "fluctuation-dressed". Let us make in Eq.(27) the variables replacements $y = q^{-1}x$, $\tau = ye^{-s}$ and $t = 1-\tau$. This transforms that equation to the following one

$$\mathcal{E}_0(q,\lambda) = \frac{D}{4}Wq(1-\lambda)^2 - \frac{D}{4}\frac{g^2}{W}q^{\frac{d+z}{2}-1}\left\langle M\left(q,\varpi,\lambda^2\right)\right\rangle \tag{68}$$

where

$$M\left(q,\varpi,\lambda^2\right) = \int_0^{q^{-1}} \frac{y^{\frac{d+z}{2}-1}e^{-\left(1-\lambda^2\right)y}}{\epsilon\left(y,q,\varpi,\lambda^2\right)}dy$$
$$+\left(1-\lambda^2\right)\int_0^1 dt\int_0^{q^{-1}} \frac{1-(1-t)^{\epsilon\left(y,q,\varpi,\lambda^2\right)}}{\epsilon\left(y,q,\varpi,\lambda^2\right)}e^{-\left(1-\lambda^2\right)ty}y^{\frac{d+z}{2}}dy, \tag{69}$$

and

$$\epsilon\left(y,q,\varpi,\lambda^2\right) = \frac{\varpi}{W}q^{\frac{z}{2}-1}y^{\frac{z}{2}} + \lambda^2 y. \tag{70}$$

To proceed, it is important to note that the function $\epsilon\left(y,q,\varpi,\lambda^2\right)$ increases, in the integration range over y, from zero to $q^{-1}\epsilon$, where $\epsilon = \frac{\varpi}{W} + \lambda^2$. Thus, at $q \gg \epsilon$ Eq.(69) may be expanded in asymptotic Laurent series in overall small $\epsilon\left(y,q,\varpi,\lambda^2\right)$

$$M\left(q,\varpi,\lambda^2\right) = \sum_{p=-1}^{\infty} M_p\left(q,\varpi,\lambda^2\right), \tag{71}$$

where

$$M_p\left(q,\varpi,\lambda^2\right) = \int_0^{q^{-1}} \left[\epsilon\left(y,q,\varpi,\lambda^2\right)\right]^p N_p\left[\left(1-\lambda^2\right)y\right] y^{\frac{d+z}{2}-1}dy \tag{72}$$

with $N_{-1}(\xi) = e^{-\xi}$,

$$N_p(\xi) = \frac{(-1)^p}{(p+1)!}\int_0^1 e^{-\xi t}\left[f(t)\right]^{p+1} t^{p+1}\xi dt,\ p \geq 0, \tag{73}$$

and

$$f(t) = -\frac{\ln(1-t)}{t} = \sum_{k=0}^{\infty} \frac{t^k}{k+1},\ 0 \leq t < 1. \tag{74}$$

The Taylor series representing $f(t)$ converges at $[0,1)$ and so does the Taylor series for any integer power of $f(t)$

$$[f(t)]^n = \sum_{m=0}^{\infty} a_{n,m} t^m. \tag{75}$$

Typically, the strong coupling-regime fluctuon binding energy $\sim Wq$ is smaller than the fluctuation energy. Hence the above-assumed relation between q and ϵ is satisfied if $\lambda^2 \ll q$. Another, weaker, criterion for expanding $M_p(q, \varpi, \lambda^2)$ in powers of $\epsilon(y, q, \varpi, \lambda^2)$ is inferred on by noting that a left vicinity of $t = 1$ is the dominant range for the integration over t in Eq.(69). Hence at $\lambda^2 \ll 1$, it is the range $y \lesssim 1$ that contributes mostly to the corresponding integral over y. In this range $\epsilon(y, q, \varpi, \lambda^2) \lesssim \frac{\varpi}{W} q^{\frac{z}{2}-1} + \lambda^2$, is small, unconditionally for $z \geq 2$, and under the condition $Wq^{1-\frac{z}{2}} \gg \varpi$ for $z < 2$. Actually, when truncating the series of Eq.(71), either $\lambda^2 \ll q$ or $\lambda^2 \ll 1$ and $Wq^{1-\frac{z}{2}} \gg \varpi$ are our the *only* approximations. We should check them at the end of our calculations.

Let us try to simplify the above-developed expansion, by picking in it up the leading terms with respect to $\kappa = (1-\lambda^2)^{-1} q \ll 1$, not imposing in advance any other restriction on q and λ^2. To this end let us transform $M_p(q, \varpi, \lambda^2)$ as follows. For $M_{-1}(q, \varpi, \lambda^2)$, we obtain directly

$$q^{\frac{d+z}{2}-1} M_{-1}\left(q, \varpi, \lambda^2\right) = \kappa^{\frac{d}{2}} \int_0^{\kappa^{-1}} \frac{u^{\frac{d}{2}-1} e^{-u}}{\frac{\varpi}{W} + \lambda^2 (\kappa u)^{\frac{2-z}{2}}} du, \tag{76}$$

Further, using in Eq.(72) the Newton's binom, we arrive at the identical but more convenient representation

$$q^{\frac{d+z}{2}-1} M_p\left(q, \varpi, \lambda^2\right) = \left(1-\lambda^2\right)^{-p-1} \sum_{k=0}^{p} C_p^k \left(\frac{\varpi}{W}\right)^k \lambda^{2(p-k)} m_{p+1,k+1}(\kappa) \tag{77}$$

where

$$m_{n,l}(\kappa) = \frac{(-1)^{n-1}}{n!}\int_0^{\kappa^{-1}} \frac{\gamma\left(\frac{1}{2}d_l + n + 2, u\right)}{u^{\frac{1}{2}d_l+1}} \left[f(\kappa u)\right]^n du,\ d_l = d + (z-2)\,l \tag{78}$$

($d_1 = d^*$ which has been introduced in Section 2 for the case of $z \geq 2$) and

$$\gamma(b,x) = \int_0^x t^{b-1}e^{-t}dt,\ b > 0 \tag{79}$$

is the incomplete gamma-function. The integral in Eq.(76) at $z \leq 2$ converges if $d > 0$ irrespective of λ, while at $z > 2$ this is so if $\lambda = 0$ strictly. For $\lambda \neq 0$, even small, the convergence condition at $z > 2$ reads $d_1 > 0$. These restictions upon the critical indexes are the same as in the weak coupling regime.

The value of $M_{-1}(q, \varpi, 0)$ is independent of z, and given by

$$q^{\frac{d+z}{2}-1} M_{-1}(q, \varpi, 0) = \frac{W}{\varpi}\gamma\left(\frac{d}{2}, \kappa^{-1}\right)\kappa^{\frac{d}{2}}. \tag{80}$$

However, estimating $M_{-1}(q, \varpi, \lambda^2)$ at $\lambda^2 \neq 0$, except for the case $z = 2$ where the factor $\left(\frac{\varpi}{W} + \lambda^2\right)^{-1}$ plainly replaces $\frac{W}{\varpi}$, depends crucially upon z. We postpone this task to consideration of specific cases. At the same time, asymptotic series in κ for $M_p(q, \varpi, \lambda^2)$ with $p \geq 0$ can be obtained by an independent of z trick.

Substituting the series of Eq.(75) into Eq.(78), integrating by parts and using the well-known asymptotic

$$\gamma(b,x) = \Gamma(b) + O\left(x^{1-b}e^{-x}\right),\ x \gg 1,$$

we obtain with an exponential accuracy

$$m_{n,l}(\kappa) = \frac{(-1)^{n-1}}{n!}\left[\Gamma\left(\frac{1}{2}d_l + n + 1\right) b_{n,l}\kappa^{\frac{1}{2}d_l} - \sum_{m\neq m_l}^{\infty} \frac{(m+n)!a_{n,m}}{m - \frac{1}{2}d_l}\kappa^m \right.$$
$$\left. + c_{n,l}(m_l+n)!\left(\ln\kappa^{-1} - \psi(m_l+n) - \frac{1}{m_l+n}\right)\kappa^{m_l}\right], \tag{81}$$

where $c_{n,l} = a_{n,m_l}$, m_l being an integer, if any, satisfying the condition $2m_l = d_l$, and otherwise $c_{n,l} = 0$,

$$b_{n,l} = \sum_{m\neq m_l}^{\infty} \frac{a_{n,m}}{m - \frac{1}{2}d_l}, \tag{82}$$

and $\psi(x)$ is the logarithmic derivative of the gamma-function. At $0 < d < 2$ no m_l emerges if $z = 2$, the only $m_1 = 0$ may appear, if $z < 2$ (e.g. for $z = d = 1$), and if $z > 2$ an infininte number of $m_l \geq 1$ may exist for some d. It is worth noting that at $z \leq 2$ and $d_1 \neq 0$

$$b_{n,l} = \int_0^1 \frac{[f(t)]^n - 1}{t^{\frac{1}{2}d_l+1}}dt - \frac{2}{d_l}. \tag{83}$$

Only the cases with $m_l = 0, 1$ may be important since the $O(\kappa^m \ln\kappa^{-1})$ terms with $m > 1$ are small compared to the kinetic-energy term in Eq.(68). By the same reason, of the series in integer powers of κ in Eqs.(81) we retain only the $O(1)$ term that exists unless $m_l = 0$. The thus approximated Eq.(68), after performing some interim summations over p and neglecting purely non-adiabatic corrections $O\left(\left(\frac{\varpi}{W}\right)^k\right)$, becomes

$$\mathcal{E}_0(q,\lambda) = \frac{D}{4}Wq(1-\lambda)^2 - \frac{D}{4}g^2\kappa^{\frac{1}{2}d}\left\langle \varpi^{-1}\Pi\left(\frac{\varpi}{W}\kappa^{\frac{z-2}{2}}, \lambda^2\right)\right\rangle - \frac{D}{4}\frac{g^2}{W}\Lambda\left(q,\lambda^2\right) + \Delta, \tag{84}$$

where

$$\Delta = -\frac{D}{2d_1}\frac{g^2}{W}(1 - \delta_{d_1,0}) \tag{85}$$

is an energy shift, independent of the variational parameters,

$$\Pi\left(x,\lambda^2\right)=\int_0^\infty\frac{u^{\frac{d}{2}-1}e^{-u}}{1+\lambda^2x^{-1}u^{\frac{2-z}{2}}}du+ \sum_{n=1}^{\infty}\sum_{l=1}^{n}\frac{(-1)^{n-1}}{n!}C_{n-1}^{l-1}\Gamma\left(\frac{1}{2}d_l+n+1\right)b_{n,l}\left(1-\lambda^2\right)^{-n}\lambda^{2(n-l)}x^l \quad (86)$$

and

$$\Lambda\left(q,\lambda^2\right)=\delta_{d_1,0}\left[\ln\frac{1}{q}+\gamma+\frac{\ln\left(1-\lambda^2\right)}{\lambda^2}\right]+\delta_{d_1,2}\left(1-\lambda^2\right)q\left(\ln\frac{1}{q}+\gamma-\frac{3}{2}\right) \quad (87)$$

with γ being the Euler constant. In Eq.(87), the first and the second term do not emerge at $z\geq 2$ (where $d_1>0$ necessarily) and at $z<2$, respectively. In all cases where $d_1>0$, $\Delta=-\mathcal{E}_B$, the band-edge shift in the lowest-order Born approximation.

Further analysis on the base of Eqs.(84) - (87) depends crucially on whether $z\geq 2$ or $z<2$. We consider these cases separately, detaching $z=2$. The peculiarity of the latter case allows us to calculate $\Pi\left(x,\lambda^2\right)$ in a closed form and, that is not feasible in other cases, to ultimately explore an impact of the spectral weight $Q\left(\varpi\right)$ on the fluctuon formation.

3.3.2 The cases with $z=2$

For $z=2$, $d_l=d$ and $b_{n,l}=b_{n,n}$, so that $\Lambda\left(q,\lambda^2\right)\equiv 0$ and Eq.(86) greatly simplifies. The answer reads

$$\mathcal{E}_0\left(q,\lambda\right)\simeq\frac{D}{4}W\left(1-\lambda\right)^2q-\frac{D}{4}\frac{g^2}{W}\Gamma\left(\frac{1}{2}d\right)\left(1-\lambda^2\right)R_d\left(\lambda^2\right)q^{\frac{1}{2}d}-\mathcal{E}_B, \quad (88)$$

where

$$R_d\left(\lambda^2\right)=\left\langle\epsilon^{-1}\left\{1+\frac{d}{2}\int_0^1\frac{1-\left[1+\epsilon h\left(t\right)\right]^{-\frac{1}{2}d-1}}{t^{\frac{1}{2}d+1}}dt\right\}\right\rangle. \quad (89)$$

and $h(t) = f(t) - 1$. Formally Eq.(88) matches the case of $\lambda = 1$, as the fluctuon binding energy obtained vanishes at $\lambda = 1$, that concords with exact Eq.(69). However, that point is likely isolated since in essential weak-coupling regime, i.e. at $0 < 1 - \lambda \ll 1$, the condition at $\kappa \ll 1$ may break down.

Minimization Eq.(88) first in q and next in λ, we find the optimal q value

$$q_0 = \left[\Gamma\left(\frac{d}{2}+1\right)\left(\frac{g}{W}\right)^2 R_d\left(\lambda_0^2\right)\left(\frac{1+\lambda_0}{1-\lambda_0}\right)\right]^{\frac{2}{2-d}} \tag{90}$$

as well as the bound energy

$$\mathcal{E}_0 \simeq -\frac{D}{4}\left(\frac{2}{d}-1\right)\left[\Gamma\left(\frac{d}{2}+1\right)\left(\frac{g}{W}\right)^2 P_d\left(\frac{\varpi}{W},\lambda_0\right)\right]^{\frac{2}{2-d}} W - \mathcal{E}_B, \tag{91}$$

where

$$P_d(\lambda) = (1+\lambda)(1-\lambda)^{1-d} R_d\left(\lambda^2\right) \tag{92}$$

and λ_0 is the maximum point of the function $P_d(\lambda)$. For $d \neq 1$, Eq.(91) presents a *singular* perturbation expansion in coupling constant. When λ_0 corresponds to an extremum, it satisfies the equation

$$2\lambda\frac{R_d'(\lambda^2)}{R_d(\lambda^2)} + \frac{d-(2-d)\lambda}{1-\lambda^2} = 0, \tag{93}$$

otherwise $\lambda_0 = 0$. For the latter case,

$$P_d(\lambda_0) = R_d\left(\lambda_0^2\right) = \frac{W}{\varpi_0} + O(1),$$

where $\varpi_0 = \langle \varpi^{-1} \rangle^{-1}$, which attains, to within $O(1)$ terms, largest of all possible values of those functions. Note that $\lim_{\varpi\to 0} Q(\varpi) = 0$, so it is likely that $\langle \varpi^{-1} \rangle < \infty$.

Let us search a solution λ_0 to Eq.(93), in the vicinity of $\lambda = 0$. Assuming that also $\langle \varpi^{-2} \rangle < \infty$, we have in the leading approximation

$$R_d\left(\lambda^2\right) \simeq W\left\langle \varpi^{-1} \right\rangle - \lambda^2 W^2 \left\langle \varpi^{-2} \right\rangle, \tag{94}$$

which yields for the sought solution

$$\lambda_0 \simeq \frac{d}{2}\frac{\varpi_1}{W},\ \varpi_1 = \frac{\langle \varpi^{-1}\rangle}{\langle \varpi^{-2}\rangle}. \tag{95}$$

For "rigid" $Q(\varpi)$, i.e. zeroing below some finite ϖ, the above-exploited assumption $\langle \varpi^{-2}\rangle < \infty$ holds automatically. Consider now "soft" $Q(\varpi)$, for which $\langle \varpi^{-2}\rangle = \infty$, but $\langle \varpi^{-1-\sigma}\rangle < \infty$ with some $0 < \sigma < 1$. Scaling the behavior of $Q(\varpi)$ at $\varpi \to 0^+$ by

$$Q(\varpi) \sim b_\sigma \left\langle \varpi^{-1-\sigma}\right\rangle \frac{\sin(\pi\sigma)}{\pi\sigma}\varpi^\sigma,\ b_\sigma = \text{const},$$

we obtain the solution to Eq.(93) at $1 > \sigma > 1/2$

$$\lambda_0 \simeq \left(\frac{d}{2b_\sigma}\right)^{\frac{1}{2\sigma-1}} \left(\frac{\varpi_\sigma}{W}\right)^{\frac{\sigma}{2\sigma-1}},\ \varpi_\sigma = \left(\frac{\langle \varpi^{-1}\rangle}{\langle \varpi^{-1-\sigma}\rangle}\right)^{\frac{1}{\sigma}}. \tag{96}$$

If $0 < \sigma \leq 1/2$, λ_0 remains zero. Since $\frac{\sigma}{2\sigma-1} > 1$ at $1 > \sigma > 1/2$, the non-adiabatic corrections resulting from $\lambda_0 \sim \left(\frac{\varpi}{W}\right)^{\frac{\sigma}{2\sigma-1}}$ are even smaller than those $\sim \frac{\varpi}{W}$ resulting from the integral term in Eq.(89).

Thus, as far as small λ_0 is concerned, either $\lambda_0^2 = o\left(\frac{\varpi}{W}\right)$ or $\lambda_0 = 0$ for all admissible $Q(\varpi)$. Neglecting the postleading non-adiabatic corrections, from Eqs.(90) and (91) we arrive at

$$q_0 = \left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{2}{2-d}},\ \mathcal{E}_0 = -\frac{D}{4}\left(\frac{2}{d}-1\right)Wq_0 - \mathcal{E}_B. \tag{97}$$

Requiring $q_0 \ll 1$, one gets the criterion of applicability of the continuum approximation

$$\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0} < 1. \tag{98}$$

Under this condition, the self-trapping term $\propto \left(\frac{g^2}{\varpi_0 W}\right)^{\frac{2}{2-d}}$ in $\mathcal{E}_0$ may be both smaller and larger than $\mathcal{E}_B$. The latter situation occurs if coupling is strong

enough to satisfy

$$\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0} > \left[\frac{2}{d}\frac{2}{2-d}\frac{1}{\Gamma\left(\frac{1}{2}d\right)}\right]^{\frac{2-d}{d}}\left(\frac{\varpi_0}{W}\right)^{\frac{2-d}{d}}. \tag{99}$$

Even though $-\mathcal{E}_B$ dominates $\mathcal{E}_0$, the self-trapping term yet lowers $\mathcal{E}_0$ more than does the correction $\propto \left(\frac{g^2}{W^2}\right)^2$ in weak coupling regime.

Consider now the singular case $d=2$, for which $m_1=1$ and

$$b_n = \int_0^1 \frac{[f(t)]^n - 1 - \frac{1}{2}nt}{t^2}dt - 1.$$

Here we obtain from Eq.(84)

$$\begin{aligned}\mathcal{E}_0(q,\lambda) =& \frac{D}{4}q\left[W(1-\lambda)^2 - \frac{g^2}{W}\left(1-\lambda^2\right)R_2\left(\lambda^2\right)\right] + \\ & \frac{D}{4}\frac{g^2}{W}\left(1-\lambda^2\right)q\ln\frac{q}{e^{\frac{3}{2}-\gamma}} - \mathcal{E}_B\end{aligned} \tag{100}$$

where

$$R_2\left(\lambda^2\right) = \left\langle \epsilon^{-1} + \int_0^1 \left[\frac{h(t)}{(1+\epsilon h(t))^2} + \frac{h(t)}{1+\epsilon h(t)} - t\right]\frac{dt}{t^2}\right\rangle$$

This expression is easily optimized first over q and afterwards over λ to yield

$$q_0 = e^{\frac{1}{2}-\gamma+S(\lambda_0)},\ \mathcal{E}_0 = -(1+q_0)\mathcal{E}_B, \tag{101}$$

where

$$S(\lambda) = R_2\left(\lambda^2\right) - \left(\frac{W}{g}\right)^2\frac{1-\lambda}{1+\lambda}.$$

and λ_0 is the maximum point of the function $S(\lambda)$. Searching again $\lambda_0 \ll 1$, we obtain

$$\lambda_0 \simeq \frac{1}{g^2\langle\varpi^{-2}\rangle},\ q_0 = e^{2-\gamma-\frac{W}{\varpi_0}\left(\frac{W\varpi_0}{g^2}-1\right)}. \tag{102}$$

It is seen that for $\lambda_0 \ll 1$ and $q_0 \ll 1$, the inequality $g^2\langle\varpi^{-2}\rangle \gg 1$ and Eq.(98) with $d=2$, respectively, should hold. $\mathcal{E}_0$ given by Eqs.(101), (102) is much above that obtained in weak-coupling regime (see case $d^*=2$ in previous

subsection) for typically $\frac{W\varpi_0}{g^2} - 1 = O(1)$, though if $\frac{W\varpi_0}{g^2} - 1 = O\left(\frac{\varpi_0}{W}\right)$ the former may gain.

But what happens if Eq.(98) doesn't hold ? The answer is easy for $2 \geq d > 1$ - in this case weak coupling regime may realize. For $d \leq 1$, however, the question cannot be answered within the present framework, as numerical study reveals no any maximum of $P_d(\lambda)$ other than that in a close vicinity of $\lambda = 0$.

3.3.3 The cases with $z \neq 2$

Using the experience with $z = 2$, in what follows we restrict ourselves to small λ, and assume $\langle \varpi^{-1-s} \rangle < \infty$, where $0 \leq s \leq 1$ throughout. The integral part of $\Pi(x, \lambda^2)$ possesses small-λ expansion at $\lambda^2 \ll x$, which we force to hold. Further, we have $x \ll 1$ unconditionally if $z > 2$. For $z < 2$ we force holding $x \ll 1$ anymore. At the end, we check those conditions both to hold. With such prerequisites, up to the first-order terms inclusive, we obtain

$$\mathcal{E}_0(q, \lambda) = \mathcal{E}_0(q, 0) - \frac{D}{2} W q \lambda + \frac{D}{4} W \Gamma \left(1 + \frac{d-z}{2}\right) g^2 \left\langle \varpi^{-2} \right\rangle q^{1+\frac{d-z}{2}} \lambda^2, \quad (103)$$

at $d > z - 2$ and

$$\mathcal{E}_0(q, \lambda) = \mathcal{E}_0(q, 0) - \frac{D}{2} W q \lambda + \frac{D}{2d} \frac{\pi\sigma}{\sin \pi\sigma} \frac{[q(0)]^{\frac{2-d}{2}}}{\Gamma\left(1 + \frac{d}{2}\right)} \left(\frac{W}{\varpi_\sigma}\right)^\sigma \lambda^{2\sigma}, \quad (104)$$

at $d > z - 2$, where $\sigma = \frac{d}{z-2}$. Here

$$\begin{aligned} \mathcal{E}_0(q, 0) = & \frac{D}{4} W q - \frac{D}{2d} [q(0)]^{\frac{2-d}{2}} q^{\frac{1}{2}d} - \frac{D}{4} [q(0)]^{\frac{2-d}{2}} \frac{\varpi_0}{W} \frac{\Gamma\left(\frac{z+d}{2}\right)}{\Gamma\left(\frac{d}{2}+1\right)} b q^{\frac{d+z}{2}-1} \\ & + \Delta - \frac{D}{4} \frac{g^2}{W} \Lambda(q, 0), \end{aligned} \quad (105)$$

$q(0)$ is q_0 obtained with $\lambda = 0$, i.e. given by Eq.(97) and

$$b = b_{1,1} = -\frac{1}{z+d}\begin{cases} 2\psi\left(1-\frac{z+d}{2}\right)+2\gamma, & z+d \neq 4 \\ 1, & z+d=4 \end{cases} \tag{106}$$

Let $d_1 \neq 0, 1$, i.e. $\Lambda(q,0) = 0$. For $d > z-2$, the minimization equation for λ is solved to give

$$\lambda(q) = \frac{q^{\frac{z-d}{2}}}{g^2\left\langle \varpi^{-2}\right\rangle \Gamma\left(1+\frac{d-z}{2}\right)}. \tag{107}$$

Then the minimization equation for q is well solved by iterations in small adiabatic parameter, to yield for the variational parameters

$$q_0 \simeq q(0) - \frac{2}{2-d}\frac{\varpi}{W}\left[q(0)\right]^{\frac{z}{2}} \tag{108}$$

$$\lambda_0 \simeq \frac{\Gamma\left(1+\frac{d}{2}\right)}{\Gamma\left(1+\frac{d-z}{2}\right)}\frac{\varpi_1}{W}\left[q(0)\right]^{\frac{z}{2}-1} \tag{109}$$

where *ad hoc* ϖ is defined by

$$\varpi = \frac{\left(1-\frac{z+d}{2}\right)\Gamma\left(\frac{z+d}{2}\right)b}{\Gamma\left(1+\frac{d}{2}\right)}\varpi_0 + \frac{\left(\frac{d-z}{2}-1\right)\Gamma\left(1+\frac{d}{2}\right)}{\Gamma\left(1+\frac{d-z}{2}\right)}\varpi_1 \tag{110}$$

For $d < z-2$ that may realize only at $z > 2$, we find the optimal λ at a given q to equal

$$\lambda(q) = \left[\frac{z-2}{2}\frac{\sin\pi\sigma}{\pi\sigma}\Gamma\left(1+\frac{d}{2}\right)\right]^{\frac{1}{2\sigma-1}}\left(\frac{\varpi_\sigma}{W}\right)^{\frac{\sigma}{2\sigma-1}}\left[q(0)\right]^{-\frac{2-d}{2}\frac{1}{2\sigma-1}}q^{\frac{1}{2\sigma-1}}, \tag{111}$$

which provides a minimum if $2\sigma > 1$(i.e. $d > \frac{z-2}{2}$), otherwise we should put $\lambda = 0$. Just as above, the equation for optimum q at the present conditions is solved by iterations, which results in

$$q \simeq q\left(0\right) - \frac{2}{2-d}\frac{\varpi}{W}\left[q\left(0\right)\right]^{\frac{z}{2}} \tag{112}$$

$$\lambda_0 \simeq \left[\frac{z-2}{2}\frac{\sin\pi\sigma}{\pi\sigma}\Gamma\left(1+\frac{d}{2}\right)\right]^{\frac{1}{2\sigma-1}}\left(\frac{\varpi_\sigma}{W}\left[q\left(0\right)\right]^{\frac{z}{2}-1}\right)^{\frac{\sigma}{2\sigma-1}}, \tag{113}$$

where here ϖ denotes only the first term in the expression given by Eq.(110). To check all necessary conditions, we consider below the cases with $z > 2$ and $z < 2$ separately.

Subcase $z > 2$ For $z > 2$, we have from Eqs.(108)-(113) $q_0 = q\left(0\right) + o\left(\frac{\varpi}{W}\right)$ and $\lambda_0 = o\left(\frac{\varpi}{W}\right)$. Both $\lambda_0 \ll 1$ and $\lambda_0^2 \ll \frac{\varpi_\sigma}{W}q_0^{\frac{z}{2}-1}$ are satisfied automatically. So the corrections to formula for $\mathcal{E}_0$ as given above for the cases with $z = 2$ are much smaller than ϖ and even not worth to be considered anymore. There remain the same conditions, given by Eqs.(98) and (99), as with $z = 2$.

Subcase $z < 2$**:** For $z < 2$ and $d + z - 2 \neq 0$, using Eq.(108) we have for original parameter $v = qW$ up to the first order corrections

$$v_0 = q_0 W \simeq W\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{2}{2-d}} - \frac{2}{2-d}\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{z}{2-d}}\varpi, \tag{114}$$

where, as introduced above,

$$\varpi = 2\frac{\left(1-\frac{z+d}{2}\right)\Gamma\left(\frac{z+d}{2}\right)b}{\Gamma\left(1+\frac{d}{2}\right)}\varpi_0 + \frac{\left(\frac{d-z}{2}-1\right)\Gamma\left(1+\frac{d}{2}\right)}{\Gamma\left(1+\frac{d-z}{2}\right)}\varpi_1, \tag{115}$$

for the parameter λ

$$\lambda_0 \simeq \frac{\Gamma\left(1+\frac{d-z}{2}\right)}{\Gamma\left(1+\frac{d}{2}\right)}\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{-\frac{2-z}{2-d}}\frac{\varpi_1}{W} \tag{116}$$

and for the fluctuon energy

$$\mathcal{E}_0 = -\frac{D}{4}\left(\frac{2}{d}-1\right)W\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{2}{2-d}} + \Delta - \frac{D}{4}\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{z}{2-d}}\varpi_{01}, \tag{117}$$

where

$$\varpi_{01} = \frac{\Gamma\left(\frac{z+d}{2}\right) b}{\Gamma\left(1+\frac{d}{2}\right)} \varpi_0 + \frac{\Gamma\left(1+\frac{d}{2}\right)}{\Gamma\left(1+\frac{d-z}{2}\right)} \varpi_1 \tag{118}$$

Now the check of necessary conditions is in order. If we require that $O\left(\lambda^2 x^{-1}\right)$ terms should be small on average, we get

$$\Gamma\left(\frac{d}{2}+1\right) \frac{g^2}{\varpi_0 W} \gg \left[|b| \frac{\Gamma\left(1+\frac{d-z}{2}\right)}{\Gamma\left(1+\frac{d}{2}\right)} \left(\frac{\varpi_0}{W}\right) \right]^{\frac{2-d}{2-z}}. \tag{119}$$

The conditions that $x \ll 1$ and $\lambda_0 \ll 1$, to within purely numerical factor, give the same inequality as Eq.(119).

Note that at $d+z-2 < 0$ the value $\Delta > 0$ and has no connection to $\mathcal{E}_B$. In these subcases, Eq.(119) proves much stronger than that of Eq.(99) that leads to total domination of the self-trapping energy term over Δ. Moreover to within the present approximation, Δ is much smaller even than the $O\left(\varpi\right)$ correction in $\mathcal{E}_0$. As an example of such a case, consider again Feynman polaron ($D = 3$, $d = 1$, $z = 0$). From Eq.(106) we have $b = 4 \ln 2$ and from Eqs.(114) - (116) we obtain, in terms of Feynman's α, for the original variational parameters $v = Wq$ and $w = \lambda v$

$$v_0 \simeq \left(\frac{4\alpha^2}{9\pi} + 1 - 8 \ln 2 \right) \varpi_0, \; w \simeq \varpi_0$$

and for the energy

$$\mathcal{E}_0 = -\left(\frac{\alpha^2}{3\pi} + 6 \ln 2 + \frac{3}{4} \right) \varpi_0,$$

These results are valid upon the conditions

$$\frac{3}{2} \sqrt{\frac{\pi W}{\varpi_0}} > \alpha \gg \frac{3}{2} \sqrt{2\pi \ln 2} \simeq 3. \tag{120}$$

The left-hand side inequality (particular case of Eq.(98)) doesn't appear in Feynman theory, since there $W = \infty$.

At the end, explore singular cases, with $m_1 = 0$, i.e. $d + z = 2$. Using Eqs.(84) - (87) we obtain

$$\mathcal{E}_0(q,0) = \frac{D}{4} W q - \frac{D}{2} W q \lambda + \frac{D}{4} W \Gamma(d)\, g^2 \left\langle \varpi^{-2} \right\rangle q^d \lambda^2 - \frac{D}{2d} \left[q(0)\right]^{\frac{2-d}{2}} q^{\frac{d}{2}} + \frac{D}{4} \frac{g^2}{W} \ln\left(\frac{q}{e^{1-\gamma}}\right). \tag{121}$$

As above, the minimization equation for λ is solved exactly

$$\lambda(q) = \frac{q^{1-d}}{g^2 \left\langle \varpi^{-2} \right\rangle \Gamma(d)}, \tag{122}$$

while that for $q = q(0)\, y$, being

$$y = \left\{ 1 - \frac{2-d}{\Gamma(d)} \frac{\varpi_1}{W} \left[q(0)\right]^{-\frac{d}{2}} y^{1-d} \Gamma\left(1 + \frac{d}{2}\right) + \frac{\varpi_0}{W} y^{-1} \Gamma\left(1 + \frac{d}{2}\right) \right\}^{-\frac{2}{2-d}}$$

is well solved by iterations around $y = 1$, to yield

$$q_0 \simeq q(0) + \left\{ \left[q(0)\right]^{1-\frac{d}{2}} \frac{2}{\Gamma(d)} \frac{\varpi_1}{W} - \frac{2}{2-d} \frac{\varpi_0}{W} q(0) \right\} \Gamma\left(1 + \frac{d}{2}\right). \tag{123}$$

Eq.(123) is valid provided that

$$\Gamma\left(1 + \frac{d}{2}\right) \frac{2-d}{\Gamma(d)} \frac{\varpi_1}{W} \left[q(0)\right]^{-\frac{d}{2}} \ll 1,$$

which means a sort of strong-coupling conditions, considered above

$$\Gamma\left(1 + \frac{d}{2}\right) \frac{g^2}{\varpi_0 W} \gg \left[\frac{2-d}{\Gamma(d)} \Gamma\left(1 + \frac{d}{2}\right) \left(\frac{\varpi_1}{W}\right) \right]^{\frac{2-d}{d}}. \tag{124}$$

Then using Eq.(121), (122), and Eq.(123) we obtain in the leading approximation

$$q_0 \simeq \left[\Gamma\left(\frac{d}{2} + 1\right) \frac{g^2}{W \varpi_0} \right]^{\frac{2}{2-d}} + \frac{2\left[\Gamma\left(1 + \frac{d}{2}\right)\right]^2}{\Gamma(d)} \left(\frac{g}{W}\right)^2 \frac{\varpi_1}{\varpi_0}, \tag{125}$$

$$\lambda_0 \simeq \frac{\Gamma\left(\frac{d}{2} + 1\right)}{\Gamma(d)} \left[\Gamma\left(\frac{d}{2} + 1\right) \frac{g^2}{W \varpi_0} \right]^{-\frac{d}{2-d}} \frac{\varpi_1}{W}, \tag{126}$$

and the energy

$$\mathcal{E}_0 = -\frac{D}{4}\left(\frac{2}{d}-1\right) W \left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{2}{2-d}} + \frac{D}{4}\frac{g^2}{W}\ln\left(e^{\gamma-1}\left[\Gamma\left(\frac{d}{2}+1\right)\frac{g^2}{W\varpi_0}\right]^{\frac{2}{2-d}}\right) - \frac{3D}{4}\frac{g^2}{W}\frac{\left[\Gamma\left(1+\frac{d}{2}\right)\right]^2}{\Gamma(d)}\frac{\varpi_1}{\varpi_0}. \tag{127}$$

As an example of the peculiar case $d+z=2$ one may consider $z=d=1$. Assuming for simplicity $\varpi_1=\varpi_0$ we obtain

$$q_0 \simeq \frac{\pi}{4}\left[\left(\frac{g}{\varpi_0}\right)^2+2\right]\left(\frac{g}{W}\right)^2,\ \lambda_0 \simeq \left(\frac{\varpi_0}{g}\right)^2,$$

and

$$\mathcal{E}_0 = -\frac{D}{16}\pi\left[\left(\frac{g}{\varpi_0}\right)^2+3\right]\frac{g^2}{W}+\frac{D}{2}\frac{g^2}{W}\ln\left(\frac{\sqrt{\pi e^{\gamma-1}}}{2}\frac{g^2}{W\varpi_0}\right). \tag{128}$$

Strong-coupling condition (124) in the present example simplifies to

$$\left(\frac{g}{\varpi_0}\right)^2 \gg 1$$

It appears that this condition and weak-coupling condition given by Eq.(67) have wide overlap, within which Eq.(128) results in much lower $\mathcal{E}_0$ than Eq.(65). Even the absolute value of logarithmic correction proves larger than that of Born shift $\frac{D}{2}\frac{g^2}{W}\ln\left(\frac{W}{\varpi_0}\right)$. This means that the strong coupling solution is energetically more favorable in the overlap region.

4 The self-trapping and electron density of states at classical critical point

4.1 Variational estimation for the electron free energy

Let us consider now the self-trapping of the electron at a *classical* critical point, CCP (or second-order phase transition) at finite temperature $T_c = \beta_c^{-1}$ (rigorously speaking, the transition can be considered as a classical one only assuming that it is not too close to QCP at zero temperature [2]). The Feynman variational approach has been applied to this problem by us earlier [21,22,23] (only for a particular case $D = 3, \eta = 0$) but here we reconsider this (for a generic situation) concentrating on some new points such as the behavior of the electron density of states (DOS) and detailed comparison with the quantum case treated above.

We start with the same general expression given by Eq.(14). Typically for CCP one has $\hbar\varpi\beta_c \ll 1$ due to well-known phenomenon of critical slowing down [31]. This is true provided that a typical wave vector of the order-parameter fluctuations is small in comparison with the reciprocal lattice vector; in our case the typical wave vectors $K^* \simeq 1/l_0$ (where l_0 is an optimal fluctuon size) should be much smaller than $K_{\max}$ and therefore, indeed, $\hbar\varpi\beta_c \simeq (K^*/K_{\max})^z \ll 1$ so we can use for our estimations long-wavelength asymtotic of *static* order-parameter correlators. Due to irrelevance of the dynamics one can put it the trial action (7) $w = 0$. We will also use the notation $C = \omega^2/2$ where ω is the frequency of the trial oscillator; the fluctuon size is

$l = (\hbar/2m\omega)^{1/2}$. We will be interested in the strong-coupling regime where

$$\beta_c \hbar\omega \gg 1 \tag{129}$$

Then instead of Eq.(19) we will have for the Gaussian case the following estimation (cf. Ref.[21])

$$\mathcal{F} \leq \frac{D\omega}{4} - \frac{\beta g^2 A_D}{2} \int_0^{K_{\max}} \mathcal{K}_2(K) \exp\left(-\frac{K^2}{2\omega}\right) K^{D-1} dK \tag{130}$$

where $\mathcal{K}_2(K)$ is the Fourier transform of the static order-parameter correlation function with a small-K expression

$$\mathcal{K}_2(K) = \left(\frac{K_{\max}}{K}\right)^{2-\eta} \tag{131}$$

A numerical factor factor in the above expression is absorbed into the coupling constant g. For the reasons which will be clear below we consider β in the partition function and, as a consequence, in Eq.(130), a running variable. Substituting Eq.(131) into Eq.(130) one promptly finds

$$\mathcal{F} \leq \frac{D\omega}{4} - \frac{D\beta g^2}{4} \Gamma\left(\frac{d}{2}\right) \left(\frac{\omega}{W}\right)^{d/2} \tag{132}$$

After minimization of the right-hand side of Eq.(132) we find for the optimal estimation of the electron free energy

$$\mathcal{F}_0(\beta, g) = -\frac{DW(2-d)}{4d} \left[\Gamma\left(\frac{d}{2}+1\right) \frac{\beta g^2}{W}\right]^{\frac{2}{2-d}} \equiv -BW \left(\frac{\beta g^2}{W}\right)^{\frac{2}{2-d}} \tag{133}$$

Similar to Ref.[21] one can show that this is an optimal estimation provided that

$$(\beta W)^{d/2} \ll (\beta g)^2 \ll (\beta W)^d \tag{134}$$

where the left inequality gives the criterion of the strong coupling, or self-trapping, and the right one gives the criterion of applicability of the Gaussian

approximation. The latter is found from the consideration of the scaling properties of higher-order cumulants in the expansion (14). For $(\beta g)^2 \ll (\beta W)^{d/2}$ (weak coupling regime) the second-order Born approximation turns out to be optimal. For $d = 1$ these results coincide with that from Ref. [21].

Comparing the result (133) with the ground-state energy estimations for strong-coupling regime (97),(117) one can see that in the leading order these expressions differ just by a natural replacement of the temperature β^{-1} for the classical critical point by a typical fluctuation energy for the quantum case. However, the physical meaning of these quantities is essentially different: whereas for the quantum case we have derived an estimation for the true boundary of the electron energy spectrum, for the classical one our result is connected with the fluctuation density of states tail which is not restricted (in the Gaussian approximation) from below. Further we will prove this important statement.

4.2 Electron density of states tail: Laplace transformation

The electron partition function (2) can be estimated, due to Eq.(133), as

$$Z \simeq \exp\left(BW^{-\frac{d}{2-d}}\beta^{\frac{4-d}{2-d}}g^{\frac{4}{2-d}}\right), \tag{135}$$

At the same time it can be rigorously expressed as a Laplace transform of the electron DOS

$$N(E) = \langle \delta(E - \mathcal{H}) \rangle_f , \tag{136}$$

namely,

$$Z = \int_0^\infty N(E)\, e^{-\beta E} dE \tag{137}$$

We can use now Eqs.(135),(137) to find the asymtotic of the electron density of states (that is why it was important to consider β formally as an independent

variable). Using the saddle point method one can prove that at large enough negative E

$$N(E) \propto \exp\left[-\frac{1}{2}\left(\frac{4}{4-d}\right)^{2-\frac{d}{2}}\left(\frac{D}{d}\right)^{\frac{d}{2}}\Gamma\left(1-\frac{d}{2}\right)\left(\frac{|E|}{E_0}\right)^{2-d/2}\right] \tag{138}$$

with a suitable choice of the energy scale E_0 as

$$E_0 = \left(\frac{\pi D}{2\sin\frac{\pi d}{2}}\right)^{\frac{2}{4-d}} g^{\frac{4}{4-d}} W^{-\frac{d}{4-d}} \tag{139}$$

(origin of a numerical factor in the definition (139) will become clear in the next Subsection). The saddle point method is applicable if the exponential in the above formula is large, which is connected with the left inequality in Eq.(134). Another restriction is obvious from the observation that the real edge of the spectrum for the Hamiltonian (1) without fluctuation dynamics equal to $E_{min} = -g\max|\varphi|$. Therefore the asymptotic (138) makes sense only for $|E| \ll |g|$. Near the edge of the spectrum the "Gaussian" tail (138) transforms into the "Lifshitz" one. Analyzing the scaling properties of the higher-order cumulants one can demonstrate that at $E \to E_{min} + 0$

$$N(E) \propto \exp\left[-\frac{const}{(E-E_{min})^{d/2}}\right]. \tag{140}$$

This result has been obtained in Ref.[23] for $d = 1$.

4.3 DOS tail: diagrammatic approach

To better appreciate the above-mentioned approximations, it is instructive to reproduce the result (138) by another way basing on the diagram technique [18,32,33]. The average Green function of the electron describing by the Hamiltonian (1) with the Gaussian random static field $\varphi(\mathbf{r})$ is written in a closed

form

$$G(E,\mathbf{P}) = \frac{1}{E - \mathbf{P}^2/2 - \Sigma(E,\mathbf{P})}$$
$$\Sigma(E,\mathbf{P}) = g^2\Omega_D \int \gamma(\mathbf{P}-\mathbf{K},\mathbf{P},\mathbf{K};E)\,\mathcal{K}_2(\mathbf{K})\,G(E,\mathbf{P}-\mathbf{K})\frac{d^DK}{(2\pi)^D} \qquad (141)$$

where Σ and γ are the self-energy and three-leg vertex, correspondingly, $\mathbf{K},\mathbf{P}$ are, as before, D-dimensional wave vectors, and static correlation function is given by the expression (131). To find asymptotic of DOS for large enough negative energies one can use a method proposed first by Keldysh for doped semiconductors [34] (the same trick was used also for magnetic semiconductors near T_c [35] and for electron topological transitions [36]). For large enough $|E|, E<0$ one can neglect momentum dependence of both Σ and γ since only the momentum transfer $\mathbf{K}\to 0$ is relevant for $d<2$. Also, we can express γ in terms of Σ via the Ward identity [32]

$$\gamma(\mathbf{P},\mathbf{P};0;E) = 1 - \frac{\partial\Sigma(E)}{\partial E}. \qquad (142)$$

Then, taking into account Eq.(131), we obtain a closed differential equation for the self-energy of the form

$$\Sigma(E) = \left(1 - \frac{\partial\Sigma(E)}{\partial E}\right) g^2 A_D \int_0^\infty \frac{K^{d-1}dK}{E - K^2/2 - \Sigma(E)}. \qquad (143)$$

Consider now the density of states (DOS)

$$N_D(E) = -\frac{A_D}{\pi}\mathrm{Im}\int_0^{K_{\max}} \frac{K^{D-1}dK}{E - \Sigma(K,E+i\delta) - \frac{1}{2}K^2} \qquad (144)$$

It is clear that at $|E-\Sigma(k,E+i\delta)| \ll \frac{1}{2}K_{\max}^2$ at least for $D\le 3$ the main contribution to $N_D(E)$ comes from small K ($K \ll K_{\max}$) region.

Let us solve now the equation (143). Integrating over K one derives

$$\Sigma(E) = \frac{\pi D}{2\sin\frac{\pi d}{2}} \frac{g^2}{W^{\frac{d}{2}}} \left[\frac{d\Sigma(E)}{dE} - 1\right] [\Sigma(E) - E]^{\frac{d}{2}-1} \tag{145}$$

Denoting

$$\Sigma(E) - E = E_0 \left[f\left(\frac{E}{E_0}\right)\right]^{\frac{2}{d}} \tag{146}$$

with E_0 given by Eq.(139) we obtain a non-linear first-order ordinary differential equation

$$\frac{2}{d}\frac{df}{dx} = f^{\frac{2}{d}} + x. \tag{147}$$

For $d = 1$ this is Riccatti equation, which was solved in a similar context earlier [35]. We consider here only the asymptotic behavior of the solution at $E < 0$ and $|E| \gg E_0$ directly from the initial equation (143). For these E

$$|\mathrm{Im}\Sigma(E)| \ll |\mathrm{Re}\Sigma(E)| \ll |E| \tag{148}$$

and we linearize this equation with respect to the imaginary part of the self-energy to obtain

$$\frac{d\mathrm{Im}\Sigma(E)}{dE} \simeq \frac{1}{E_0}\left(\frac{-E}{E_0}\right)^{1-\frac{d}{2}} \mathrm{Im}\Sigma(E) \tag{149}$$

Thus, we have

$$\mathrm{Im}\Sigma(E) \simeq CE_0 \exp\left[-\frac{2}{4-d}\left|\frac{E}{E_0}\right|^{2-\frac{d}{2}}\right],\ |E| \gg E_0 \tag{150}$$

where C is an undetermined integration constant. At these energies, the density of states becomes

$$N_D(E) \simeq \frac{CD(2-D)}{2\sin\frac{\pi D}{2}} \frac{E_0}{W^{\frac{D}{2}}|E|^{2-\frac{D}{2}}} \exp\left[-\frac{2}{4-d}\left|\frac{E}{E_0}\right|^{2-\frac{d}{2}}\right] \tag{151}$$

which coincides with the result (138), with an accuracy of a numerical factor of order of 1 in the exponent. This may be considered as a justification of our treatment basing on the Feynman variational approach.

The physical meaning of the self-trapping energy for quantum and classical fluctuons are essentially different. For the fluctuon near QCP, as well as for the Feynman polaron, we calculate approximately the ground state electron energy, or the edge of the spectrum. If we will calculate next-order corrections to the electron free energy in $T = \beta^{-1}$ we will find just a temperature shift of this energy rather than any exponential tail of DOS. The energy of the classical fluctuon is just a position of the chemical potential at small enough electron concentration n. For

$$n < \int_{-\infty}^{0} N(E)\, dE \propto \left(\frac{g}{W}\right)^{\frac{2D}{4-d}}, \tag{152}$$

which is a capacity of the tail, the chemical potential level is "pinned" to the fluctuon energy and almost independent on n due to exponential dependence of the DOS (138) on E.

5 Conclusions

Let us resume on the main results obtained. Due to complexity of the problem of the electron states near quantum critical point (QCP) it is hardly believable that this problem can be treated rigorously. To obtain first insight into this we used variational approach within Feynman path integral formalism. Originally, this approach was developed in the connection with polaron in ionic crystals and proved to give excellent results [24,25]. For the case of classical critical point (CCP) we have checked the reliability of this approach by fairly independent Green function method.

The results on the electron ground state at QCP turn out to be crucially dependent on the anomalous space dimensionality $d = D - 2 + \eta$ and dy-

namical critical exponent z. The most interesting result is nonexistence of regular perturbation theory for the ground state energy for arbitrary small coupling constant g. In such cases singular perturbation theory emerges with the expansion in non-integer powers of g. For $z \geq 2$, those cases fall into range $d + z - 2 \leq 1$. For $z < 2$ it occurs at $z \geq \frac{2}{3}(d + 2)$ which is consistent if $0 < d < 1$.

In the above mentioned singular perturbation-theory cases, as well as in general situation at large enough g (strong coupling regime) the leading term in the ground state energy is independent of z and is given by Eq.(97). This result is valid for $g^2 \ll W\omega$ (W is the electron bandwidth and ω is a typical fluctuation energy) which in fact is a criterion of consistence of continuum approximation. Physically this means that the size of self-trapped state (fluctuon) is much larger than interatomic distance. Otherwise a small-radius fluctuon likely forms, which should be considered by different methods.

In contrast with the quantum case, at CCP the fluctuon states form a continuum in the DOS tail. In this case the variational fluctuon's free energy by Feynman method simply gives a position of the electron chemical potential in the tail counted from the bare band edge. The tail capacity proves $\left(\frac{g}{W}\right)^{\frac{2D}{4-d}}$ times a numerical constant; if the electron concentration is much larger than this estimate the fluctuons can scarcely contribute to the electron properties of material near CCP.

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