Quantum diffusion in two-dimensional random systems with particle–hole symmetry

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Abstract

We study the scattering dynamics of an *n*-component spinor wavefunction in a random environment on a two-dimensional lattice. If the particle–hole symmetry of the Hamiltonian is spontaneously broken the dynamics of the quantum particles becomes diffusive on large scales. The latter is described by a non-interacting Grassmann field, indicating a special kind of asymptotic freedom on large scales in d = 2.

1. Introduction

Conventional wisdom is that a classical approach of a randomly scattered particle leads to diffusion. Diffusion in quantum systems can either be caused by particle–particle collisions or collisions with (static) impurity scatterers. If the latter are randomly distributed, however, this may lead to Anderson localization rather than to diffusion [1, 2]. This effect is particularly strong in low-dimensional systems such as in two-dimensional graphene sheets. The scaling approach to generic random scattering [2] indicates that diffusion is suppressed by Anderson localization for dimension $d \leq 2$. On the other hand, ballistic motion can also be ruled out, even for a finite system with random scattering [4]. It was pointed out by Kaveh, however, that diffusion cannot be obtained in random-phase approximation applied to the disordered system [3].

Inspired by the recent observation of metallic behavior (i.e. diffusive or even ballistic transport) in disordered two-dimensional systems (graphene) [5, 6], a general discussion of a diffusive quantum particle is required, which takes into account a spinor structure of the wavefunction. There are two possibilities, ballistic transport for finite systems [7, 8] or diffusive transport for infinite systems [9]. Here we will focus on infinite systems and study a quantum *n*-component spinor particle on a two-dimensional lattice with particle–hole symmetry. It will be shown that on large scales the particle diffuses on the lattice with d = 2. This work presents a generalization of the idea that a spontaneously broken supersymmetry can lead to diffusion in a system with particle–hole symmetry [9, 10].

The motion of a quantum particle is characterized by the transition probability $P_{\mathbf{r},\mathbf{r}'}(i\epsilon)$ for an *n*-component spinor particle at site \mathbf{r}' that moves to site \mathbf{r} with frequency $i\epsilon$:

$$P_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon) = \frac{K_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon)}{\sum_{\mathbf{r}} K_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon)} \quad \text{with} \quad K_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon) = \left\langle \operatorname{Tr}_n \left[G_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon) G_{\mathbf{r}',\mathbf{r}}^{\dagger}(\mathbf{i}\epsilon) \right] \right\rangle_v$$
$$= \left\langle \operatorname{Tr}_n \left[G_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon) G_{\mathbf{r}',\mathbf{r}}(-\mathbf{i}\epsilon) \right] \right\rangle_v, \tag{1}$$

where $G(i\epsilon) = (i\epsilon + H)^{-1}$ is the one-particle Green function of the Hamiltonian H and $\langle \cdots \rangle_v$ is the average with respect to some random scatterers. $Tr_n(...)$ is the trace with respect to the n spinor components. The last equation in equation (1) follows from the Hermitian Hamiltonian: $H^{\dagger} = H$.

After Fourier transformation of the two-particle Green function $K_{\mathbf{r},\mathbf{r}'}(\mathbf{i}\epsilon) \rightarrow k_{\mathbf{r},\mathbf{r}'}(t)$ we study the motion of the quantum particle with the mean-square displacement of the coordinate r_k

$$\langle r_k^2 \rangle = \frac{\sum_{\mathbf{r}} r_k^2 k_{\mathbf{r},0}(t)}{\sum_{\mathbf{r}} k_{\mathbf{r},0}(t)}.$$
(2)

This expression grows linearly with time t in the case of diffusion.

2. Model

We consider an *n*-component spinor wavefunction described by the Hamiltonian matrix

 $H = H_0 + vH_1, \quad H_0 = (h_{\mathbf{r},\alpha;\mathbf{r}',\alpha'}), \quad H_1 = (h_{\alpha,\alpha'}\delta_{\mathbf{r},\mathbf{r}'}), \quad v = (v_{\mathbf{r}}\delta_{\alpha,\alpha'}\delta_{\mathbf{r},\mathbf{r}'}), \quad (3)$

where \mathbf{r}, \mathbf{r}' are coordinates on the two-dimensional lattice and $\alpha, \alpha' = 1, 2, ..., n$ refer to the *n* spinor components. $v_{\mathbf{r}}$ is a random variable with an uncorrelated Gaussian distribution: $\langle v_{\mathbf{r}} \rangle_v = 0, \langle v_{\mathbf{r}} v_{\mathbf{r}'} \rangle_v = g \delta_{\mathbf{r},\mathbf{r}'}$. In the following we assume that the Hamiltonian satisfies the generalized particle-hole symmetry $H_j \rightarrow -UH_j^*U^{\dagger} = H_j$ (j = 0, 1), which belongs to class D according to Cartan's classification scheme [11]. In terms of the Green functions, this transformation provides a sign change of the frequency:

$$G(i\epsilon) \to -UG^T(i\epsilon)U^{\dagger} = G(-i\epsilon),$$
(4)

since $H_j^{\dagger} = H_j$ implies $H_j = -UH_j^T U^{\dagger}$ (^{*T*} is the matrix transposition). The Green functions $G(i\epsilon)$ and the transposed Green function $G^T(i\epsilon)$ can be expressed in a functional-integral representation of a free complex (boson) field $\phi_{\mathbf{r},k}^1$ and a Grassmann (fermion) field $\phi_{\mathbf{r},k}^2$, respectively. This allows us to construct the Bose–Fermi functional integral [12]

$$\langle f(\phi) \rangle_{\phi} = \int f(\phi) \,\mathrm{e}^{-S} \mathcal{D}[\phi],$$
(5)

which is normalized:

$$\int e^{-S} \mathcal{D}[\phi] = 1. \tag{6}$$

The action S is

$$S = -i(\phi \cdot (\ddot{H}_0 + i\epsilon)\phi) + g(\phi \cdot \ddot{H}_1\phi)^2 \quad (\epsilon > 0), \tag{7}$$

with respect to the boson-fermion vector field $\phi = (\phi_{\mathbf{r},k}^1, \phi_{\mathbf{r},k}^2)$ (k = 1, 2, ..., n) and with the block-diagonal Hermitian matrices $\hat{H}_j = \text{diag}(H_j, H_j^T)$. After averaging over the random variables $v_{\mathbf{r}}$ we can write

$$\left\langle G_{\mathbf{r},k;\mathbf{r}',l}(\mathbf{i}\epsilon)G_{\mathbf{r}',m;\mathbf{r},n}^{T}(\mathbf{i}\epsilon)\right\rangle_{v} = -\left\langle \phi_{\mathbf{r}',l}^{1}\bar{\phi}_{\mathbf{r},k}^{1}\phi_{\mathbf{r},n}^{2}\bar{\phi}_{\mathbf{r}',m}^{2}\right\rangle_{\phi}$$
(8)

with $\langle \cdots \rangle_{\phi} = \int \cdots e^{-S} \mathcal{D}[\phi]$. The normalization can easily be seen by performing the ϕ integration before averaging over $v_{\mathbf{r}}$.

An integral of the form (6) describes a supersymmetric field theory, meaning that it is a field theory for bosons as well as fermions which appear with the *same* Green functions [12]. However, it should be noticed that supersymmetry is sufficient for the normalized integral but not necessary [9]. In the present case the boson and the fermion Green functions are different, provided that $H^T \neq H$. The choice of different Green functions in the action (7) has profound consequences in comparison with the model, where fermions and bosons appear symmetrically with the same Green function, because the latter is subject to a larger symmetry group. This will be discussed at the end of the paper.

Using the relation in equation (8), we can write for the expression in equation (1)

$$K_{\mathbf{r},\mathbf{r}'} = \langle \operatorname{Tr}_{n}[G_{\mathbf{r},\mathbf{r}'}(i\epsilon)G_{\mathbf{r}',\mathbf{r}}(-i\epsilon)] \rangle_{v} = - \langle \operatorname{Tr}_{n}\left[G_{\mathbf{r},\mathbf{r}'}(i\epsilon)UG_{\mathbf{r}',\mathbf{r}}^{T}(i\epsilon)U^{\dagger}\right] \rangle_{v}$$

$$= \sum_{l,m,n,n'} U_{m,n}U_{l,n'}^{*} \langle \phi_{\mathbf{r}',m}^{1} \bar{\phi}_{\mathbf{r},l}^{2} \phi_{\mathbf{r}',n}^{2} \bar{\phi}_{\mathbf{r}',n}^{2} \rangle_{\phi} = -\sum_{l,m,n,n'} U_{m,n}U_{l,n'}^{*} \langle \phi_{\mathbf{r}',m}^{1} \bar{\phi}_{\mathbf{r},n'}^{2} \phi_{\mathbf{r},n'}^{1} \rangle_{\phi}.$$
(9)

This expression will be used subsequently to study diffusion in the particle-hole symmetric system.

3. Summary of the subsequent calculation

Before embarking to the detailed calculation of $K_{\mathbf{r},\mathbf{r}'}$, that will lead us to a simple expression for the functional integral on large scales $|\mathbf{r} - \mathbf{r}'|$ in terms of a saddle-point approximation, a brief outlook on the lengthy calculation is given in this section. In a first step we identify a symmetry in terms of a similarity transformation with respect to the boson-fermion structure. After introducing a new field in the functional integral, we apply a saddle-point approximation to the latter. It turns out that the above mentioned symmetry creates a two-dimensional fermionic saddle-point manifold, given by a two-component Grassmann field (φ, φ'). For large scales this becomes a free field and provides a diffusion propagator. In other words, our approximation scheme allows us to prove that the Fourier components of $K_{\mathbf{r},\mathbf{r}'}(i\epsilon)$ describe diffusion in the large distance asymptotics:

$$K_{\mathbf{q}}(\mathbf{i}\epsilon) \sim \frac{K}{\mathbf{i}b\epsilon + \tilde{c}_0 - \tilde{c}_{\mathbf{q}}}$$
(10)

with finite constants b and \bar{K} , which is determined by the solution of the saddle-point equation. Moreover, \tilde{c}_q are the Fourier components of

$$c_{\mathbf{r},\mathbf{r}'} = 16 \operatorname{Tr}_{n}[g_{+,\mathbf{r}',\mathbf{r}}Q_{2}H_{1}g_{-,\mathbf{r},\mathbf{r}'}Q_{2}H_{1}],$$

where the Green functions g_{\pm} are defined as

$$g_{\pm} = [H_0 \pm i\epsilon + 2(Q_1 \pm Q_2)H_1]^{-1}.$$
(11)

 Q_1, Q_2 are determined by saddle-point equations.

Remark. The Green functions g_{\pm} can be considered as the self-consistent Born approximation (SCBA) of the random Green functions $G(\pm i\epsilon)$, where Q_1, Q_2 are self-energies [13, 14].

4. Diffusion on large scales

In the following we derive the asymptotic form of $K_{\mathbf{r},\mathbf{r}'}$ in equation (10).

4.1. Boson-fermion symmetry

Considering the block matrix

$$\begin{pmatrix} A & \Theta \\ \bar{\Theta} & B \end{pmatrix},$$

where the elements of the matrices A, B are complex and the elements of the matrices Θ , $\overline{\Theta}$ are Grassmannian, we introduce the graded trace

$$\operatorname{Tr} g \begin{pmatrix} A & \Theta \\ \bar{\Theta} & B \end{pmatrix} = \operatorname{Tr} A - \operatorname{Tr} B,$$

where Tr is the conventional trace, and the graded determinant detg [9]:

$$\det\left(\begin{array}{cc} A & \Theta \\ \bar{\Theta} & B \end{array}\right) = \frac{\det(A)}{\det(B)} \det(\mathbf{1} - \Theta B^{-1}\bar{\Theta}A^{-1}) = \frac{\det(A - \Theta B^{-1}\bar{\Theta})}{\det(B)}.$$
 (12)

For the special matrix $\hat{H} = \text{diag}(H, H^T)$ this gives $\text{Trg}(\hat{H}) = 0$ and $\text{detg}(\hat{H} + i\epsilon) = 1$. Trg and detg have the same properties as the conventional trace and determinant. In particular, we have the relations $\text{detg}(\hat{A})\text{detg}(\hat{B}) = \text{detg}(\hat{A}\hat{B})$ and $\text{detg}(\hat{A}) = \exp(\text{Trg}(\log \hat{A}))$.

Now we consider the special matrix

$$\hat{S} = \begin{pmatrix} 0 & \varphi U \\ \varphi' U^{\dagger} & 0 \end{pmatrix} \quad (\varphi, \varphi' \in G),$$
(13)

where G is a Grassmann algebra (i.e. $\varphi \varphi' = -\varphi' \varphi$). \hat{H}_i and \hat{S} anticommute:

$$\hat{H}_{j}\hat{S} = \begin{pmatrix} 0 & H_{j}\varphi U \\ H_{j}^{T}\varphi'U^{\dagger} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varphi H_{j}U \\ \varphi'H_{j}^{T}U^{\dagger} & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\varphi UH_{j}^{T} \\ -\varphi'U^{\dagger}H_{j} & 0 \end{pmatrix} = -\hat{S}\hat{H}_{j},$$

where the second equation follows from the assumption that φ , φ' commute with H_j . This relation implies that for a global \hat{S} (i.e. \hat{S} is constant on the lattice)

$$e^{\hat{S}}\hat{H}_j e^{\hat{S}} = \hat{H}_j, \tag{14}$$

which can be considered the supersymmetry of the model defined in (7) because the transformation connects the fermionic and the bosonic sector of the theory. For the subsequent calculations, it is useful to notice that with Trg $\hat{S} = 0$ we have

$$detg(e^{S}) = exp(Trg \hat{S}) = 1.$$
(15)

4.2. Functional integral with nonlinear field

Defining the tensor field

$$\hat{\Phi}_{kk'}^{j,j'} = \bar{\phi}_k^j \phi_{k'}^{j'} \quad (j, j' = 1, 2; \ k, k' = 1, \dots, n),$$

we rewrite the terms in equation (7) as

$$(\phi \cdot \hat{H}_0 \bar{\phi}) = \operatorname{Trg}(\hat{H}_0 \hat{\Phi}), \quad (\phi \cdot \hat{H}_1 \bar{\phi})^2 = \operatorname{Trg}(\hat{H}_1 \hat{\Phi} \hat{H}_1 \hat{\Phi}).$$

Then, the identity

 $g\operatorname{Trg}(\hat{H}_1\hat{\Phi}\hat{H}_1\hat{\Phi}) + g^{-1}\operatorname{Trg}[(\mathrm{i}g\hat{H}_1\hat{\Phi} - \hat{Q})(\mathrm{i}g\hat{H}_1\hat{\Phi} - \hat{Q})] = g^{-1}\operatorname{Trg}(\hat{Q}^2) - 2\mathrm{i}\operatorname{Trg}(\hat{Q}\hat{H}_1\hat{\Phi})$ with matrix field

$$\hat{Q} = \begin{pmatrix} Q_{\mathbf{r}} & \Theta_{\mathbf{r}} \\ \bar{\Theta}_{\mathbf{r}} & iP_{\mathbf{r}} \end{pmatrix}$$

allows us to write the interaction term as a \hat{Q} integral:

$$\exp[-g\operatorname{Trg}(\hat{H}_{1}\hat{\Phi}\hat{H}_{1}\hat{\Phi})] = \int \exp[-g\operatorname{Trg}(\hat{H}_{1}\hat{\Phi}\hat{H}_{1}\hat{\Phi}) -g^{-1}\operatorname{Trg}[(ig\hat{H}_{1}\hat{\Phi} - \hat{Q})(gi\hat{H}_{1}\hat{\Phi} - \hat{Q})]]\mathcal{D}[\hat{Q}] = \int \exp[-g^{-1}\operatorname{Trg}(\hat{Q}^{2}) + 2i\operatorname{Trg}(\hat{Q}\hat{H}_{1}\hat{\Phi})]\mathcal{D}[\hat{Q}].$$

With the expression on the right-hand side we can perform the ϕ integration in the functional integral of equation (5), since ϕ appears only as a quadratic form in the exponent. Thus we remain with a functional integral over \hat{Q} :

$$\int F(\hat{\Phi}) \,\mathrm{e}^{-S} \mathcal{D}[\phi] = \int G(\hat{Q}) \mathrm{detg}(\hat{H}_0 + \mathrm{i}\epsilon + 2\hat{Q}\hat{H}_1)^{-1} \,\mathrm{e}^{-g^{-1} \operatorname{Trg}(\hat{Q}^2)} \mathcal{D}[\hat{Q}]$$
(16)

because of

$$\int e^{-\operatorname{Trg}(\hat{A}\hat{\Phi})} \mathcal{D}[\phi] = \operatorname{detg}(\hat{A})^{-1}.$$

The determinant

$$J = \det(\hat{H}_0 + i\epsilon + 2\hat{Q}\hat{H}_1)^{-1}$$
(17)

is the Jacobian for the transformation $\phi \rightarrow \hat{Q}$ in the functional integration. The function G can be obtained from F by directly calculating the integrals on both sides. This, however, is a complex task for a general F. Here we consider only one specific case which is sufficient for a diffusive mode:

$$K_{\mathbf{r},\mathbf{r}'} = -\frac{1}{g^2} \sum_{l,m,n,n'} U_{m,n} U_{l,n'}^* \langle \left(H_1^{-1} \Theta_{\mathbf{r}'}\right)_{mn} \left(H_1^{T-1} \bar{\Theta}_{\mathbf{r}}\right)_{n'l} \rangle_{\hat{\mathcal{Q}}}$$

with $\langle \cdots \rangle_{\hat{Q}} = \int \cdots J e^{-g^{-1} \operatorname{Trg}(\hat{Q}^2))} \mathcal{D}[\hat{Q}]$. Moreover, we have $H_1^T = -U^{\dagger} H_1 U$ such that

$$K_{\mathbf{r},\mathbf{r}'} = \frac{1}{g^2} \sum_{l,m,n,n'} U_{m,n} U_{l,n'}^* \langle \left(H_1^{-1} \Theta_{\mathbf{r}'} \right)_{mn} \left(U^{\dagger} H_1^{-1} U \bar{\Theta}_{\mathbf{r}} \right)_{n'l} \rangle_{\hat{Q}}.$$
 (18)

4.3. Saddle-point approximation

The saddle-point approximation of the functional integral (16) is given by a solution of the saddle-point equation $\delta_{\hat{O}}S' = 0$ with

$$S' = g^{-1} \operatorname{Trg}(\hat{Q}_0^2) + \log \operatorname{detg}(\hat{H}_0 + i\epsilon + 2\hat{Q}\hat{H}_1).$$
(19)

The saddle point is degenerate with respect to the similarity transformation

$$e^{\hat{S}}\hat{Q}_0 e^{-\hat{S}}$$
 with $\hat{Q}_0 = \begin{pmatrix} Q_0 & 0\\ 0 & iP_0 \end{pmatrix}$

This covers the entire saddle-point degeneracy because we assume here that there is no additional symmetry of H.

 \hat{Q}_0 consists of two terms, namely $\hat{Q}_0 = \hat{Q}_1 + \hat{Q}_2$, where $\hat{Q}_1(\hat{Q}_2)$ commutes (anticommutes) with \hat{S} :

$$e^{\hat{S}}\hat{Q}_0 e^{-\hat{S}} = \hat{Q}_1 + \hat{Q}_2 e^{-2\hat{S}},$$
(20)

which implies $\text{Trg}(\hat{Q}_0^2) = 0$. Then the saddle-point solution contributes to the action (19) the two terms

$$U(Q_1H_1)^T U^{\dagger} = -Q_1H_1, \quad U(Q_2H_1)^T U^{\dagger} = Q_2H_1, \tag{21}$$

where the first (second) term preserves (breaks) the symmetry of the Jacobian. These properties imply

$$Ug_{-}^{T}U^{\dagger} = -g_{+}, \qquad (22)$$

which is consistent with equation (4).

Inserting the expression (20) into the functional integral of equation (16) results in

$$\int G(e^{\hat{S}}\hat{Q}_0 e^{-\hat{S}}) \det[\hat{H}_0 + i\epsilon + 2\hat{Q}_1\hat{H}_1 + 2\hat{Q}_2\hat{H}_1 e^{2\hat{S}}]^{-1}\mathcal{D}[\hat{Q}'].$$
(23)

This indicates that \hat{Q}_2 is the order parameter for spontaneous symmetry breaking. Thus we have reduced the integration to the nonlinear field $\hat{Q}' = \hat{Q}_2 \exp(2\hat{S})$, while \hat{Q}_0 is determined by the saddle-point condition.

Now we use the identity $e^{2\hat{s}} = 2(1 - \hat{s})^{-1} - 1$ and define $\gamma_{\pm} = 4g_{\pm}Q_2H_1$ with the help of the Green functions g_{\pm} in equation (11) to obtain for the inverse Jacobian (cf appendix A)

$$J^{-1} = \bar{J}^{-1} \det(\mathbf{1} + \gamma_+ \varphi \varphi' - \varphi \gamma_- \varphi' + \gamma_+ \varphi \gamma_- \varphi') \quad \text{with}$$
$$\bar{J} = \frac{\det(-[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1])}{\det(H_0 + i\epsilon + 2Q_0H_1)}. \tag{24}$$

Using the identity $det(A) = exp{Tr[log(A)]}$, we eventually have

$$J = \overline{J} \exp\{-\mathrm{Tr}[\log(1 + \gamma_{+}\varphi\varphi' - \varphi\gamma_{-}\varphi' + \gamma_{+}\varphi\gamma_{-}\varphi')]\}.$$
(25)

4.4. Large-scale properties

The spatial diagonal elements of $\gamma_+\varphi\varphi'-\varphi\gamma_-\varphi'+\gamma_+\varphi\gamma_-\varphi'$ can be written as

$$(\gamma_{+}\varphi\varphi' - \varphi\gamma_{-}\varphi' + \gamma_{+}\varphi\gamma_{-}\varphi')_{\mathbf{r},\mathbf{r}} = (\gamma_{+} - \gamma_{-} + \gamma_{+}\gamma_{-})_{\mathbf{r},\mathbf{r}}\varphi_{\mathbf{r}}\varphi'_{\mathbf{r}} + \sum_{\mathbf{r}'}\gamma_{+,\mathbf{r},\mathbf{r}'}\gamma_{-,\mathbf{r}',\mathbf{r}}(\varphi_{\mathbf{r}'} - \varphi_{\mathbf{r}})\varphi'_{\mathbf{r}},$$
(26)

where the first part is proportional to ϵ :

$$(\gamma_+ - \gamma_- + \gamma_+ \gamma_-)_{\mathbf{r},\mathbf{r}} = -8i\epsilon g_+ g_- Q_2 H_1.$$
⁽²⁷⁾

The second term can also be expressed as

$$\sum_{\mathbf{r}'} \operatorname{Tr}_{n} \gamma_{+,\mathbf{r},\mathbf{r}'} \gamma_{-,\mathbf{r}',\mathbf{r}} (\varphi_{\mathbf{r}'} - \varphi_{\mathbf{r}}) \varphi_{\mathbf{r}}' = -\sum_{\mathbf{r}'} d_{\mathbf{r},\mathbf{r}'} \varphi_{\mathbf{r}} \varphi_{\mathbf{r}'}'$$
(28)

with

$$d_{\mathbf{r},\mathbf{r}'} = \delta_{\mathbf{r},\mathbf{r}'} \sum_{\mathbf{r}''} c_{\mathbf{r}'',\mathbf{r}'} - c_{\mathbf{r},\mathbf{r}'} \quad \text{with} \quad c_{\mathbf{r},\mathbf{r}'} = \mathrm{Tr}_n[\gamma_{+,\mathbf{r}',\mathbf{r}}\gamma_{-,\mathbf{r},\mathbf{r}'}].$$
(29)

It should be noticed in equation (28) that the spatial diagonal elements $\gamma_{\pm,\mathbf{r},\mathbf{r}}$ do not contribute. Moreover, $(\gamma_+\varphi\varphi'-\varphi\gamma_-\varphi'+\gamma_+\varphi\gamma_-\varphi')_{\mathbf{r},\mathbf{r}'}$ ($\mathbf{r}' \neq \mathbf{r}$) has at least one spatial off-diagonal factor $\gamma_{\pm,\mathbf{r},\mathbf{r}'}$ in each term. Therefore, all matrix elements $(\gamma_+\varphi\varphi'-\varphi\gamma_-\varphi'+\gamma_+\varphi\gamma_-\varphi')_{\mathbf{r},\mathbf{r}'}$ have at least one factor $\gamma_{\pm,\mathbf{r},\mathbf{r}'}$ with $\mathbf{r}' \neq \mathbf{r}$, except for the diagonal term in (27) which is proportional to ϵ .

In the next step we analyze terms that depend on the off-diagonal elements $\gamma_{\pm,\mathbf{r},\mathbf{r}'}$ ($\mathbf{r}' \neq \mathbf{r}$). Under a change of the length scale $\mathbf{r} \to \Delta \mathbf{r}$ on the two-dimensional lattice these off-diagonal terms scale as (cf appendix B)

$$\gamma_{\pm,\mathbf{r},\mathbf{r}'} \to \Delta^{-2} \gamma_{\pm,\mathbf{r},\mathbf{r}'} \quad (\mathbf{r}' \neq \mathbf{r}).$$
(30)

 ϵ is an arbitrarily small parameter which should be sent to zero. This allows us to replace $\epsilon \rightarrow \Delta^{-2}\epsilon$ here. Moreover, products of *n* matrices are of order Δ^{-2n} because $\gamma_{\pm,\mathbf{r},\mathbf{r}'}$ decays

exponentially in space due to the nonzero symmetry breaking term Q_2 . Therefore, the intermediate **r** summations do not contribute a factor Δ . Finally, the trace scales as $\text{Tr} \rightarrow \Delta^2 \text{Tr}$, and we obtain from equation (25) for the scaled Jacobian

$$J \to J_{\Delta} = \bar{J}_{\Delta} \exp\{-\Delta^{2} \operatorname{Tr}[\log(1 + \Delta^{-2}(\gamma_{+}\varphi\varphi' - \varphi\gamma_{-}\varphi' + \gamma_{+}\varphi\gamma_{-}\varphi'))]\}.$$

Thus the large-scale limit $\Delta \sim \infty$ reads

$$J_{\Delta} \sim \bar{J}_{\Delta} \exp\{-\mathrm{Tr}(\gamma_{+}\varphi\varphi' - \varphi\gamma_{-}\varphi' + \gamma_{+}\varphi\gamma_{-}\varphi')\},\tag{31}$$

which is a quadratic form of φ , φ' in the exponent (i.e. (φ, φ') is a free field). This reads with equations (27), (28)

$$J_{\Delta} \sim \bar{J}_{\Delta} \exp\left[-\sum_{\mathbf{r},\mathbf{r}'} (\mathbf{i}\epsilon b\delta_{\mathbf{r},\mathbf{r}'} + d_{\mathbf{r},\mathbf{r}'})\varphi_{\mathbf{r}}\varphi_{\mathbf{r}'}'\right] \equiv \bar{J}_{\Delta} \exp\left(-\sum_{\mathbf{r},\mathbf{r}'} \kappa_{\mathbf{r},\mathbf{r}'}^{-1}\varphi_{\mathbf{r}}\varphi_{\mathbf{r}'}'\right),\tag{32}$$

where $b = 8 \text{Tr}_n[(g_+g_-Q_2H_1)_{\mathbf{r},\mathbf{r}}]$. After Fourier transformation $\mathbf{r} \to \mathbf{q}$ we obtain

$$\tilde{d}_{\mathbf{q}} = \tilde{c}_0 - \tilde{c}_{\mathbf{q}} \text{ and } \kappa_{\mathbf{q}} = \frac{1}{\mathbf{i}b\epsilon + \tilde{c}_0 - \tilde{c}_{\mathbf{q}}}.$$
(33)

Returning to the functional integral in equation (18) we now have an integration over φ , φ' with

$$\Theta_{\mathbf{r}} = -2Q_2U\varphi_{\mathbf{r}}, \quad \bar{\Theta}_{\mathbf{r}} = 2U^{\dagger}Q_2\varphi_{\mathbf{r}}',$$

such that

$$egin{aligned} &K_{\mathbf{r},\mathbf{r}'} \sim rac{4 J_\Delta}{g^2} \sum_{m,n} U_{m,n} ig(H_1^{-1} Q_2 U ig)_{mn} \sum_{l,n'} U_{l,n'}^* ig(U^\dagger H_1^{-1} Q_2 ig)_{n'l} ig\langle arphi_{\mathbf{r}} arphi_{\mathbf{r}'}^\prime ig
angle \ &= rac{4 ar{J}_\Delta}{g^2} \mathrm{Tr}_n ig(U U^T H_1^{-1} Q_2 ig) \mathrm{Tr}_n (U^* U^\dagger H_1^{-1} Q_2) ig\langle arphi_{\mathbf{r}} arphi_{\mathbf{r}'}^\prime ig
angle \end{aligned}$$

with $\langle \varphi_{\mathbf{r}} \varphi'_{\mathbf{r}'} \rangle = -\kappa_{\mathbf{r}',\mathbf{r}'}/\det(\kappa)$. Using the Fourier components in equation (33), the Fourier transformation of $K_{\mathbf{r},\mathbf{r}'}$ reads

$$\tilde{K}_{\mathbf{q}} \sim \frac{\bar{K}}{\mathrm{i}b\epsilon + \tilde{c}_0 - \tilde{c}_{\mathbf{q}}},\tag{34}$$

where

$$\bar{K} = \frac{4\bar{J}_{\Delta}}{\det(\kappa)g^2} \operatorname{Tr}_n(UU^T H_1^{-1}Q_2) \operatorname{Tr}_n(U^* U^{\dagger} H_1^{-1}Q_2).$$

This concludes our calculation of the large-scale properties of $K_{\mathbf{r},\mathbf{r}'}$.

4.5. Alternative approach: nonlinear sigma model

Returning to the expression in equation (23), we can expand the logarithm of the Jacobian in powers of \hat{Q}_2 up to second order. This approximation is referred to as the nonlinear sigma model approach which is believed to provide a good description of the transport properties of disordered systems [15, 16]. For our model we derive the nonlinear sigma model for the action

$$S' = \log[\det(\hat{H}_0 + i\epsilon + 2\hat{Q}_1\hat{H}_1 + 2\hat{Q}_2\hat{H}_1e^{2\hat{S}})]$$

= $\log[\det(\hat{H}_0 + i\epsilon + 2(\hat{Q}_1 + \hat{Q}_2)\hat{H}_1 + 2\hat{Q}_2\hat{H}_1(e^{2\hat{S}} - \mathbf{1}))],$

where $e^{2\hat{S}} - 1 = 2(\hat{S} + \hat{S}^2)$. With

$$\hat{G}_0 = \begin{pmatrix} g_+ & 0 \\ 0 & -U^{\dagger}g_-U \end{pmatrix}^{-1} = \begin{pmatrix} g_+ & 0 \\ 0 & g_+^T \end{pmatrix}^{-1}$$

we can expand the action up to second order in \hat{Q}_2 as $S' \approx S_0 + S''$ with

$$S'' = 4 \operatorname{Trg}(\hat{G}_0 \hat{Q}_2 \hat{H}_1 (\hat{S} + \hat{S}^2)) + 8 \operatorname{Trg}[(\hat{G}_0 \hat{Q}_2 \hat{H}_1 (\hat{S} + \hat{S}^2))^2]$$

= 4 \text{Trg}(\text{\text{G}}_0 \hat{Q}_2 \hat{H}_1 \hat{S}^2) + 8 \text{Trg}[(\text{G}_0 \hat{Q}_2 \hat{H}_1 \hat{S})^2] + 8 \text{Trg}[(\text{G}_0 \hat{Q}_2 \hat{H}_1 \hat{S}^2)^2]. (35)

 $\hat{G}_0\hat{Q}_2\hat{H}_1$ can be approximated by a gradient operator. This gives the standard form of the nonlinear sigma model for the last two terms, whereas the first term contributes to the symmetry-breaking term which is proportional to i ϵ . Moreover, a straightforward calculation shows that the last term vanishes for our model

$$\operatorname{Trg}[(\hat{G}_0 \hat{Q}_2 \hat{H}_1 \hat{S}^2)^2] = 0, \tag{36}$$

such that only the quadratic terms in φ survive in the nonlinear sigma model. This is in agreement with the exponent in equations (31) and (32).

5. Discussion

Our derivation of $K_{\mathbf{r},\mathbf{r}'}$ in the previous section was obtained without specifying H_0 , H_1 of the Hamiltonian. This prevents us from determining Q_1 , Q_2 here because this requires the solution of the saddle-point equation. It is crucial though that the symmetry breaking term Q_2 represents a mass to the Green functions γ_{\pm} such that the latter decay exponentially. There is no diffusion but localization for saddle-point solutions with $Q_2 = 0$, as discussed for the case of Weyl fermions in [10].

We leave the determination of Q_1 , Q_2 for specific Hamiltonians to further work and study only the general structure of the diffusion propagator in equation (34). For the large-scale behavior of the latter we consider $q \sim 0$

$$\tilde{K}_{\mathbf{q}} \sim \frac{\bar{K}}{b} \frac{1}{\mathbf{i}\epsilon + \sum_{i,j} D_{ij} q_i q_j} \tag{37}$$

with

$$ilde{d}_{\mathbf{q}} = ilde{c}_0 - ilde{c}_{\mathbf{q}} \sim b \sum_{i,j} D_{ij} q_i q_j$$

and with the diffusion coefficients

$$D_{ij} = -\frac{1}{2b} \frac{\partial^2 \tilde{c}_q}{\partial q_i \partial q_j} \Big|_{q=0} = \frac{\sum_{\mathbf{r}} r_i r_j \operatorname{Tr}_n [g_{+,0,\mathbf{r}} Q_2 H_1 g_{-,\mathbf{r},0} Q_2 H_1]}{\operatorname{Tr}_n [(g_{+} g_{-} Q_2 H_1)_{\mathbf{r},\mathbf{r}}]}.$$

In the isotropic case (i.e. for $D_{ij} = D\delta_{ij}$) we have

$$\tilde{d}_{\mathbf{q}} = \tilde{c}_0 - \tilde{c}_{\mathbf{q}} \sim bDq^2, \quad D = -\frac{1}{2b} \frac{\partial^2 \tilde{c}_{\mathbf{q}}}{\partial q_k^2} \Big|_{q=0} = \frac{1}{2b} \sum_{\mathbf{r}} r_k^2 c_{\mathbf{r},0}$$

such that the diffusion propagator reads

$$\tilde{K}_{\mathbf{q}}(\mathbf{i}\epsilon) = \frac{\bar{K}}{\mathbf{i}b\epsilon + \tilde{c}_0 - \tilde{c}_{\mathbf{q}}} \sim \frac{\bar{K}}{b} \frac{1}{\mathbf{i}\epsilon + Dq^2}.$$
(38)

From the diffusion propagator we can evaluate the dynamics of the quantum walk. We apply a Fourier transformation from frequency ϵ to time *t* and get

$$\tilde{K}_{\mathbf{q}}(\mathbf{i}\epsilon) \to K_{\mathbf{q}}(t) = \frac{K}{b} \mathrm{e}^{-Dq^2t},$$

and a Fourier transformation from momentum q to real space coordinates r gives

$$K_{\mathbf{q}}(t) \rightarrow k_{\mathbf{r}}(t) = \frac{\bar{K}}{b} \frac{\mathrm{e}^{-r^2/4Dt}}{\pi Dt}$$

This provides the mean-square displacement as a function of time:

$$\langle r_k^2 \rangle = \frac{\sum_{\mathbf{r}} r_k^2 k_{\mathbf{r}}(t)}{\sum_{\mathbf{r}} k_{\mathbf{r}}(t)} \sim 2Dt.$$
(39)

There is a simple scaling relation between the two-particle Green function $K_{r,0}$ in equation (1) and saddle-point expression $c_{r,0}$ in equation (29) as

$$\sum_{\mathbf{r}} r_k^2 K_{\mathbf{r},0}(\mathbf{i}\epsilon) \sim \frac{\bar{K}}{b^2 \epsilon^2} \sum_{\mathbf{r}} r_k^2 c_{\mathbf{r},0}.$$
(40)

This result can be considered as an extension of the self-consistent Born approximation to $K_{\mathbf{r},\mathbf{r}'}$.

Example. Weyl fermions with random gap: n = 2, $H_0 = i\partial_x\sigma_1 + i\partial_y\sigma_2$, $H_1 = \sigma_3$, $U = \sigma_1$, $Q_1 = 0$, $Q_2 = -i(\eta/2)\sigma_3$, where $\{\sigma_j\}$ are Pauli matrices. The saddle-point equation reads in this case [10]

$$\operatorname{Tr}_{2}[(g_{+}g_{-})_{\mathbf{r},\mathbf{r}}] = g^{-1}.$$

Inserting this in our expressions above, we obtain $b = 4i\eta/g$, $\bar{K}/b^2 = -1/4$,

$$c_{\mathbf{r},0} = -4\eta^2 \operatorname{Tr}_2[g_{+,0,\mathbf{r}}g_{-,\mathbf{r},0}], \quad \sum_{\mathbf{r}} r_k^2 K_{\mathbf{r},0}(\mathbf{i}\epsilon) \sim -\frac{1}{4\epsilon^2} \sum_{\mathbf{r}} r_k^2 c_{\mathbf{r},0} = \frac{1}{2\pi\epsilon^2}.$$

Here we have fixed the cut-off Λ in equation (B.1) such that det(κ) = 1. The conductivity σ can be calculated from this expression via the Kubo approach by an analytic continuation $\epsilon \rightarrow i\omega/2$ [10]:

$$\sigma \sim -\frac{e^2}{2h}\omega^2 \sum_{\mathbf{r}} r_k^2 K_{\mathbf{r},0}(-\omega/2) = \frac{e^2}{\pi h},\tag{41}$$

which is the well-known minimal conductivity of graphene (except for an additional degeneracy factor 4) [5]. The disorder independent conductivity reflects the well-known fact that the conductivity can not distinguish between ballistic and diffusive transport of Weyl fermions [13]. The diffusive behavior was also found in recent numerical simulations by Chalker *et al* [17] and Medvedyeva *et al* [18].

5.1. Broken particle-hole symmetry

We introduce a chemical potential μ that shifts away from particle-hole symmetry point by $\pm \mu$ in the Hamiltonian

$$\bar{H} = \begin{pmatrix} H + \mu\sigma_0 & 0 & 0 & 0 \\ 0 & H - \mu\sigma_0 & 0 & 0 \\ 0 & 0 & H^T - \mu\sigma_0 & 0 \\ 0 & 0 & 0 & H^T + \mu\sigma_0 \end{pmatrix}.$$
 (42)

Then we define the Green function in analogy to $\hat{G}(i\epsilon)$ as

$$\bar{G}(i\epsilon) = (\bar{H} + i\epsilon)^{-1}.$$
(43)

The generalization of transformation matrix \hat{S} in equation (13) then is

$$\bar{S} = \begin{pmatrix} 0 & 0 & \varphi_1 U & 0 \\ 0 & 0 & 0 & \varphi_2 U \\ \varphi_1' U^{\dagger} & 0 & 0 & 0 \\ 0 & \varphi_2' U^{\dagger} & 0 & 0 \end{pmatrix}$$
(44)

which anticommutes with \overline{H} : $\overline{S}\overline{H} = -\overline{H}\overline{S}$. This implies the symmetry transformation

$$e^{\bar{S}}\bar{H}e^{\bar{S}}=\bar{H}$$

and detg($e^{\bar{S}}$) = exp(Trg \bar{S}) = 1. Now we can employ the expansion of equation (35) to obtain the nonlinear sigma model. It turns out that the fourth-order term in \bar{S} does not vanish for $\mu \neq 0$, in contrast to the result in equation (36).

6. Conclusions

We have seen that the discrete particle-hole symmetry of the Hamiltonian $H \rightarrow -UH^*U^{\dagger} = H$ can lead to a diffusive behavior. For this result it is crucial that no additional continuous symmetry exists for the *H*. A typical realization of this case are two-dimensional Weyl-Dirac fermions with random gap [9]. The diffusive behavior requires a non-vanishing symmetrybreaking term \hat{Q}_2 , which reflects spontaneous breaking of the symmetry in equation (14). \hat{Q}_2 must be determined as a solution of the saddle-point equation. This can, depending on the specific Hamiltonian *H*, generate a complex phase diagram with metallic (i.e. diffusive), insulating and quantum-Hall phases (cf [10]).

A central fact in section 4.4 is that the saddle-point integration in equation (23) is restricted to a two-component Grassmann field (φ , φ'). This is crucial for the derivation of the main result. The integration would be over a larger manifold when the underlying Hamiltonian has additional symmetries or in the absence of particle–hole symmetry. The latter case was briefly discussed in section 5.1 where we introduced a shift away from the particle–hole symmetry point. The integration over a larger manifold may result in a non-diffusive behavior.

There is a large number of publications on the subject of disordered particle–hole symmetric Hamiltonians (class D), which are based on (i) field theory (in particular, nonlinear sigma models), (ii) related network models and (iii) numerical simulations. A discussion with many references can be found, for instance, in [19]. Unfortunately, there is no simple conclusion from all the publications because the details of the results depend on the specific form of the Hamiltonians or the network models, the distribution of disorder as well as on the approximations used in analytic treatments. Moreover, the mapping from network models onto Hamiltonian models is only understood on an approximative level [20, 21].

The approach discussed in this paper, which was originally proposed in [9], offers an alternative to the nonlinear sigma model used in [22]. The main difference between the two approaches is that the former is not supersymmetric, in contrast to the latter. The reason is that we started from the asymmetric two-particle (Bose–Fermi) Hamiltonian $\hat{H} = \text{diag}(H, H^T)$ in the construction of the functional integral in equation (7), whereas Bocquet et al used the symmetric two-particle (Bose–Fermi) Hamiltonian $\hat{H} = \text{diag}(H, H)$. This difference has several consequences for the effective field theory of the average Green functions. First, the saddle-point manifold defined in equation (20) is different from the ortho-symplectic Lee group OSp(2n|2n)/GL(n|n) which generates the manifold of the symmetric approach [22]. Second, the massless mode is only the two-component Grassmann field (φ, φ') in the asymmetric approach, whereas it consists of Grassmann and Goldstone (bosonic) components in the symmetric approach. Thus the saddle-point integration is more complex in the latter. It was treated within a renormalization-group approach, which provides an ideal metallic fixed point with infinite conductivity, in contrast to our finite conductivity in equation (41). Besides its technical simplicity, the asymmetric approach provides a metal-insulator phase diagram [10], which agrees qualitatively with the numerically determined phase diagram of Chalker et al [17].

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Appendix A. Jacobian

The inverse Jacobian in equation (23) reads

$$\begin{split} J^{-1} &= \det(\hat{H}_0 + i\epsilon + 2\hat{Q}_1\hat{H}_1 + 2\hat{Q}_2\hat{H}_1e^{2\hat{S}}) \\ &= \det(\hat{H}_0 + i\epsilon + 2\hat{Q}_1\hat{H}_1 - 2\hat{Q}_2\hat{H}_1 + 4\hat{Q}_2\hat{H}_1(1-\hat{S})^{-1}). \quad (A.1) \end{split}$$
 After pulling out the factor $(1-\hat{S})^{-1}$ we get

$$J^{-1} &= \det(1-\hat{S})^{-1}\det(\hat{H}_0 + i\epsilon + 2\hat{Q}_0\hat{H}_1 - [\hat{H}_0 + i\epsilon + 2(\hat{Q}_1 - \hat{Q}_2)\hat{H}_1]\hat{S}). \end{split}$$
 The (anti) commutation relation of \hat{Q}_1 (\hat{Q}_2) implies

$$iUP_j = -(-1)^j Q_j U, \quad U^{\dagger}Q_j = -i(-1)^j P_j U^{\dagger} \quad (j = 1, 2) \end{cases}$$
 and yields

$$J^{-1} = \det[1(1-\varphi\varphi')]^{-1}\frac{\det(H_0 + i\epsilon + 2Q_0H_1)}{\det(H_0^{\intercal} + i\epsilon + 2iP_0H_1^{\intercal})}\det(1-[H_0 + i\epsilon + 2(Q_1 - Q_2)H_1]\varphi) \\ \times [H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}(H_0 - i\epsilon + 2Q_0H_1)\varphi'(H_0 + i\epsilon + 2Q_0H_1)^{-1}). \end{split}$$
 In the second factor, P_j can be expressed by Q_j such that

$$\det(H_0^{\intercal} + i\epsilon + 2iP_0H_1^{\intercal}) = \det(U(H_0^{\intercal} + i\epsilon + 2iP_0H_1^{\intercal})U^{\dagger}) \\ = \det(-[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}(H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]). \end{split}$$
With the identities

$$[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}(H_0 - i\epsilon + 2(Q_1 + Q_2)H_1) \\ = 1 + [H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}4Q_2H_1 \\ =: 1 + 4g_-Q_2H_1$$
and

$$[H_0 + i\epsilon + 2(Q_1 + Q_2)H_1]^{-1}(H_0 - i\epsilon + 2(Q_1 + Q_2)H_1) \\ = 1 - [H_0 + i\epsilon + 2(Q_1 + Q_2)H_1]^{-1}Q_2H_1 \\ =: 1 - 4g_+Q_2H_1$$
and with det $(1 - \varphi\varphi')^{-1} = \det(1 + \varphi\varphi')$ we get eventually

$$J^{-1} = \frac{\det(H_0 + i\epsilon + 2Q_0H_0)}{\det(-[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1} \\ \times \varphi\{1 + 4[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1\} \\ \times \varphi\{1 + 4[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1]\varphi'). \qquad (A.2)$$
Moreover, we have

$$\det(1 - [4 - 4[H_0 + i\epsilon + 2(Q_1 + Q_2)H_1]^{-1}Q_2H_1]\varphi') \\ = \det(1 - \varphi\varphi' + 4[H_0 + i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1]\varphi') \\ = \det(1 - \varphi\varphi' + 4[H_0 + i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1\varphi') \\ + 16[H_0 + i\epsilon + 2(Q_1 - Q_2)H_1]^{-1}Q_2H_1\varphi'$$

 $= \det(\mathbf{1} - \varphi \varphi' + 4g_+ Q_2 H_1 \varphi \varphi' - 4\varphi g_- Q_2 H_1 \varphi' + 16g_+ Q_2 H_1 \varphi g_- Q_2 H_1 \varphi').$

Thus, we get for the expression in equation (A.2)

$$J^{-1} = \frac{\det(H_0 + i\epsilon + 2Q_0H_1)}{\det(-[H_0 - i\epsilon + 2(Q_1 - Q_2)H_1])} \det(1 + 4g_+Q_2H_1\varphi\varphi' - 4\varphi g_-Q_2H_1\varphi' + 16g_+Q_2H_1\varphi g_-Q_2H_1\varphi').$$

Appendix B. Scaling transformation

The Green function of the saddle-point approximation in equation (11) reads in Fourier representation

$$g_r = \int_0^{\Lambda} \frac{\int_0^{2\pi} e^{iqr\cos\alpha} d\alpha}{i\epsilon + m + q^2} q dq, \qquad (B.1)$$

where *m* is an effective mass that is created by the saddle-point matrices $Q_1 \pm Q_2$. Rescaling $r \rightarrow \Delta r$ then gives

$$g_{\Delta r} = \int_0^{\Lambda} \frac{\int_0^{2\pi} e^{i\Delta qr\cos\alpha} d\alpha}{i\epsilon + m + q^2} q dq = \Delta^{-2} \int_0^{\Delta\Lambda} \frac{\int_0^{2\pi} e^{ipr\cos\alpha} d\alpha}{i\epsilon + m + p^2/\Delta^2} p dp \sim \Delta^{-2} g_r$$
(B.2)

if $m \sim 1$, since the integral is dominated by small p and does not depend on the cut-off $\Delta \Lambda$.

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