Instanton calculus of Lifshitz tails

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Some degree of quenched disorder is present in nearly all solids, and can have a marked impact on their macroscopic properties. A manifestation of this effect is the Lifshitz tail of localized states that then gets attached to the energy spectrum, resulting in the nonzero density of states in the band gap. We present here a systematic approach for deriving the asymptotic behavior of the density of states and of the typical shape of the disorder potentials in the Lifshitz tail. The analysis is carried out first for the well-controlled case of noninteracting particles moving in a Gaussian random potential and then for a broad class of disordered scale-invariant models—pertinent to a variety of systems ranging from semiconductors to semimetals to quantum critical systems. For relevant Gaussian disorder, we obtain the general expression for the density of states deep in the tail, with the rate of exponential suppression governed by the dynamical exponent and spatial dimensions. For marginally relevant disorder, however, we would expect a power-law scaling. We discuss the implications of these results for understanding conduction in disordered materials.

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I. INTRODUCTION

In forming solids, it is practically impossible to avoid quenched disorder such as lattice vacancies or quenched impurities. These microscopic imperfections effectively act as randomly frozen degrees of freedom, which often measurably affects the macroscopic properties of solids. A dramatic example of such an effect is provided by Anderson localization, where quenched disorder traps quasiparticles and consequently turns a conducting metal into an insulating Fermi glass [1–4]. Although the resulting material is insulating at sufficiently low temperatures, the temperature dependence of its direct current conductivity $\sigma(T)$ can be very different from that of an intrinsic insulator. When the chemical potential lies within the band gap of a very pure insulator with band gap energy $E_{\rm g}$, we naively expect

$$\sigma(T) \sim \sigma_0 \exp\left(-\frac{E_{\rm g}}{2k_{\rm B}T}\right), \tag{1}$$

mediated by rarely activated conduction quasiparticles [5]. By contrast, for sufficiently disordered materials, we expect Mott's law [6],

$$\sigma(T) \sim \sigma_0 \exp\left\{-\left(\frac{E_0}{k_{\rm B}T}\right)^{1/(d+1)}\right\}, \tag{2}$$

to hold in spatial dimension d [7]. After accepting a few physically reasonable assumptions and neglecting the role of interactions, the estimation of the direct current conductivity can indeed be mapped to a percolation problem [8]. In this picture, conduction is mediated by variable-range hopping of localized quasiparticles that exist in the band gap due to deep disorder potential wells that trap them there. This tail of localized quasiparticles in the energy spectrum is known as the Lifshitz tail [9], and its characterization is the main object of the present paper.

Various methods for obtaining an asymptotic expression of the Lifshitz tail exist. Building on the work of Halperin and Lax [10], Zittartz and Langer [11] obtained an asymptotic expression for the density of states deep in the tail of the band,

$$\rho(E) \approx A(E) e^{-B(E)}, \tag{3}$$

for noninteracting quasiparticles moving in a random potential (see also Ref. [12]). Cardy derived the same result through the replica trick [13] and a supersymmetry-based derivation also exists [14,15]. All these techniques and results, however, are confined to the noninteracting regime. As usual, once interactions are included our theoretical machinery and understanding remain rather primitive, especially for strongly correlated systems. Because localized states deep in the Lifshitz tail constitute the basis from which to understand conduction in disordered materials, a method that is applicable for a class of systems broader than a collection of simple noninteracting systems would be desirable.

In order to go beyond the noninteracting regime, we develop a systematic approach that enables us to analyze the effect of quenched disorder deep in the Lifshitz tail. The plan for the rest of this paper is as follows. In Sec. II we first take the well-understood case of noninteracting particles governed by the standard Schrödinger equation and present the disorder saddle method, emphasizing that this approach is more generically applicable than supersymmetric and replica methods (reviewed in Appendix B). In particular, in Sec. III we use the disorder saddle approach to study a broad class of noninteracting and interacting systems whose low-energy excitations are governed by scale-invariant theories. We then derive the form of the Lifshitz tail induced by relevant Gaussian disorder, which generalizes the result for noninteracting systems to a host of quantum critical materials. In Sec. IV, we conclude with a brief discussion of irrelevant and marginally relevant disorder, and the general implications of our results for understanding conduction in disordered materials.

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II. DISORDER SADDLE APPROACH

Let us consider a system of noninteracting quasiparticles in spatial dimensions $d < 4$, governed by the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi_n^V(\mathbf{x}) + V(\mathbf{x})\psi_n^V(\mathbf{x}) = E_n^V\psi_n^V(\mathbf{x}), \tag{4}$$

with a Gaussian random potential $V(\mathbf{x})$. Intensive observables, when scanned over a macroscopic sample, typically self-average [16]. In particular we can then legitimately estimate the disorder-averaged density of states as

$$[\rho(E)]_{\text{d.a.}} = \frac{1}{\mathcal{N}_\gamma}\int[\mathcal{D}V]e^{-\frac{1}{2\gamma}\int d\mathbf{x}V^2(\mathbf{x})}\rho^V(E), \tag{5}$$

where

$$\rho^V(E) = \frac{1}{V_d}\sum_n \delta\big(E - E_n^V\big). \tag{6}$$

Here, $\mathcal{N}_\gamma \equiv \int[\mathcal{D}V]e^{-\frac{1}{2\gamma}\int d\mathbf{x}V^2(\mathbf{x})}$ is the normalization constant and γ characterizes the strength of the disorder. We are interested in the asymptotic behavior of $[\rho(E)]_{\text{d.a.}}$ in the limit of large negative E.

In the following we present a simple derivation that focuses on disorder saddles, building upon classic work by Lifshitz, Halperin, Lax, Zittartz, and Langer [9–12,18]. Namely we evaluate the disorder integral through the saddle-point approximation, seeking a localizing disorder saddle which minimizes the cost $\frac{1}{2\gamma}\int d\mathbf{x}V^2(\mathbf{x})$ with the constraint that it holds an eigenfunction with the negative eigenenergy E. In order to ensure that the saddle point is the absolute minimum of the cost, the corresponding eigenfunction must have the lowest energy. To see this, let us suppose that there exists an eigenfunction $\tilde{\psi}(\mathbf{x})$ with lower energy $\tilde{E} < E < 0$. Then, setting $s \equiv \sqrt{E/\tilde{E}} < 1$, we would be able to lower the cost by replacing $V(\mathbf{x})$ with $s^2V(s\mathbf{x})$, which holds $\tilde{\psi}(s\mathbf{x})$ as an eigenfunction with energy E. Note that for $d \leqslant 4$ a square-integrable potential always has a unique normalizable ground state [20]. We henceforth seek a normalized ground-state wave function, which we further set to be real without loss of generality.

To solve the constrained minimization problem at hand, we introduce a Lagrange multiplier field $\lambda(\mathbf{x})$ and a Lagrange multiplier μ_0. The problem then becomes equivalent to the minimization of the cost action,

$$\begin{aligned}&I[V(\mathbf{x}),\psi(\mathbf{x}),\lambda(\mathbf{x}),\mu_0]\\ &\equiv +\frac{1}{2\gamma}\int d\mathbf{x}V^2(\mathbf{x})\\ &\quad -\frac{1}{\gamma}\int d\mathbf{x}\lambda(\mathbf{x})\left\{E + \frac{\hbar^2}{2m}\nabla^2 - V(\mathbf{x})\right\}\psi(\mathbf{x})\\ &\quad +\mu_0\left\{\int d\mathbf{x}\psi^2(\mathbf{x}) - 1\right\}.\end{aligned} \tag{7}$$

Extremizing it yields

$$V(\mathbf{x}) = -\lambda(\mathbf{x})\psi(\mathbf{x}), \tag{8}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}), \tag{9}$$

$\int d\mathbf{x}\psi^2(\mathbf{x}) = 1$, $\mu_0 = 0$, and

$$-\frac{\hbar^2}{2m}\nabla^2\lambda(\mathbf{x}) + V(\mathbf{x})\lambda(\mathbf{x}) = E\lambda(\mathbf{x}). \tag{10}$$

The last equality (10), combined with the uniqueness of the ground state, dictates that $\lambda(\mathbf{x}) = \lambda_0\psi(\mathbf{x})$ with a constant λ_0. Consequently, Eq. (8) tells us that $V(\mathbf{x}) = -\lambda_0\psi^2(\mathbf{x})$ and the Schrödinger equation (9) morphs into the instanton problem with a single real scalar field,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) - \lambda_0\psi^3(\mathbf{x}) = E\psi(\mathbf{x}). \tag{11}$$

From the study of the instanton problem, for $d < 4$, we know that this equation has spherically symmetric solutions which minimize the action among all the nontrivial stationary points [21]. We thus have the cost minimizing solutions,

$$V_\star(\mathbf{x}) = Ef^2\left(\sqrt{\frac{-2mE}{\hbar^2}}|\mathbf{x}-\mathbf{x}_0|\right), \tag{12}$$

$$\psi_\star(\mathbf{x}) = \sqrt{\frac{-E}{\lambda_0}}f\left(\sqrt{\frac{-2mE}{\hbar^2}}|\mathbf{x}-\mathbf{x}_0|\right), \tag{13}$$

where $f(\tilde{r})$ satisfies

$$\frac{d^2f}{d\tilde{r}^2} + \frac{d-1}{\tilde{r}}\frac{df}{d\tilde{r}} - f + f^3 = 0, \tag{14}$$

with the regularity condition $\frac{df}{d\tilde{r}}|_{\tilde{r}=0} = 0$ and the normalizability condition $\lim_{\tilde{r}\to\infty} f(\tilde{r}) = 0$. The normalization condition on $\psi_\star$ fixes $\lambda_0 = c_\lambda(-E)^{1-\frac{d}{2}}(\frac{2m}{\hbar^2})^{-\frac{d}{2}}$ with

$$c_\lambda = \frac{2\pi^{\frac{d}{2}}}{\Gamma\big(\frac{d}{2}\big)}\int_0^\infty d\tilde{r}\tilde{r}^{d-1}f^2. \tag{15}$$

Finally, evaluating the cost action for these solutions yields the leading exponential factor,

$$[\rho(E)]_{\text{d.a.}} \sim \exp\left\{-\frac{a_d}{g(E)}\right\}, \tag{16}$$

with the dimensionless number,

$$a_d = \frac{\pi^{\frac{d}{2}}}{\Gamma\big(\frac{d}{2}\big)}\int_0^\infty d\tilde{r}\tilde{r}^{d-1}f^4, \tag{17}$$

and the dimensionless coupling,

$$g(E) = \gamma(-E)^{\frac{d}{2}-2}\left(\frac{2m}{\hbar^2}\right)^{\frac{d}{2}}. \tag{18}$$

We can further obtain the subleading prefactor through the fluctuation analysis (Appendix A). The result is that

$$[\rho(E)]_{\text{d.a.}} \approx A(E)e^{-\frac{a_d}{g(E)}} \tag{19}$$

with the prefactor,

$$A(E) = c\left(\frac{2m}{\hbar^2}\right)^{\frac{d}{2}}(-E)^{\frac{d}{2}-1}\{g(E)\}^{-\frac{(d+1)}{2}}, \tag{20}$$

where c is another dimensionless constant. This expression is asymptotically valid for $d < 4$ in the regime $E \ll$

$-\gamma^{\frac{2}{4-d}}(\frac{2m}{\hbar^2})^{\frac{d}{4-d}}$ where the disorder coupling $g(E)$ is small, akin to the dilute instanton gas limit.

The same result can also be derived through supersymmetric and replica methods (Appendix B). The above derivation clearly shows that the saddle point appearing in these two methods corresponds to the most likely form of a localized wave function of large negative energy E, dilutely distributed; the disorder saddle depicts the shape of the associated trapping potential. As we shall see next, the approach taken here generalizes to a broad class of systems where supersymmetric and replica methods are not readily applicable.

III. DISORDERED SCALE-INVARIANT MODELS

The noninteracting model considered above, relevant in the vicinity of a band edge for conventional semiconductors, is a special case of scale-invariant models. Other examples of scale-invariant models include noninteracting models with more general scaling relation $E \propto |\mathbf{k}|^z$, as in semimetals, and interacting models in the vicinity of quantum critical points [25]. Taking the disorder saddle approach laid out in the last section, we compute the Lifshtiz tails for disordered scale-invariant models.

A clean scale-invariant model possesses a dilatation operator $\hat{D}$ along with a time-translation operator $\hat{H}_0$ and space-translation operators $\hat{P}_i$ for $i = 1,\ldots,d$. These operators obey commutation relations,

$$[\hat{H}_0,\hat{P}_i] = 0, \quad [\hat{P}_i,\hat{P}_j] = 0, \quad [\hat{D},\hat{P}_i] = i\hat{P}_i, \tag{21}$$

and

$$[\hat{D},\hat{H}_0] = iz\hat{H}_0, \tag{22}$$

where z is a dynamical exponent. We suppose that the model has a conserved current with a local density operator $\hat{J}^t(\mathbf{x}) = e^{-i\hat{\mathbf{P}}\cdot\mathbf{x}}\hat{J}^t(\mathbf{0})e^{+i\hat{\mathbf{P}}\cdot\mathbf{x}}$ obeying $[\hat{J}^t(\mathbf{x}),\hat{J}^t(\mathbf{y})] = 0$ and

$$[\hat{D},\hat{J}^t(\mathbf{0})] = id\hat{J}^t(\mathbf{0}). \tag{23}$$

A number operator $\hat{Q} \equiv \int d\mathbf{x}\hat{J}^t(\mathbf{x})$ in particular satisfies $[\hat{H}_0,\hat{Q}] = [\hat{D},\hat{Q}] = 0$. We also suppose that there is a local operator $\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{x}) = e^{-i\hat{\mathbf{P}}\cdot\mathbf{x}}\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{0})e^{+i\hat{\mathbf{P}}\cdot\mathbf{x}}$ with scaling dimension $\Delta_{\rm pro}$ and unit, minimal, number $q_{\rm unit}$. In other words,

$$[\hat{D},\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{0})] = i\Delta_{\rm pro}\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{0}), \tag{24}$$

and

$$[\hat{Q},\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{0})] = q_{\rm unit}\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{0}). \tag{25}$$

We set $\hbar = 1$ and $q_{\rm unit} \equiv 1$ henceforth.

Let us now sprinkle impurities into the clean system, deforming the Hamiltonian to

$$\hat{H}_V = \hat{H}_0 + \int d\mathbf{x} V(\mathbf{x})\hat{J}^t(\mathbf{x}), \tag{26}$$

where for now we suppose that a random potential $V(\mathbf{x})$ again obeys Gaussian statistics. We probe this dirty system by injecting a unit-number excitation through $\hat{\mathcal{O}}^\dagger_{\rm pro}$ and observing how it propagates. Specifically we look at a local density of states defined via

$$\rho^V_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(E,\mathbf{x}) \equiv -\frac{1}{\pi}{\rm Im}\big\{G^V_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(\mathbf{x},\mathbf{x};E)\big\}, \tag{27}$$

where

$$G^V_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(\mathbf{x},\mathbf{y};E) \equiv -i\int dt e^{iEt}\theta(t) \times {}_V\langle 0;0|\hat{\mathcal{O}}^V_{\rm pro}(t,\mathbf{x})\hat{\mathcal{O}}^{V\,\dagger}_{\rm pro}(0,\mathbf{y})|0;0\rangle_V, \tag{28}$$

with $\hat{\mathcal{O}}^{V\,\dagger}_{\rm pro}(t,\mathbf{x}) \equiv e^{+i\hat{H}_V t}\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{x})e^{-i\hat{H}_V t}$ [26]. Here, $|0;0\rangle_V$ denotes a state of the lowest energy among states with zero total number. In general we label eigenstates as

$$\hat{Q}|Q;n\rangle_V = Q|Q;n\rangle_V, \tag{29}$$

and

$$\hat{H}_V|Q;n\rangle_V = E^V_{Q;n}|Q;n\rangle_V \tag{30}$$

for each realization of $V(\mathbf{x})$. The density of states defined above generalizes the standard definition for noninteracting systems and in general admits the spectral representation [27],

$$\sum_n |{}_V\langle 1;n|\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{x})|0;0\rangle_V|^2\delta\big(E - E^V_{1;n} + E^V_{0;0}\big). \tag{31}$$

Contributions for negative energy E, if any, come from bound states with $E^V_{1;n} - E^V_{0;0} = E < 0$ and a nonzero overlap ${}_V\langle 1;n|\hat{\mathcal{O}}^\dagger_{\rm pro}(\mathbf{x})|0;0\rangle_V \neq 0$. When disorder-averaged, they give rise to a smooth Lifshitz tail. We are interested in the asymptotic behavior of $[\rho_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(E)]_{\rm d.a.}$ in the limit of large negative energy E, which we obtain through the disorder saddle approach.

At this point we make two hypotheses, both of which can be rigorously established for a noninteracting scale-invariant theory with $z = 2$ considered in the last section. First we assume that for any square-integrable potential $V(\mathbf{x}) \neq 0$, when $d \leqslant 2z$, there exists a state of the lowest energy $E^V_{1;0}$ among states with a unit number excited by $\hat{\mathcal{O}}^\dagger_{\rm pro}$ (and similarly the existence of the vacuum state $|0;0\rangle_V$). Then, as emphasized in the last section, the game is to seek a localizing potential saddle which minimizes the cost $\int d\mathbf{x}V^2(\mathbf{x})$ while still holding a bound state with $E^V_{1;0} - E^V_{0;0} = E$ for a fixed negative energy E. Generically we expect that the competition between the cost, preferring narrower and shallower potential wells, and the demand for trapping a bound state with a large negative energy, preferring broader and deeper wells, settles into such minimizers. Hence we expect the following, second, hypothesis to hold: There exists a family of square-integrable potentials $V^E_\star(\mathbf{x})$ which minimizes the cost among all the square-integrable potentials with $E^V_{1;0} - E^V_{0;0} = E$ for $d < 2z$. In the saddle-point approximation,

$$[\rho_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(E)]_{\rm d.a.} \sim \exp\left[-\frac{1}{2\gamma}\int d\mathbf{x}\{V^E_\star(\mathbf{x})\}^2\right] \tag{32}$$

then yields the leading exponential factor.

Accepting these two hypotheses, we can obtain the asymptotic expression for the density of states in the tail via simple dimensional analysis. Let us be as pedantic as possible, however. First we can use commutation relations to show that

$$e^{-i\lambda\hat{D}}\hat{H}_V e^{+i\lambda\hat{D}} = e^{z\lambda}\hat{H}_{V^{(\lambda)}}, \tag{33}$$

with

$$V^{(\lambda)}(\mathbf{x}) = e^{-z\lambda} V(e^{-\lambda}\mathbf{x}), \tag{34}$$

from which we deduce that

$$e^{-i\lambda\hat{D}}|Q;n\rangle_V = |Q;n\rangle_{V^{(\lambda)}} \tag{35}$$

with the scaling relation of the spectra,

$$E^{V^{(\lambda)}}_{Q;n} = e^{-z\lambda} E^{V}_{Q;n}. \tag{36}$$

Combined with the scaling relation of the cost,

$$\int d\mathbf{x}\{V^{(\lambda)}(\mathbf{x})\}^2 = e^{(d-2z)\lambda}\left[\int d\mathbf{x}\{V(\mathbf{x})\}^2\right], \tag{37}$$

we conclude that for $E^{(\lambda)} = e^{-z\lambda}E$

$$V_\star^{E^{(\lambda)}}(\mathbf{x}) = \{V_\star^{E}(\mathbf{x})\}^{(\lambda)} = e^{-z\lambda} V_\star^{E}(e^{-\lambda}\mathbf{x}). \tag{38}$$

From Eqs. (37) and (38) it then follows that

$$\frac{1}{2\gamma}\int d\mathbf{x}\left\{V_\star^{E}(\mathbf{x})\right\}^2 = \frac{a_0}{g(E)}, \tag{39}$$

with the dimensionless constant a_0 and the dimensionless disorder coupling,

$$g(E) = \gamma(-E)^{\frac{d}{z}-2}. \tag{40}$$

Thus in the saddle-point approximation,

$$[\rho_{\hat{\mathcal{O}}^\dagger_{\rm pro}}(E)]_{\rm d.a.} \sim \exp\left\{-\frac{a_0}{g(E)}\right\} \tag{41}$$

for $d < 2z$, valid in the regime $E \ll -\gamma^{\frac{z}{2z-d}}$.

We see that the asymptotic scaling of the Lifshitz tail is dictated by the spatial dimensions and the dynamical exponent, ordaining the dispersion relation of the low-energy excitations. The scaling dimension $\Delta_{\rm pro}$ enters only into the subleading prefactor. Our result conforms with the result for noninteracting scale-invariant systems with $z = 2$. It is also in accord with the Harris criterion [28] which stipulates that the disorder is relevant for $d < 2z$. Further insight can be obtained through the use of a Lagrange multiplier (Appendix C).

In passing we note that the same derivation can be repeated for non-Gaussian disorder distributions, for example, those governed by the cost functional of the form,

$$\frac{1}{2\gamma}\int d\mathbf{x}|V(\mathbf{x})|^p, \tag{42}$$

as long as we restrict ourselves to the square-integrable potentials. Such a disorder is relevant for $d < pz$.

We also point out limitations of the current approach. First, it does not provide a systematic way of analyzing fluctuations around the saddle and thus a prefactor in front of the exponential is beyond its scope in general. Another notable restriction is that the method does not apply to the class of strictly bounded disorders for which there exists no obvious large negative energy regime. For example, for the disorder uniformly distributed in bounded interval, our second hypothesis is not justified as there is no apparent penalty for creating broad potential wells. Viewing such disorder as the suitable $p = \infty$ limit of the above non-Gaussian disorder, the interesting essential singularity near the band edge [29–31] sits right at the border of the applicability of the dilute saddle regime.

IV. CONCLUSION

We have presented the systematic approach for analyzing observables deep in the Lifshitz tail, focusing on disorder saddles rather than integrating them out at the onset. This approach clearly illuminates the physical origin of the Lifshitz tail, attributing it to rare regions of deep potential wells that trap and localize wave functions. We have further obtained the form of Lifshitz tails for general scale-invariant models deformed by relevant disorder, including conventional semiconductors and some quantum critical materials. For marginal disorder—for example, Gaussian-disordered semimetal such as graphene with $z = 1$ in $d = 2$ dimensions—the answer depends on whether the disorder is marginally relevant or marginally irrelevant. For the former, positing the existence of saddle points in appropriate disorder integrals, the logarithmic running of the disorder coupling would result in the power-law behavior of the tails and weakly localized states. It is worth carrying out detailed analysis of the tail within the disorder saddle framework for concrete models with marginally relevant disorder. For marginally irrelevant—or, more generally, irrelevant—disorders, there instead exists no clean ultraviolet fixed point and thus the form of the Lifshitz tail sensitively depends on microscopic details of the disorder distribution. This is indeed what happens in the case of Gaussian-disordered semimetals with $z = 1$ in $d = 3$ dimensions [32] and, more generally, Gaussian-disordered systems in higher dimensions $d > 2z$ [33]. Even in such cases, the disorder saddle approach nonetheless seems to provide a good starting point [32].

More wildly, it would be interesting to seek the generalized Mott's law for generic disordered scale-invariant models. When the disorder is relevant and exponentially localized states are only dilutely populated, we would expect the variable-range hopping picture to roughly hold with insulation at sufficiently low temperature. A systematic derivation of this picture is nonetheless desirable in order to put the theory of conduction in disordered materials on the same footing as that for the Lifshitz tail. It would then be particularly interesting to ponder how the effect of interaction could possibly halt the percolation at finite temperature, resulting in many-body localization.

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APPENDIX A: FLUCTUATION ANALYSIS

To evaluate the subleading prefactor, let us first expand around each saddle $V_\star(\mathbf{x})$ as

$$V - V_\star = \sum_{l=0}^{\infty} \xi_l v_l, \tag{A1}$$

where v_l's are a set of orthonormal functions. We choose

$$v_0 = A_{\rm E} f^2\left(\sqrt{\frac{-2mE}{\hbar^2}}|\mathbf{x}-\mathbf{x}_0|\right), \tag{A2}$$

with $A_{\rm E} = (2a_d)^{-\frac{1}{2}}(-E)^{\frac{d}{4}}(\frac{2m}{\hbar^2})^{\frac{d}{4}}$ so that all the other modes will not change the ground-state energy to first order in ξ_l. Integration over ξ_0, hitting the energy delta function in the density of states, leaves us with the factor,

$$\left(\sqrt{2\pi\gamma}\frac{\partial E}{\partial \xi_0}\right)^{-1} = \left(\sqrt{2\pi\gamma}\int d\mathbf{x}\psi_\star^2 v_0\right)^{-1} = \left(\frac{c_\lambda}{2\pi^{\frac{1}{2}}a_d^{\frac{1}{2}}}\right) g^{-\frac{1}{2}}\frac{1}{(-E)}, \tag{A3}$$

where we also took care of the factor coming from $\mathcal{N}_\gamma$.

Next for $i = 1,\ldots,d$ we choose

$$v_i = A_{\rm T}\partial_i V_\star, \tag{A4}$$

where $A_{\rm T} = c_{\rm T}(-E)^{\frac{d}{4}-\frac{3}{2}}(\frac{2m}{\hbar^2})^{\frac{d}{4}-\frac{1}{2}}$ with

$$c_{\rm T} = \left\{\frac{8\pi^{\frac{d}{2}}}{d\times\Gamma\left(\frac{d}{2}\right)}\int_0^\infty d\tilde{r}\tilde{r}^{d-1}f^2\left(\frac{df}{d\tilde{r}}\right)^2\right\}^{-\frac{1}{2}}. \tag{A5}$$

They are d translational zero modes and integration over these modes should be traded for integration over the collective coordinates $\mathbf{x}_0$, sweeping along the saddle submanifold in the field space. The Jacobian involved in this coordinate transformation is $A_{\rm T}^{-1}$ for each mode as can be seen by comparing changes in the field induced by $(\delta\mathbf{x}_0)_i$ and by $\delta\xi_i$. After dividing by the volume V_d and again taking $\mathcal{N}_\gamma$ into account, we receive

$$(A_{\rm T}\sqrt{2\pi\gamma})^{-d} = g^{-\frac{d}{2}}\left(\frac{-2mE}{\hbar^2}\right)^{\frac{d}{2}}\left(2\pi c_{\rm T}^2\right)^{-\frac{d}{2}} \tag{A6}$$

from these modes.

For $l \geqslant d+1$, we have the ground-state energy shift,

$$\sum_{l=d+1}^{\infty}\sum_{l'=d+1}^{\infty}\xi_l\xi_{l'}\sum_n \frac{\langle 0|v_l|n\rangle\langle n|v_{l'}|0\rangle}{E_0^{V_\star}-E_n^{V_\star}}, \tag{A7}$$

to second order in ξ_l's. We compensate it by setting

$$\xi_0 = -\frac{1}{\langle 0|v_0|0\rangle}\sum_{l=d+1}^{\infty}\sum_{l'=d+1}^{\infty}\xi_l\xi_{l'}\sum_n \frac{\langle 0|v_l|n\rangle\langle n|v_{l'}|0\rangle}{E_0^{V_\star}-E_n^{V_\star}} \tag{A8}$$

so as to keep the ground-state energy intact to this order. The resulting disorder cost is

$$\frac{1}{2\gamma}\sum_{l=d+1}^{\infty}\sum_{l'=d+1}^{\infty}\xi_l\xi_{l'}\left(\delta_{l,l'} - 2\lambda_0\sum_n \frac{\langle 0|v_l|n\rangle\langle n|v_{l'}|0\rangle}{E_n^{V_\star}-E}\right). \tag{A9}$$

Imitating Ref. [11], we proceed by choosing $v_l = f u_l$ with

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - E + (1+c_l)V_\star\right]u_l = 0. \tag{A10}$$

(Corresponding to v_0 and v_i, we have $u_0 \propto f$ and $u_i \propto \partial_i f$ with $c_0 = 0$ and $c_i = 2$, respectively.) With this trick we evaluate the cost to be

$$\frac{1}{2\gamma}\sum_{l=d+1}^{\infty}\xi_l^2\left(1-\frac{2}{c_l}\right). \tag{A11}$$

Performing Gaussian integrals over ξ_l's for $l \geqslant d+1$ and taking $\mathcal{N}_\gamma$ into account yields their contributions.

All in all we find the prefactor,

$$A(E) = c\left(\frac{2m}{\hbar^2}\right)^{\frac{d}{2}}(-E)^{\frac{d}{2}-1}\{g(E)\}^{-\frac{(d+1)}{2}}, \tag{A12}$$

with

$$c = \left(\frac{c_\lambda}{2\pi^{\frac{1}{2}}a_d^{\frac{1}{2}}}\right)\left(2\pi c_{\rm T}^2\right)^{-\frac{d}{2}}\prod_{l=d+1}^{\infty}\left(1-\frac{2}{c_l}\right)^{-\frac{1}{2}}. \tag{A13}$$

Another expression for c is given in Ref. [19].

For $d = 1$, we get $a_d = \frac{8}{3}$, $c_\lambda = 4$, $c_{\rm T} = \frac{\sqrt{15}}{8}$, and $c_l = \frac{l(l+3)}{2}$, the last of which can be obtained through the use of Gegenbauer polynomials of order $\frac{3}{2}$ [11]. Thus $c = \frac{4}{\pi}$, conforming with the exact result obtained by Halperin [34]. For $d = 2,3$, the product is actually divergent and needs to be regularized [35].

APPENDIX B: SUPERSYMMETRIC AND REPLICA METHODS

Here we review the supersymmetric and replica derivations of Lifshitz tails. Before doing so, let us mention the original motivation for this study. A decade after the work by Zittartz and Langer [11], Cardy revisited the Lifshitz tail problem using the replica trick [13]. An instanton yielded the same exponential factor $e^{-B(E)}$, but zero-mode counting showed that the way the prefactor $A(E)$ scales with E is different from the one presented in Ref. [11]. To confirm our understanding of these methods, it is important to reconcile the dispute. The supersymmetric method was brought into this study as a judge. It turns out that the source of the disagreement lies in a minor algebraic mistake. Correcting Eq. (5.24) of Ref. [11] to

$$|\det(\nabla\nabla D)| = \left|\det\left\{2\int d\mathbf{x}V(\mathbf{x})\nabla\nabla\bar{V}(\mathbf{x})\right\}\right| \approx \left|\det\left\{2\int d\mathbf{x}\bar{V}(\mathbf{x})\nabla\nabla\bar{V}(\mathbf{x})\right\}\right| \equiv c, \tag{B1}$$

the apparent discrepancy between Refs. [11] and [13] is resolved. The eventual agreement adds confidence to the use of the replica trick in the nonperturbative regime.

Without further ado, let us present the supersymmetric derivation [14,15,36]. First we express the density of state as

$$\rho^V(E) = -\frac{1}{\pi}\lim_{\delta\to+0}{\rm Im}\left[\frac{1}{V_d}\int d\mathbf{x}G_{\rm R}^V(\mathbf{x},\mathbf{x};E+i\delta)\right]. \tag{B2}$$

The retarded one-particle Green function $G_{\mathrm{R}}^{V}(\mathbf{x},\mathbf{x}';E+i\delta)$ can be represented as

$$(-i)\frac{\int[\mathcal{D}\phi]\phi(\mathbf{x})\phi(\mathbf{x}')e^{iS_V[\phi]}}{\int[\mathcal{D}\phi]e^{iS_V[\phi]}} \tag{B3}$$

with

$$S_V[\phi]=\frac{1}{2}\int d\mathbf{x}\phi\left\{E+i\delta+\frac{\hbar^2}{2m}\nabla^2-V\right\}\phi. \tag{B4}$$

The supersymmetric method proceeds by rewriting the expression (B3) as

$$\left(\frac{-i}{2}\right)\int[\mathcal{D}\vec{\phi}\mathcal{D}\chi_1\mathcal{D}\chi_2]\vec{\phi}(\mathbf{x})\cdot\vec{\phi}(\mathbf{x}')e^{\sum_{a=1}^{2}iS_V[\phi_a]+iS_V[\chi_1,\chi_2]} \tag{B5}$$

with

$$S_V[\chi_1,\chi_2]=\frac{1}{2}\int d\mathbf{x}\chi_2\left\{E+i\delta+\frac{\hbar^2}{2m}\nabla^2-V\right\}\chi_1, \tag{B6}$$

where we doubled the bosonic field ϕ to $\vec{\phi}=(\phi_1,\phi_2)$ and introduced fermionic fields χ_1 and χ_2. Now that there is no denominator containing the random potential, we can perform functional integration over V and obtain

$$[\rho(E)]_{\mathrm{d.a.}}=\frac{1}{2\pi V_d}\mathrm{Im}\int[\mathcal{D}\vec{\tilde{\phi}}\mathcal{D}\tilde{\chi}_2\mathcal{D}\tilde{\chi}_1]\int d\mathbf{x}\vec{\tilde{\phi}}(\mathbf{x})\cdot\vec{\tilde{\phi}}(\mathbf{x}) \times e^{-S_{\mathrm{b}}[\vec{\tilde{\phi}}]-S_{2\mathrm{f}}[\tilde{\chi}_1,\tilde{\chi}_2,\vec{\tilde{\phi}}]-S_{4\mathrm{f}}[\tilde{\chi}_1,\tilde{\chi}_2]}, \tag{B7}$$

with

$$S_{\mathrm{b}}[\vec{\tilde{\phi}}]=\frac{1}{2}\int d\mathbf{x}\left[\vec{\tilde{\phi}}\cdot\left(-\frac{\hbar^2}{2m}\nabla^2-E-\frac{\gamma}{4}\vec{\tilde{\phi}}^2\right)\vec{\tilde{\phi}}\right], \tag{B8}$$

$$S_{2\mathrm{f}}[\tilde{\chi}_1,\tilde{\chi}_2,\vec{\tilde{\phi}}]=\frac{1}{2}\int d\mathbf{x}\tilde{\chi}_2\left(-\frac{\hbar^2}{2m}\nabla^2-E-\frac{\gamma}{2}\vec{\tilde{\phi}}^2\right)\tilde{\chi}_1, \tag{B9}$$

and

$$S_{4\mathrm{f}}[\tilde{\chi}_1,\tilde{\chi}_2]=-\frac{\gamma}{8}\int d\mathbf{x}(\tilde{\chi}_2\tilde{\chi}_1)^2. \tag{B10}$$

We have defined $\vec{\tilde{\phi}}\equiv e^{+\frac{i\pi}{4}}\vec{\phi}$ and $\tilde{\chi}_a\equiv e^{+\frac{i\pi}{4}}\chi_a$ for $E<0$ and the expression (B7) should be viewed with appropriate analytic continuation in mind [37,38].

To evaluate $[\rho(E)]_{\mathrm{d.a.}}$ for large negative E, we use the method of steepest descent, extremizing S_{b}. The trivial saddle $\vec{\tilde{\phi}}=0$ gives no contribution to $[\rho(E)]_{\mathrm{d.a.}}$ due to the absence of negative modes. Among nontrivial saddles, we assume that the saddles,

$$\vec{\tilde{\phi}}_{\mathrm{cl}}(\mathbf{x})=\vec{e}\sqrt{\frac{-2E}{\gamma}}f\left(\sqrt{\frac{-2mE}{\hbar^2}}|\mathbf{x}-\mathbf{x}_0|\right), \tag{B11}$$

minimize the action, where $\vec{e}$ is a constant unit vector and $f(\tilde{r})$ was defined around Eq. (14) [39]. Evaluating the action for these solutions gives the same leading exponential factor $e^{-\frac{a_d}{g}}$ as before.

In regards to the subleading prefactor, one contribution comes from

$$\int d\mathbf{x}\vec{\tilde{\phi}}_{\mathrm{cl}}(\mathbf{x})\cdot\vec{\tilde{\phi}}_{\mathrm{cl}}(\mathbf{x})\sim g^{-1}(-E)^{-1} \tag{B12}$$

in front. (We will not keep track of the overall dimensionless constant in this derivation.) To evaluate the remaining contributions, we expand around each saddle as

$$\vec{\tilde{\phi}}-\vec{\tilde{\phi}}_{\mathrm{cl}}=\vec{e}\sum_{l=0}^{\infty}\xi_l^{\mathrm{B}\parallel}\varphi_l^{\mathrm{B}\parallel}+\vec{e}_\perp\sum_{l=0}^{\infty}\xi_l^{\mathrm{B}\perp}\varphi_l^{\mathrm{B}\perp}, \tag{B13}$$

and

$$\tilde{\chi}_a=\sum_{l=0}^{\infty}\left(\xi_l^{\mathrm{F}}\right)_a\varphi_l^{\mathrm{F}}. \tag{B14}$$

Here, $\vec{e}_\perp$ is a unit vector perpendicular to $\vec{e}$, and $\varphi_l^{\mathrm{B}\parallel}$'s are a set of orthonormal functions satisfying

$$\left(-\frac{\hbar^2}{2m}\nabla^2-E-\frac{3\gamma}{2}\vec{\tilde{\phi}}_{\mathrm{cl}}^2\right)\varphi_l^{\mathrm{B}\parallel}=(-E)c_l^{\parallel}\varphi_l^{\mathrm{B}\parallel}, \tag{B15}$$

and $\varphi_l^{\mathrm{B}\perp}=\varphi_l^{\mathrm{F}}\equiv\varphi_l^{\perp}$'s are another set of orthonormal functions satisfying

$$\left(-\frac{\hbar^2}{2m}\nabla^2-E-\frac{\gamma}{2}\vec{\tilde{\phi}}_{\mathrm{cl}}^2\right)\varphi_l^{\perp}=(-E)c_l^{\perp}\varphi_l^{\perp}, \tag{B16}$$

with dimensionless numbers $c_l^{\parallel}$'s and $c_l^{\perp}$'s. We deal first with $\xi_l^{\mathrm{B}\parallel}$ fluctuations and then with the rest.

Analyzing $\varphi_l^{\mathrm{B}\parallel}$ modes, we find that the lowest mode has a negative eigenvalue $c_0^{\parallel}<0$, giving rise to a factor of

$$i(-E)^{-\frac{1}{2}}, \tag{B17}$$

and allowing the saddles to contribute to the density of states. Next come d translational zero modes. Trading integration over these modes for integration over $\mathbf{x}_0$ and dividing by the volume, we receive the Jacobian,

$$\left\{\frac{1}{d}\int d\mathbf{x}\left(\nabla\vec{\tilde{\phi}}_{\mathrm{cl}}\right)^2\right\}^{\frac{d}{2}}\sim\left\{g^{-\frac{d}{2}}\left(\frac{-2mE}{\hbar^2}\right)^{\frac{d}{2}}\right\}. \tag{B18}$$

Finally all the other modes have positive eigenvalues, each of which gives a factor of $(-E)^{-\frac{1}{2}}$.

Analyzing the other set of fluctuations, except the lowest modes, all the modes have positive eigenvalues, each of which gives a factor of $(-E)^{-\frac{1}{2}+\frac{1}{2}+\frac{1}{2}}=(-E)^{+\frac{1}{2}}$. The lowest modes are the zero modes arising from $O(2)$-rotational symmetry, proportional to $|\vec{\tilde{\phi}}_{\mathrm{cl}}(\mathbf{x})|$. The bosonic zero mode, upon trading integration over $\xi_0^{\mathrm{B}\perp}$ for integration over $\vec{e}$, yields the Jacobian,

$$\left\{\int d\mathbf{x}\vec{\tilde{\phi}}_{\mathrm{cl}}^2\right\}^{\frac{1}{2}}\sim(-E)^{-\frac{1}{2}}(g^{-\frac{1}{2}}). \tag{B19}$$

We also need to saturate fermionic zero modes by expanding the action to the quartic order in fluctuations: If we kept only quadratic terms in the expansion of the action, integration over $(\xi_0^{\mathrm{F}})_a$'s would give zero. Thus we must bring down either a factor of $\gamma\int d\mathbf{x}\tilde{\chi}_2(\vec{\tilde{\phi}}^2-\vec{\tilde{\phi}}_{\mathrm{cl}}^2)\tilde{\chi}_1$ or $\gamma\int d\mathbf{x}(\tilde{\chi}_2\tilde{\chi}_1)^2$.

After appropriate Gaussian integrations, we obtain a factor of

$$(-E)^{+\frac{2}{2}}(g^{+\frac{2}{2}}). \tag{B20}$$

Putting them all together, we recover the same result (19) as before.

Finally let us turn to the replica derivation [13]. The replica trick proceeds by rewriting the expression (B3) as

$$\left(\frac{-i}{N_{\rm r}}\right)\int[\mathcal{D}\vec{\phi}]\vec{\phi}(\mathbf{x})\cdot\vec{\phi}(\mathbf{x}')e^{i\sum_{a=1}^{N_{\rm r}}S_V[\phi_a]}, \tag{B21}$$

where we introduced $(N_{\rm r}-1)$ replicas, promoting ϕ to $\vec{\phi}=(\phi_1,\phi_2,\ldots,\phi_{N_{\rm r}})$, and took the dicey limit in which $N_{\rm r}\to 0$ to eliminate the denominator. After integrating over V and making analytic continuation, we find instantons of the same form (B11), but zero-mode analysis is slightly different from the one in the supersymmetric derivation. Besides d translational zero modes, there are $\lim_{N_{\rm r}\to 0}(N_{\rm r}-1)=-1$ bosonic zero modes coming from $O(N_{\rm r})$-rotational symmetry. The latter is replaced by the combination of one bosonic zero mode and two fermionic zero modes in the supersymmetric derivation.

We note that the instantons (B11) appearing in replica and supersymmetric derivations and the localized wave functions (13) have exactly the same shape. Thus we interpret the instantons as most likely forms of localized wave functions or square roots of localizing potentials [cf. Eq. (12)], dilutely distributed for large negative E. It may be more appropriate to call all these solutions "localons."

APPENDIX C: GENERAL FORM OF DISORDER SADDLE

In this appendix we derive coupled equations which determine saddle points of the disorder integral for scale-invariant models. Recall that we are seeking minima of the cost $\int d\mathbf{x}V^2(\mathbf{x})$ with the constraint $E^V_{1;0}-E^V_{0;0}=E$. Through the introduction of a Lagrange multiplier λ_0, the problem becomes equivalent to the minimization of

$$I[V(\mathbf{x}),\lambda_0]\equiv+\frac{1}{2}\int d\mathbf{x}V^2(\mathbf{x})+\lambda_0\big(E^V_{1;0}-E^V_{0;0}-E\big).$$

Extremizing it with respect to λ_0 reproduces the constraint

$$E^V_{1;0}-E^V_{0;0}=E, \tag{C1}$$

while extremizing it with respect to $V(\mathbf{x})$ yields

$$V(\mathbf{x})=-\lambda_0[{}_V\langle 1;0|\hat{J}^t(\mathbf{x})|1;0\rangle_V-{}_V\langle 0;0|\hat{J}^t(\mathbf{x})|0;0\rangle_V]. \tag{C2}$$

Here

$$\hat{H}_V|0;0\rangle_V=E^V_{0;0}|0;0\rangle_V, \tag{C3}$$

$$\hat{H}_V|1;0\rangle_V=E^V_{1;0}|1;0\rangle_V, \tag{C4}$$

and we used the Hellmann-Feynman relation [41,42],

$$\frac{\delta}{\delta V(\mathbf{x})}E^V_{Q;0}={}_V\langle Q;0|\hat{J}^t(\mathbf{x})|Q;0\rangle_V.$$

We can see from Eq. (C2) that the disorder saddle in general is proportional to the excess density profile of the localized state, as is the case for noninteracting systems.

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