Electron self-trapping and fluctuation density-of-states tail at the critical point

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We consider electron self-trapping due to its interaction with order-parameter fluctuations at the second-order phase-transition or critical point (for example, at the Curie temperature in magnetic or ferroelectric semiconductors). Using Feynman path integral approach the autolocalization energy and the size of the self-trapped state (fluctuon) are estimated. It is shown that the fluctuon states are connected with the Lifshitz tail of the electron density-of-states, the parameters of this tail being determined by the critical exponents.

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The interaction of the charge carrier in a semiconductor with some order-parameter fluctuations can drastically change its state leading to a self-trapping, or autolocalization [1, 2, 3, 4, 5, 6, 7]. This phenomenon is of crucial importance, for example, for so hot subject as phase separation in magnetic semiconductors and colossal magnetoresistance materials [5, 6, 7], where the magnetization plays the role of the order parameter. Since the band motion of the electron is easier (and, hence, the bandwidth is larger) for ferromagnetically ordered state the electron in antiferromagnetic or magnetically disordered surrounding creates a ferromagnetic region (magnetic polaron, "ferron" [6], or "fluctuon" [2]) and turns our to be self-trapped in this region. Recently, the formation of the magnetic polaron in ferromagnetic semiconductors EuB_6 and, possibly, EuO, has been observed (see Refs.8, 9 and references therein). The order parameter can be also of different origin, e.g., electric polarization in ferroelectric semiconductors, or crystallographic order parameter in ordered alloys [2]. Phase transitions in helium monolayers [10] and ultracold atom systems in optical lattices [11] might be novel interesting examples.

The "driving force" of the self-trapping is always a band narrowing in disordered state in comparison with the completely ordered one. This intuitive view [12] can be confirmed by a rigorous consideration for the classical $s-d$ exchange ("Kondo lattice") model on the Bethe lattice [5]; however, for the real lattices it is actually not very accurate. It was demonstrated already in a seminal paper by Brinkman and Rice [1] that the band *edges* do not depend on the degree of spin disorder and the band narrowing means rather the decrease of the electron density-of-states (DOS) momenta, the DOS near the edges being exponentially small in the disordered state (Lifshitz tails [13, 14]). The fluctuons (we will use this term to emphasize that the magnetic origin of the order parameter is actually not relevant for the problem under consideration) are connected with the Lifshitz tails.

The autolocalization region becomes larger when the energy goes closer to the band edge (and the edge itself corresponds to the state with complete ordering in the whole crystal) [1]. The consideration of the fluctuon problem is crucially dependent on the ratio of the autolocalization radius l to another scale of the system, namely, the correlation length ξ. In particular, a standard phenomenological consideration [2] is inapplicable at the critical point (or the point of the second-order phase transition), where $\xi \to \infty$. At the same time, this case is especially interesting since the fluctuations near the critical point are strongest and the self-trapping conditions fulfill much easier in this case. Here we present a theory for the Lifshitz DOS tails and fluctuon states at the critical point $T = T_c$.

Following Refs. 3, 4 we will use the path integral variational approach developed by Feynman for the problem of polaron in ionic crystal [15, 16]. For simplicity, we start with 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 critical point in ferroelectrics); some generalization will be considered further. 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

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

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 order-parameter field with its own Hamiltonian $\mathcal{H}_f(\varphi)$ and g is the coupling constant; we will choose it in such a way that φ varies between -1 and 1. The partition function of the whole system may be transformed to

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

where $\beta = T^{-1}$ is the inverse temperature, $Z_f = \mathrm{Tr}_\varphi e^{-\beta\mathcal{H}_f(\varphi)}$ 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

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

is the average over the field states. Here we will consider only classical case where τ-dependence of the field can be neglected. Using Feynman path-integral approach [16, 17, 18] and taking average over φ yields for the electron-only free energy

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

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

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

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

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

etc. Further we consider only the case of $\mathcal{K}_1 = 0$.

To estimate $\mathcal{F}$ we use the same trial action as in Refs.3, 4, $\mathcal{S}_t = \mathcal{S}_0 + \mathcal{S}_{pot}$ where

$$\mathcal{S}_{pot} = \frac{\omega^2}{4\beta}\int_0^\beta\int_0^\beta \left[\mathbf{r}\left(\tau\right) - \mathbf{r}\left(\sigma\right)\right]^2 d\tau d\sigma, \tag{7}$$

the oscillator frequency ω being trial parameter (in contrast with Ref.15 we do not introduce any retardation in the trial action since our field is supposed to be static). Then the Peierls-Feynman-Bogoliubov inequality applied to Eq. (4) reads

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

where

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

which is equivalent to

$$\begin{aligned} \mathcal{F} \leq \mathcal{F}_t &- \frac{\omega^2}{4\beta^2}\int_0^\beta\int_0^\beta \left\langle\left[\mathbf{r}\left(\tau\right) - \mathbf{r}\left(\sigma\right)\right]^2\right\rangle_t d\tau d\sigma \\ &- \sum_{m=2}^{\infty}\frac{g^m}{m!\beta}\int_0^\beta ... \int_0^\beta \left\langle\mathcal{K}_m\left(\mathbf{r}\left(\tau_1\right),...,\mathbf{r}\left(\tau_m\right)\right)\right\rangle_t \prod_{j=1}^{m} d\tau_j \end{aligned} \tag{10}$$

To proceed, we will pass to the Fourier transforms of the cumulants $\mathcal{K}_m\left(\mathbf{K}_1,..,\mathbf{K}_{m-1}\right)$ and take into account that for the Gaussian trial action $\mathcal{S}_t$ one has

$$\begin{aligned} &\left\langle \exp\left\{ i\sum_{j=1}^{m-1}\mathbf{K}_j\left[\mathbf{r}\left(\tau_j\right) - \mathbf{r}\left(\tau_m\right)\right]\right\}\right\rangle_t = \\ &\exp\left\{ -\sum_{j,k=1}^{m-1}\frac{\mathbf{K}_j\mathbf{K}_k}{2D}\left\langle\left[\mathbf{r}\left(\tau_j\right) - \mathbf{r}\left(\tau_m\right)\right]\left[\mathbf{r}\left(\tau_k\right) - \mathbf{r}\left(\tau_m\right)\right]\right\rangle_t\right\}, \end{aligned} \tag{11}$$

where D is the space dimensionality, $\mathbf{K}_j$ are the wave-vectors.

For the states in the tail the variational parameter ω satisfies the inequalities $\beta\omega \gg 1$ and $\omega << W = \frac{1}{2}K_{\max}^2$ where $K_{\max}$ is the Debye wave vector and W is of order of the electron bandwidth (the last inequality just means that the fluctuon size $l = 1/\sqrt{2\omega}$ is much larger than interatomic distance). Thus we have [3, 4]

$$\begin{aligned} \mathcal{F} \leq \frac{D}{4}\omega - \sum_{m=2}^{\infty}\frac{1}{m!}\left(g\beta\right)^m \int ... \int \mathcal{K}_m\left(\mathbf{K}_1,...,\mathbf{K}_{m-1}\right) \times \\ \exp\left[-\frac{1}{4\omega}\sum_{j=1}^{m}\mathbf{K}_j^2 - \frac{1}{4\omega}\left(\sum_{j=1}^{m}\mathbf{K}_j\right)^2\right]\prod_{j=1}^{m-1}\frac{\Omega_D d^D K_j}{\left(2\pi\right)^D} \end{aligned} \tag{12}$$

where Ω_D is the unit lattice volume. If one can neglect the $\mathbf{K}$-dependence of the cumulants this sum can be transformed [3, 4] to the phenomenological expression [2] in terms of the fluctuation free energy in *homogeneous* field created by the electron. This assumption works not too close to the critical point where $l \gg \xi$. At the critical point this assumption can be never used. Instead, the scaling properties hold [19]

$$\mathcal{K}_m\left(\mathbf{K}_1,...,\mathbf{K}_{m-1}\right) = a^{(2-\eta)(m-1)}\mathcal{K}_m\left(a\mathbf{K}_1,...,a\mathbf{K}_{m-1}\right) \tag{13}$$

where η is the anomalous dimensionality critical exponent. Making replacement of variables by $\mathbf{K}_j = \sqrt{q}\varkappa_j$, where $q = \omega/W$, and further returning to the real space coordinates conjugate to $\varkappa_j$, we get

$$\begin{aligned} \mathcal{F} \leqslant \frac{DW}{4}q - q^{-d/2}\beta^{-1}\sum_{m=2}^{\infty}\frac{\left(\beta q^{d/2}\right)^m}{m!}\times \\ \int ... \int K_m\left(\mathbf{r}_1,...,\mathbf{r}_m\right)\prod_{j=1}^{m}u_D(r_j)d^D r_j \\ = \frac{DW}{4}q - q^{-d/2}f\left[q^{d/2}u_D\left(r\right)\right], \end{aligned} \tag{14}$$

where $d = D - 2 + \eta$ is the anomalous space dimensionality,

$$u_D\left(r\right) = g\left(\frac{K_{\max}}{2\pi}\right)^{D/2}\exp\left(-\frac{1}{2}K_{\max}^2 r^2\right) \tag{15}$$

is the potential localized within Debye sphere around $\mathbf{r} = 0$; $f[U(\mathbf{r})]$ is the change of the free energy of the fluctuations bath upon switching an external potential $U(\mathbf{r})$ on.

Earlier [3] we considered the Gaussian approximation (only the term with $m = 2$ in Eq.(14)) which is applicable for not too large coupling constants. To consider the states near the band edge $E = -g$ we have to sum up the series (14). To this end, we employ the fact that $u_D(r)$ is virtually D-dimensional delta function for typical $r \gtrsim l$. Further, to avoid ultraviolet divergencies, we return to the discrete-lattice Ising model, where $\varphi_{\mathbf{r}_i} = \pm 1$. In this framework we adopt that the above potential acts only at site $\mathbf{r}_i = \mathbf{0}$, viz. $u_D(\mathbf{r}_i) = g\delta_{\mathbf{r}_i,\mathbf{0}}$. This assumption can only affect some numerical coefficients of order of unity in the following estimations. Then in the limit of $gq^{d/2} \gg 1$ corresponding to the states near the band edge one obtains

$$f\left[q^{d/2}u_D(r)\right] \simeq -gq^{d/2} + \frac{1}{\beta}\ln G_D \tag{16}$$

where $G_D = \left\langle \delta_{\varphi(\mathbf{0}),1} \right\rangle_f^{-1}$. This is just a number larger than 1 which can be calculated if all necessary correlation functions are known. For the Ising model with nearest-neighbor interaction J, one can easily derive

$$G_D^{-1} = \exp(\beta_c \mathcal{F}_f) \left\langle \prod_{i=1}^{z} (\cosh \beta_c J + \varphi_{\mathbf{r}_i} \sinh \beta_c J) \right\rangle_f \tag{17}$$

where z is the nearest-neighbor number and $\mathcal{F}_f$ is the Ising model free energy per site at $T = T_c = \beta_c^{-1}$.

Substituting Eq.(16) into Eq.(14) and minimizing with respect to q one finds for the optimal fluctuon size

$$l_0 = \frac{1}{K_{\max}\sqrt{q_0}} = \frac{1}{K_{\max}} \left(\frac{W}{T_c} \frac{D}{2d \ln G_D} \right)^{\frac{1}{d+2}} \tag{18}$$

and for the fluctuon energy

$$\mathcal{F}_0 = -g + \frac{d+2}{2} (T_c \ln G_D)^{\frac{2}{d+2}} \left(\frac{DW}{2d} \right)^{\frac{d}{d+2}}. \tag{19}$$

The fluctuon forms only at $\mathcal{F}_0 < 0$. This requirement yields necessary condition for the self-trapping, which reads

$$\frac{T_c}{W} < \frac{D}{2d \ln G_D} \left(\frac{2}{D+\eta} \frac{2d}{D} \frac{g}{W} \right)^{\frac{D+\eta}{2}}, \tag{20}$$

where the band is assumed wide in the sense that $W \gg g$. In the case opposite to one given by Eq.(20) the Gaussian approximation works [3].

The estimation (16) does not work for the systems with continuous broken symmetry such as XY or Heisenberg model; in that case some logarithmic corrections arise. To be specific, let us consider the case of the XY model where $\varphi = \cos\theta$ with the angle θ distributed on the interval $[0, 2\pi)$. Then, instead of Eq.(15), the following asymptotic takes place

$$f[q^{d/2}u_D(r)] \simeq -gq^{d/2} + \frac{1}{\beta}\ln\frac{gq^{d/2}\beta G_D}{2} \tag{21}$$

with a constant G_D given by $G_D^{-1} = \langle \delta(\theta_{\mathbf{0}}) \rangle_f$, where the average is with XY model on discrete lattice. After minimization one has, instead of Eq.(19)

$$\begin{aligned} \mathcal{F}_0 &= -g + \frac{d+2}{4d} DW q_0, \\ q_0 &= \left(\frac{2d}{D}\frac{T}{W} \right)^{\frac{2}{d+2}} \left\{ \ln \left[\frac{G_D}{2e}\frac{g}{T} \left(\frac{2d}{D}\frac{T}{W} \right)^{\frac{d}{d+2}} \right] \right\}^{\frac{2}{d+2}} \end{aligned} \tag{22}$$

This expression can be applied, for example, for the case of two-dimensional XY model up to the Kosterlitz-Thouless transition [19, 20] where the correlation functions decay by power-low with the distance and $d = \eta$ grows linearly with the temperature.

Using the results obtained for the fluctuon energy one can restore the asymptotic of DOS $N(E)$ near the band edge $E = -g$. To this end we use the Laplace transformation connecting the partition function $Z(\beta) = \exp[-\beta\mathcal{F}(\beta)]$ and the DOS

$$Z(\beta) = \int_{-g}^{\infty} N(E)\, e^{-\beta E} dE, \tag{23}$$

inverse transformation, and the saddle point method; the corresponding asymptotics are connected by the so called Tauberian theorems; this approach was used by Friedberg and Luttinger [21] to obtain the Lifshitz tail for disordered systems. To employ this in our treatment, we consider the inverse temperature β in Eqs. (19), (22) as a parameter, except the constant G_D and, possibly, critical exponents. Acting similarly to the derivation of Eq.(2.19) of Ref.[21] one can find the Lifshitz tail in the critical point for the discrete order parameter

$$N(E) \propto \exp\left[-\left(\frac{DW}{4\epsilon} \right)^{d/2} \ln G_D \right] \tag{24}$$

and for the XY model

$$\ln N(E) \propto -\left(\frac{DW}{4\epsilon} \right)^{d/2} \left\{ \ln \left[\frac{g}{W} \left(\frac{W}{\epsilon} \right)^{d/2} G_D \right] \right\}^{\frac{1}{d+1}},$$

where in both cases $\epsilon = E + g$.

Our final results mean that for the case of discrete order parameter such as in the Ising model the main difference between the Lifshitz tails at the critical point and above the critical region is just a replacement of the space dimensionality D by the anomalous space dimensionality

$d = D - 2 + \eta$. For the case of continuous order parameter additional logarithmic stretching of Lifshitz exponent emerge.

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