Quantum-Classical Transitions in Lifshitz Tails with Magnetic Fields

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We consider Lifshitz's model of a quantum particle subject to a repulsive Poissonian random potential and address various issues related to the influence of a constant magnetic field on the leading low-energy tail of the integrated density of states. In particular, we propose the magnetic analog of a 40-year-old landmark result of Lifshitz for short-ranged single-impurity potentials U. The Lifshitz tail is shown to change its character from purely quantum, through quantum classical, to purely classical with an increasing range of U. This systematics is explained by the increasing importance of the classical fluctuations of the particle's potential energy in comparison to the quantum fluctuations associated with its kinetic energy.

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The exponential distortion of van Hove singularities of the (integrated) density of states (IDOS) near band edges is a fundamental feature of disordered electronic systems. The associated leading (band-edge) falloff of the IDOS is commonly referred to as a Lifshitz tail (LT). For an unadulterated theoretical understanding of this phenomenon, Lifshitz studied an idealized statistical model of a quantum particle in three-dimensional configuration space $\mathbb{R}^3$ subject to macroscopically many repulsive impurities which are distributed completely at random [1]. Within this model the (low-energy) falloff of the IDOS originates in exponentially rare realizations of the randomness with large impurity-free regions, where the particle's potential energy is solely due to the impurities outside. It therefore depends on the range of the impurities. Lifshitz argued that all impurities of short range create the same tail [universally given by (8) below with $d = 3$]. A proof of this result turned out to be difficult [2–4]. It was achieved with the help of Donsker and Varadhan's celebrated large-deviation theorem for the long-time asymptotics of certain Wiener path integrals [2]. Shortly after, Pastur observed that the LT ceases to be universal in case of long-ranged impurities, but rather depends on details of the potential created by a single impurity [3].

Apart from its obvious relevance to highly doped semiconductors, the phenomenon of Lifshitz tailing is of interest for a variety of other disordered systems. An example is Brownian motion in random media for which the long-time survival probability is related to the low-energy behavior of the IDOS by Laplace transformation and a Tauberian theorem [2,5,6]. Another example is the random-bond Ising model exhibiting Griffiths singularities [7]. The basic large-deviation mechanism responsible for the creation of LTs is also claimed to be the reason for the suppression of superconductivity in systems with magnetic impurities [8] and for the disorder-induced rounding of certain quantum phase transitions [9].

In the present Letter we report on new theoretical, mostly rigorous results on the fate of LTs in a constant magnetic field. Rigorous studies of Lifshitz's model for a two-dimensional configuration space $\mathbb{R}^2$ have already revealed that the presence of a magnetic field brings about remarkable changes in comparison to the nonmagnetic case [10–13]. In $\mathbb{R}^3$ an additional feature comes into play: apart from universal and nonuniversal LTs of purely quantum and purely classical character, respectively, there exists a wide class of LTs with coexistence of both characters. They occur for impurities of intermediate range. Our main goal is to develop the physical heuristics behind these results for $\mathbb{R}^2$ and $\mathbb{R}^3$. Hereby the new facet lies in both, the inclusion of a magnetic field and the consideration of non-short-ranged impurities. Proofs for the case $\mathbb{R}^3$ will be published elsewhere.

Model.—Lifshitz's model concerns a spinless particle with mass $m > 0$ and electric charge $q \neq 0$, which we will suppose to move in d-dimensional Euclidean space $\mathbb{R}^d$. Its total energy is represented by a random Schrödinger operator on the Hilbert space $L^2(\mathbb{R}^d)$ which is informally defined as

$$H(V) := \frac{1}{2m}\sum_{k=1}^{d}\left(-i\hbar\frac{\partial}{\partial x_k} - qA_k\right)^2 + V. \tag{1}$$

Here $2\pi\hbar > 0$ denotes Planck's constant, $-i\hbar\partial/\partial x_k$ the kth component of the canonical-momentum operator, and A_k the kth component of a vector potential $A:\mathbb{R}^d \to \mathbb{R}^d$ describing a constant magnetic field of strength $B \geq 0$. Repulsive impurities generate the Poissonian random potential $V:\mathbb{R}^d \to \mathbb{R}$ informally given by $V(x) := \sum_j U(x - p^{(j)})$, $U \geq 0$. For a fixed realization of the randomness, the point $p^{(j)} \in \mathbb{R}^d$ stands for the position of the jth impurity repelling the particle at $x \in \mathbb{R}^d$ through a nonrandom, non-negative single-impurity potential $U:\mathbb{R}^d \to \mathbb{R}$, which we assume to be integrable, square integrable, and strictly positive on some nonempty open subset of $\mathbb{R}^d$ [14]. The impurity positions are independently, identically, and uniformly distributed throughout $\mathbb{R}^d$ with mean concentration $\varrho > 0$ such that the probability of finding $J \in \{0, 1, 2, \ldots\}$ impurities in a region $\Lambda \subset \mathbb{R}^d$ of volume $|\Lambda| := \int_\Lambda d^d x$ is given by Poisson's law $\exp[-\varrho|\Lambda|](\varrho|\Lambda|)^J/J!$. Denoting the corresponding probabilistic (ensemble) average with an overbar, the IDOS resulting from (1) at a fixed energy $E \in \mathbb{R}$ can be defined [15] as

$$N(E) := \overline{\langle x|\Theta[E - H(V)]|x\rangle}, \tag{2}$$

in terms of Heaviside's unit-step function Θ. Thanks to unitary invariance of the kinetic-energy operator $H(0)$ under magnetic translations and because of the $\mathbb{R}^d$ homogeneity of the Poisson potential, $N(E)$ is independent of the chosen $x \in \mathbb{R}^d$ labeling the position representation. By the decay of U at infinity the half-line $[\varepsilon_0, \infty[\subset \mathbb{R}$ is not only the set of growth points of the function $N:\mathbb{R} \to \mathbb{R}$ but also coincides with the spectrum of $H(V)$ almost surely, that is, with probability one. Here $\varepsilon_0 \geq 0$ denotes the ground-state energy of $H(0)$, which is zero for $d = 1$ and equal to the lowest Landau-level energy $\hbar|q|B/2m$ for $d = 2$ and 3.

Quantum-classical transitions.—At energies $E \downarrow \varepsilon_0$, the particle will be localized [16] in a large region $\Lambda_0 \subset \mathbb{R}^d$ without impurities. If U is short ranged, its potential energy in Λ_0 is to a good approximation zero. By the spatial confinement its kinetic energy is not smaller than the lowest eigenvalue of $H(0)$ when the latter is Dirichlet restricted to Λ_0. Lifshitz suggested that at low energies $N(E)$ is determined by the region $\Lambda_0(E) \subset \mathbb{R}^d$ with the smallest volume $|\Lambda_0(E)|$ for which the lowest Dirichlet eigenvalue of $H(0)$ coincides with the given E [17]. He therefore proposed the following asymptotic formula [18] for the leading low-energy falloff of the IDOS as $E \downarrow \varepsilon_0$

$$\begin{aligned} \ln N(E) &\sim \ln \mathrm{Prob}\{\Lambda_0(E) \text{ is free of impurities}\} \\ &= -\varrho|\Lambda_0(E)| \end{aligned} \tag{3}$$

if U is short ranged. If U is long ranged, the particle inside Λ_0 acquires a potential energy due to the long-distance decay of potentials U generated by impurities located outside Λ_0, that is, in $\mathbb{R}^d \backslash \Lambda_0$. Given the impurity-free region Λ_0, this potential energy is on average of the order of magnitude

$$\varrho \int_{\mathbb{R}^d \backslash \Lambda_0} d^d x U(x). \tag{4}$$

Supposing that U varies slowly on the scale of the particle's de Broglie wavelength, the kinetic energy of the particle inside Λ_0 will still be given approximately by the lowest Dirichlet eigenvalue of $H(0)$. Therefore, a basic question is whether this kinetic energy, caused by the spatial confinement to Λ_0, dominates (4) or not as $|\Lambda_0| \to \infty$. If yes, the LT has a purely quantum character and is universally given by (3). If no, it, in general, depends on details of the decay of U and exhibits classical features. Moreover, if the quantum fluctuations related to the kinetic energy can be neglected completely, the LT has a purely classical character in the sense that

$$\ln N(\varepsilon_0 + E) \sim \ln N_{cl}(E) \tag{5}$$

as $E \downarrow 0$. Here

$$N_{cl}(E) := \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \frac{\overline{[E - V(0)]^{d/2}\Theta[E - V(0)]}}{\Gamma(1 + d/2)} \tag{6}$$

is the (quasi-) classical IDOS [15,19] with Γ denoting Euler's gamma function.

Case $B = 0$.—It is instructive to briefly recall what happens in the zero-field case. Here the isoperimetric inequality of Strutt (=Rayleigh), Faber, and Krahn [20] shows that balls have the smallest volume for a given lowest Dirichlet eigenvalue of $H(0)$. But the volume $|\Lambda_0|$ of a ball Λ_0 whose associated lowest Dirichlet eigenvalue is $E_0(\Lambda_0)$ can be inferred from a scaling argument:

$$E_0(\Lambda_0) = \frac{\kappa_d \hbar^2}{2m} |\Lambda_0|^{-2/d}. \tag{7}$$

Here κ_d is the lowest eigenvalue of the negative Laplacian when Dirichlet restricted to a ball in $\mathbb{R}^d$ of unit volume, for example, $\kappa_1 = \pi^2$, $\kappa_2 = \pi\xi_0^2$, with $\xi_0 = 2.404\ldots$ being the smallest positive zero of the zeroth Bessel function of the first kind, and $\kappa_3 = \pi^2(4\pi/3)^{2/3}$. Combining (3) and (7) one obtains Lifshitz's landmark result [1] for the leading low-energy falloff of the IDOS as $E \downarrow 0 (= \varepsilon_0)$ if U is short ranged:

$$\ln N(E) \sim -\varrho\left(\frac{\kappa_d \hbar^2}{2mE}\right)^{d/2}. \tag{8}$$

If U is long ranged in the sense that it has an (integrable) algebraic decay proportional to $|x|^{-\alpha}$ as $|x| \to \infty$ with some exponent α ($> d$), the potential energy (4) is proportional to $|\Lambda_0|^{1-\alpha/d}$. As $|\Lambda_0| \to \infty$, it is therefore negligible in comparison to the kinetic energy (7) if and only if $\alpha > d + 2$. More generally, if the decay is faster than algebraic with exponent $d + 2$, the LT was proven [2–4] to be universally given by (8). If $\alpha < d + 2$ the total energy is dominated by the potential energy and the LT has, indeed, a purely clasical character in the sense that (5) holds [3]. Algebraic decay with exponent $\alpha = d + 2$ therefore discriminates between LTs of purely quantum and those of purely classical character if $B = 0$. In this borderline case, $\alpha = d + 2$, coexistence of both quantum and classical behavior is expected [15].

Case $B > 0$.—What changes when a constant magnetic field is turned on? First of all, a magnetic field of strength B introduces the length scale $\ell := \sqrt{\hbar/|q|B}$ and the energy scale $\hbar^2/2m\ell^2$ ($= \varepsilon_0$ for $d = 2$ and 3). Of course, Eq. (3) continues to hold in the short-ranged case. It is the shape and mainly the volume of the region $\Lambda_0(E)$ through which the magnetic field enters. Physical intuition suggests that an external magnetic field favors localization effects. Hence, the energy of a particle which is confined to some region is dramatically diminished in comparison to the case $B = 0$. To discuss this in more detail, it is helpful to consider first the (idealized) quantum Hall situation with the particle and all impurities confined to a plane $\mathbb{R}^2$ perpendicular to the magnetic field.

Case $B > 0$ and $d = 2$.—Because of the rotational symmetry about the magnetic-field direction it is plausible that balls in $\mathbb{R}^2$, that is, disks, still yield the smallest area for a given lowest eigenvalue of $H(0)$. The underlying magnetic isoperimetric inequality was proven in [20]. Moreover, the increase of the kinetic ground-state energy $E_0(\Lambda_0) - E_0(\mathbb{R}^2) = E_0(\Lambda_0) - \varepsilon_0$ by spatial confinement to a large disk $\Lambda_0 \subset \mathbb{R}^2$ with area $|\Lambda_0|$ is asymptotically given by [11]

$$E_0(\Lambda_0) - \varepsilon_0 = \varepsilon_0 \exp\left[-\frac{|\Lambda_0|}{2\pi\ell^2}[1 + o(1)] \right], \qquad (9)$$

where "little oh" $o(1)$ tends to zero as $|\Lambda_0| \to \infty$. The exponential dependence on the area $|\Lambda_0|$ is a consequence of the fact that the circularly symmetric ground-state wave function of the infinite-area kinetic-energy operator $H(0)$ for $B > 0$ is (in contrast to the case $B = 0$) square integrable and even exponentially localized. For short-ranged U a combination of (3) and (9) yields a power-law falloff of the IDOS near the (almost sure) ground-state energy $\varepsilon_0 > 0$ of $H(V)$ in the sense that

$$\ln N(\varepsilon_0 + E) \sim \ln E^{2\pi\varrho\ell^2} \sim -2\pi\varrho\ell^2 |\ln E| \qquad (10)$$

as $E \downarrow 0$. This stands in sharp contrast to the exponential falloff (8) if $B = 0$. Given (3), the difference is because of the fact that the finite-area kinetic ground-state energy [see (9) and (7)] approaches its infinite-area limit ε_0 exponentially if $B > 0$ but only algebraically if $B = 0$, as the disk Λ_0 is blown up to exhaust all of the plane $\mathbb{R}^2$. Depending on whether the exponent $2\pi\varrho\ell^2$ in (10), which is just the mean number of impurities in a disk of radius $\sqrt{2}\ell$, is smaller or larger than 1, the IDOS exhibits a rootlike or true power-law falloff. The resultant divergence of the DOS dN/dE at ε_0 if $2\pi\varrho\ell^2 < 1$ should be observable in suitable experiments. We note that in the limiting case of point impurities [14] the lowest-Landau-band approximation to N is known exactly [21] with a LT (see also [22]) differing from (10).

A nontrivial proof of (10) was given by Erdős [11] for U with compact support. Building on his result, Eq. (10) was shown to hold for any U which decays faster than any Gaussian at infinity [12]. In fact, this is plausible from the heuristic point of view. When estimating the potential energy of a particle in a large impurity-free disk $\Lambda_0 \subset \mathbb{R}^2$ by (4), it turns out to be negligible in comparison to the increase of the kinetic energy given by (9) if and only if U decays faster than any Gaussian. Conversely, if U decays slower than any Gaussian, the LT is dominated by the potential energy and hence of classical character in the sense that (5) holds [10,12]. The discriminating decay of U for the quantum-classical transition is therefore Gaussian if $B > 0$ and not algebraic (as in the case $B = 0$). In the borderline case of Gaussian decay quantum and classical behavior coexist [12,13].

Case $B > 0$ and $d = 3$.—In contrast to the two-dimensional situation, the presence of a constant magnetic field in $\mathbb{R}^3$ introduces an anisotropy. Here the isoperimetric problem of finding those regions which yield the smallest volume for a given lowest Dirichlet eigenvalue of $H(0)$ seems to be unsolved. It is natural to assume that its solution is found among convex regions which are axially symmetric about the magnetic-field direction. Assuming right circular cylinders as the solution, one may argue as follows. For a large confining cylinder $D \times I \subset \mathbb{R}^3$ with base disk $D \subset \mathbb{R}^2$ and altitude interval $I \subset \mathbb{R}$ parallel to the magnetic-field direction, the increase of the kinetic ground-state energy $E_0(D \times I)$—ε_0 is just a sum of two terms in accordance with (9) and (7):

$$E_0(D \times I) - \varepsilon_0 = \varepsilon_0 \exp\left[-\frac{|D|}{2\pi\ell^2}[1 + o(1)] \right] + \frac{\pi^2\hbar^2}{2m|I|^2}. \qquad (11)$$

As a consequence, among all right circular cylinders the one (to be denoted as $\Lambda_0 \subset \mathbb{R}^3$) which yields the smallest volume for a given lowest Dirichlet eigenvalue of $H(0)$ can be inferred asymptotically from the equation

$$E_0(\Lambda_0) - \varepsilon_0 = \inf_{|I|>0} E_0((\Lambda_0/I) \times I) - \varepsilon_0$$
$$= \frac{\pi^2\hbar^2}{2m}\left(\frac{2\pi\ell^2}{|\Lambda_0|}\ln|\Lambda_0|^2\right)^2 [1 + o(1)]. \qquad (12)$$

Inserting this result into (3), we conclude that for short-ranged impurities the IDOS drops down to zero near the ground-state energy $\varepsilon_0 > 0$ of $H(V)$ according to

$$\ln N(\varepsilon_0 + E) \sim -2\pi\varrho\ell^2 |\ln E| \left(\frac{\pi^2\hbar^2}{2mE}\right)^{1/2} \qquad (13)$$

as $E \downarrow 0$. The right-hand side (rhs) is the product [23] of the rhs of (10) and (8) with $d = 1$, provided one notes that ϱ in (13) is the mean bulk concentration. The dominant second factor may be attributed to the effective zero-field motion of the particle parallel to the magnetic field. A leading asymptotic behavior proportional to $E^{-1/2} \ln E$ was also suggested [24] in case of point impurities [14] for the DOS within the lowest-Landau-band approximation. So far we do not have a complete proof of (13), the magnetic analog of Lifshitz's 40-year-old result (8) (with $d = 3$). We have a lower bound [25] on the IDOS, which coincides with the so-called optimal-fluctuation formula [26] and has the same leading asymptotics as the rhs of (13). The asymptotics of our upper bound [25], however, dismisses the logarithmic factor. To sharpen the upper bound one should extend Erdős's proof [11] from $d = 2$ to $d = 3$.

What changes if U is long ranged? The potential energy (4) of the particle inside $\Lambda_0 = D \times I$ is of the same order of magnitude as the sum of two terms

$$\varrho \int_{\mathbb{R}^2 \setminus D} d^2 x_\perp U_\perp(x_\perp) + \varrho \int_{\mathbb{R}\setminus I} dx_\| U_\|(x_\|) \qquad (14)$$

containing D and I separately. Here we have introduced marginal impurity potentials of the directions perpendicular and parallel to the magnetic field, $U_\perp(x_\perp) := \int_{\mathbb{R}} dx_\| U(x_\perp, x_\|)$ and $U_\|(x_\|) := \int_{\mathbb{R}^2} d^2x_\perp U(x_\perp, x_\|)$. As $|D|, |I| \to \infty$, each of the two terms of the potential energy in (14) competes with its corresponding term of the kinetic energy in (11). As a consequence, apart from LTs with either purely quantum or purely classical character, there emerges a wide class of impurity potentials U yielding LTs with coexistence of these characters. Of physical relevance in the context of screening of charged impurities is the example in which U decays proportional to $\exp\{-(|x|/\lambda)^\beta[1 + o(1)]\}$ as $|x| = (|x_\perp|^2 + x_\|^2)^{1/2} \to \infty$ with some decay length $\lambda > 0$ and some exponent $\beta > 0$. Here the potential energy coming from $U_\|$ in (14) is negligible in comparison to the corresponding kinetic energy in (11) as $|I| \to \infty$. However, the analogous assertion concerning the perpendicular directions as $|D| \to \infty$ is true if and only if $\beta > 2$. In other words, we expect (13) to hold as long as U decays faster than any Gaussian. If $\beta < 2$, the LT was proven to be [25]

$$\ln N(\varepsilon_0 + E) \sim -\pi\varrho\lambda^2 |\ln E|^{2/\beta}\left(\frac{\pi^2\hbar^2}{2mE}\right)^{1/2} \qquad (15)$$

as $E \downarrow 0$. Like (13) it coincides with the product [23] of the logarithms of corresponding tails for $d = 2$ and 1, as follows from (5) (see [12]) and (8), respectively. It incorporates (through $\hbar$ and λ) both quantum and classical features. For the borderline case $\beta = 2$ we conjecture in analogy to Eq. (15) and Ref. [13] that the LT is given by (15) with $\beta = 2$ and λ^2 replaced by $\lambda^2 + 2\ell^2$. To summarize, in $\mathbb{R}^3$ Gaussian decay discriminates between magnetic LTs with purely quantum and those with coexisting quantum-classical behavior.

A transition from the coexistence regime to the purely classical one can be found, for example, within the class of single-impurity potentials U with (integrable) algebraic decay proportional to $|x|^{-\alpha}$ as $|x| \to \infty$ with some exponent α ($>3 = d$). Here the particle's potential energy stemming from $U_\perp$ in (14) always dominates the corresponding kinetic energy in (11). Since $U_\|$ decays proportional to $|x_\||^{2-\alpha}$ as $|x_\|| \to \infty$, the second term in (14) dominates its kinetic counterpart in (11) if and only if $\alpha < 5$. In the latter case, the LT was, indeed, proven to have a purely classical character in the sense that (5) holds [27]. Algebraic decay with exponent $\alpha = 5$ ($= d + 2$) therefore discriminates between magnetic LTs with coexisting quantum-classical and those with purely classical character.

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