Zero-energy states in corrugated bilayer graphene

M. I. Katsnelson[1,*] and M. F. Prokhorova[2,†]

[1]*Institute for Molecules and Materials, Radboud University of Nijmegen, 6525ED Nijmegen, The Netherlands*
[2]*Institute of Mathematics and Mechanics, Kovalevskaya strasse 16, 620219 Ekaterinburg, Russia*

Anomalous quantum Hall effects in single-layer and bilayer graphene are related with nontrivial topological properties of electron states (Berry phases π and 2π, respectively). It was known that the Atiyah-Singer index theorem guarantees, for the case of the single layer, existence of zero-energy states for the case of inhomogeneous magnetic fields assuming that the total flux is nonzero. This leads, in particular, to the appearance of midgap states in corrugated graphene and topologically protects zero-energy Landau level in corrugated single-layer graphene. Here we apply this theorem to the case of bilayer graphene and prove the existence of zero-energy modes for this case.

I. INTRODUCTION

Graphene, which is a two-dimensional allotrope of carbon formed by a single carbon atom sheet is a subject of hot interest now (for review, see Refs. [1–4]). One of the most interesting aspects of the graphene physics, from a theoretical point of view, is a deep and fruitful relation with the quantum electrodynamics and quantum field theory.[5–12] As was proven experimentally in Refs. [13] and [14] charge carriers in the single-layer graphene are massless Dirac fermions characterized by "chirality," or "Berry phase" π. As a consequence, graphene demonstrates anomalous quantum Hall effect due to the existence of the zero-energy Landau level. The latter can be considered[2,11,13] as a simple consequence of the famous Atiyah-Singer index theorem,[15] which plays an important role in the modern quantum field theory and theory of superstrings.[16,17]

Charge carriers in bilayer graphene, formed by *two* graphite atomic sheets,[18] can be, in a good approximation, considered as chiral fermions with the Berry phase 2π, which leads to another type of anomalous quantum Hall effect[18,19] and to a very unusual character of electron transmission through potential barriers.[9] Exact solution of the Schrödinger equation for the bilayer graphene in homogeneous magnetic field[19] demonstrates the existence of the zero-energy Landau level with twice larger degeneracy than for the case of a single layer. However, the topological origin of this feature was not clarified yet. This is the aim of the present work. We will prove that the existence of the zero-energy states in bilayer graphene is also a consequence of the Atiyah-Singer index theorem and thus is topologically protected.

This is an important question since it is known[20–25] that graphene is always corrugated and covered by ripples, which can be either intrinsic[21,22,25,26] or induced by a roughness of substrate.[23,24] In general, nonflatness of graphene leads to the appearance of the pseudomagnetic *inhomogeneous* gauge field[20,27] acting on the charge carriers. Based on the topological arguments one can demonstrate that this pseudomagnetic field should also result in the appearance of zero-energy states (pseudo-Landau levels) as was recently confirmed by model[28] and first-principles[29] electronic structure calculations. This can provide a mechanism of formation of charge

inhomogeneity in corrugated graphene[28] and thus essentially will have an effect on its electronic properties. Also, this "topological protectorate" of the zero-energy Landau level can explain why it is narrower than the higher-energy levels as was recently observed experimentally.[30] The ripples in bilayer graphene have already been observed experimentally,[22] but it is still not clear whether this leads to the formation of zero-energy states, similar to the case of single layer (or not). Here we give a positive answer to this question based on a very general topological consideration.

II. FORMULATION OF THE PROBLEM

The corrugation leads to important consequences for the electronic structure of graphene. The nearest-neighbor hopping integral γ turns out to be fluctuating due to its dependence on the deformation tensor[26]

$$\bar{u}_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j} + \frac{\partial h}{\partial x_i}\frac{\partial h}{\partial x_j}\right), \qquad (1)$$

where h is the displacement in the direction perpendicular to the graphene plane, $x_i = (x,y)$ are coordinates in the plane, and u_i are the corresponding components of the displacement vector,

$$\gamma = \gamma_0 + \left(\frac{\partial \gamma}{\partial \bar{u}_{ij}}\right)_0 \bar{u}_{ij}. \qquad (2)$$

Taking into account this inhomogeneity in a standard tight-binding description of the electronic structure of graphene[4] one can obtain an effective Dirac-type Hamiltonian describing electron states near the conical K point as follows:

$$H = v_F \sigma(-i\hbar\,\nabla - \mathcal{A}), \qquad (3)$$

where $v_F = \sqrt{3}\gamma_0 a/2\hbar$ and $\mathcal{A}$ is the "vector potential" connected with the deviations of the hopping parameters γ_i from their unperturbed value γ_0.

$$\mathcal{A}_x = \frac{1}{2v_F}(\gamma_2 + \gamma_3 - 2\gamma_1), \quad \mathcal{A}_y = \frac{\sqrt{3}}{2v_F}(\gamma_3 - \gamma_2), \qquad (4)$$

where the nearest neighbors with vectors $(-a/\sqrt{3},0)$, $(a/2\sqrt{3},-a/2)$, and $(a/2\sqrt{3},a/2)$ are labeled 1, 2, and 3, re-

spectively. a is the lattice constant.[11] This means that the flexural fluctuations act on the electronic structure near the K point as an Abelian gauge field, which is equivalent to the action of a random magnetic field. Thus, the bending of graphene violates the time-reversal symmetry for a given valley; of course, the Umklapp processes between the K and K' points will restore this symmetry. As was suggested in Ref. 20 these effective magnetic fields might be responsible for suppression of the weak localization effects in graphene.

Whereas a smooth deformation of the graphene sheets produces the gauge field similar to the electromagnetic one, different topological defects in graphene inducing intervalley (Umklapp) processes can be considered as sources of a non-Abelian gauge field; corresponding analogy with gravitation was discussed in Refs. 31 and 32.

The bilayer graphene in the simplest approximation can be considered as a zero-gap semiconductor with parabolic touching of the electron and hole bands described by the single-particle Hamiltonian[18,19]

$$H = \begin{pmatrix} 0 & -(p_x - ip_y)^2/2m \\ -(p_x + ip_y)^2/2m & 0 \end{pmatrix}, \quad (5)$$

where $p_i = -i\hbar \, \partial/\partial x_i - \mathcal{A}_i$ are electron momenta operators and $m \simeq 0.054 m_e$ is the effective mass, with m_e being the free-electron mass. This description is accurate at the energy scale larger than a few meV, otherwise a more complicated picture including trigonal warping takes place;[19] we will restrict ourselves only by the case of not too small doping when the approximate Hamiltonian (5) works. Two components of the wave function originated from the crystallographic structure of graphite sheets with two carbon atoms in the sheet per elementary cell. There are two touching points per Brillouin zone: K and K'. For smooth enough external potential, no Umklapp processes between these points are allowed and thus they can be considered independently.

We will prove that the zero-energy states in the case of the bilayer found by the exact solution for the case of homogeneous magnetic field[19] are topologically protected and their number is determined only by the total flux per sample, irrespective to whether the field is homogeneous or not, exactly as in the case of the single layer.[2,11,13]

III. RESULTS AND DISCUSSION

The proof is based on the theory of elliptic operators and on the Atiyah-Singer index theorem. Let us first be reminded of some facts about these theories. Let X be a smooth compact manifold and E and E' be smooth complex bundles over X (we shall use the word "smooth" in the sense of "infinitely differentiable"). Let D be a smooth linear differential operator of order m acting from $C^\infty(E)$ to $C^\infty(E')$, where $C^\infty(E)$ is the vector space of smooth sections of E. Here smoothness of the operator is regarded as smoothness of its coefficients in any smooth local coordinates.

In local coordinates (x^i) on X the highest-order terms of D have a form $\sum a^{i_1 \cdots i_m}(x) \frac{\partial}{\partial x^{i_1}} \cdots \frac{\partial}{\partial x^{i_m}}$. Let us consider the expression $\sum a^{i_1 \cdots i_m}(x) \xi_{i_1} \cdots \xi_{i_m}$, $\xi \in T^*X$, with T^*X being the cotangent bundle of X. It is independent of the choice of local

coordinates and defines the homomorphism of vector bundles $\pi_* E \to \pi_* E'$, which is homogeneous of degree m by ξ. Here $\pi_* E$, $\pi_* E'$ are the liftings of the bundles E, E' to T^*X (see the commutative diagrams below; vertices on the diagrams are smooth manifolds and arrows are smooth maps).

$$
\begin{array}{ccc}
\pi_* E & \xrightarrow{\pi_*} & E \\
\downarrow & & \downarrow \\
T^*X & \xrightarrow{\pi} & X
\end{array}
\qquad
\begin{array}{ccc}
\pi_* E & \xrightarrow{\sigma(D)} & \pi_* E' \\
\searrow & & \swarrow \\
& T^*X &
\end{array}
$$

This homomorphism $\pi_* E \to \pi_* E'$ is called *symbol* $\sigma(D)$ of differential operator D. The latter is called *elliptic* if $\sigma(D)$ is invertible outside the zero section of T^*X (that is invertible at $\xi \neq 0$ in local coordinates).

Elliptic operators have a good behavior:[15] if D: $C^\infty(E) \to C^\infty(E')$ is a smooth elliptic operator, then

(1) All distributional solutions of D are smooth.

(2) Ker D (the space of solutions of the equation $D\psi=0$) and Coker D (the factor space of $C^\infty(E')$ by the image $\{D\psi\}$ of D) are finite dimensional.

(3) The value index$D \triangleq \dim$ Ker $D - \dim$ Coker D depends only on the symbol of D; moreover, index$D$ depends only on the homotopy class of symbol in the space of continuous invertible symbols of a given order.

The rough idea of the proof is the following. We consider the two-periodic case (a justification of this choice will be discussed below); a wave function is the section of complex linear bundle E over two-dimensional torus X. The vector potential $\mathcal{A}$ defines the connection $\nabla_j = \frac{\partial}{\partial x_j} - \frac{i}{\hbar} \mathcal{A}_j$ on E; its flux $\hbar^{-1} \int_X d\mathcal{A}$ defines the bundle E up to isomorphism.

The differential operators $p_x \pm ip_y$ are elliptic operators acting on $C^\infty(E)$. They are conjugated so the cokernel of $p_x + ip_y$ is isomorphic to the kernel of $p_x - ip_y$ and vice versa. Therefore the difference of dimensions of the kernels of $p_x + ip_y$ and $p_x - ip_y$ is equal to the index of operator $p_x + ip_y$. The same is valid for the squares of these operators, thus $\dim \text{Ker}(p_x + ip_y)^2 - \dim \text{Ker}(p_x - ip_y)^2 = \text{index}(p_x + ip_y)^2$.

The desired result follows just from the fact that the index of the composition of elliptic operators is equal to the sum of their indices,[33] so we have index$(p_x+ip_y)^2 = 2$ index$(p_x + ip_y)$.

According to the Atiyah-Singer theorem the index of operator $p_x + ip_y$ depends only on the symbol of $p_x + ip_y$ determined by the integer number $N = (2\pi\hbar)^{-1} \int_X d\mathcal{A}$ and does not depend on the choice of the field $\mathcal{A}$ for a given number of this integral. We obtain index$(p_x+ip_y)=N$ from purely topological considerations, replacing operator $p_x + ip_y$ by the other operator with the same symbol and known index. In physical terms, N is the total flux of the (pseudo)magnetic field per torus in the units of the flux quantum.

It is worth stressing that the "vector potentials" $\mathcal{A}$ are assumed not to be very smooth in our proof, but just continuously differentiable, which makes the result rather general.

The choice of the torus can be justified by standard arguments used at the introduction of the Born–von Karman periodic boundary conditions in solid state theory.[34] Namely, the total number of zero-energy modes, assuming that N

$\neq 0$ is proportional to the total number of atoms in the sample N_0. At the same time, if one replaces "realistic" boundary conditions by the periodic ones the total density of states can be changed by a quantity proportional to the number of edge atoms; that is, $\sqrt{N_0}$. This means that the total number of states with the energy *close* to zero should be, in the limit of large crystallite, correctly described by the periodic case; that is, the case of torus. Note that the torus has zero Gaussian curvature, which physically means the absence of topological defects, such as disclinations (pentagons of heptagons in the original hexagonal lattice).[31,32]

The physical consequences are straightforward: for the case of bilayer graphene as well as for the case of the single-layer graphene, (i) corrugations can result in the appearance of the midgap states[28] and (ii) pseudomagnetic fields due to corrugations will not broaden the zero-energy Landau level in the case of the quantum Hall effect.[30] It would be very interesting to experimentally check the second statement by measurements of the quantum Hall activation gaps for the bilayer graphene, similar to Ref. 30 for the case of single-layer graphene. A mathematical proof of the statement is presented in the Appendix.

ACKNOWLEDGMENTS

APPENDIX

Let Γ be a lattice in the two-dimensional Euclidean space $\mathbb{R}^2$, $X = \mathbb{R}^2$ mod Γ be the two-dimensional torus, and E be a smooth linear complex vector bundle over X with structure group $U(1)$. Let us have a C^1-connection on E; that is, corresponding covariant derivatives are written as $\nabla_x = \frac{\partial}{\partial x} - iA_x$, $\nabla_y = \frac{\partial}{\partial y} - iA_y$, where A_x and A_y are *continuously differentiable* real functions in local coordinates (x, y) on X (these coordinates we choose as the usual coordinates on universal covering $\mathbb{R}^2$ of X, so they are defined up to the addition of vectors from Γ).

Although the connection form $A = A_x dx + A_y dy$ depends on the choice of local coordinates, its curvature dA is globally defined on X. We can integrate dA over X; this integral depends only on the isomorphism class of E and does not depend on the choice of connection on E. Let

$$N(E) = (2\pi)^{-1} \int_X dA. \qquad (A1)$$

This number must be an integer.

Following Ref. 15, we consider Hilbert spaces $H_s(E)$ of those distributional sections u of E for which $Du \in L_2(X)$ for all differential operators $D: C^\infty(E) \to C^\infty(1_X)$ with smooth coefficients, and of order $\leq s$. Here, $C^\infty(E)$ is the space of smooth sections of E and 1_X is the trivial linear complex bundle over X. The Hermitian product in $H_s(E)$ can be defined at $s=0$ as $\langle u, v \rangle_0 = \int_X \langle u, v \rangle dx dy$ and at $s>0$ as $\langle u, v \rangle_s$

$= \int_X \langle \Delta^s u, v \rangle dx dy$. Here $\Delta = 1 + D^* D$, $D: C^\infty(E) \to C^\infty(E \otimes T^*X)$ is the covariant derivative given by some fixed smooth connection on E (the precise choice of this connection is irrelevant for our aims).

We can consider differential operators $P^\pm = \nabla_x \pm i\nabla_y$ as continuous linear operators from $H_s(E)$ to $H_{s-1}(E)$ at $s \leq 2$; let us denote these linear operators as $P_s^\pm$. Similarly, we can consider differential operators $Q^\pm = (\nabla_x \pm i\nabla_y)^2$ as continuous linear operators $Q_2^\pm$ from $H_2(E)$ to $H_0(E)$.

Theorem.

$$\dim \text{Ker } P_1^+ - \dim \text{Ker } P_1^- = N(E),$$

$$\dim \text{Ker } Q_2^+ - \dim \text{Ker } Q_2^- = 2N(E). \qquad (A2)$$

Remark. If the connection (that is, the functions A_x, A_y) is *smooth* then all distributional solutions of the operators $P_1^\pm$, $Q_2^\pm$ are also smooth,[15] and for the differential operators $P^\pm$, $Q^\pm$ acting on $C^\infty(E)$ we have from Eq. (A2),

$$\dim \text{Ker } P^+ - \dim \text{Ker } P^- = N(E),$$

$$\dim \text{Ker } Q^+ - \dim \text{Ker } Q^- = 2N(E).$$

Proof. Note that in our case when X is the two-dimensional torus the cotangent bundle $\pi: T^*X \to X$ is a trivial two-dimensional real bundle over X and can be identified with the trivial linear complex bundle $X \times \mathbb{C} \to X$. So lift of the bundle E over X to the bundle $\pi_* E$ over T^*X can be identified with linear complex bundle $E \times \mathbb{C} \to X \times \mathbb{C}$. At this identification, symbols $\sigma^\pm: \pi_* E \to \pi_* E$ of the operators $P^\pm$ become the following form: for $e \in E$, $\xi \in \mathbb{C}$ we have $\sigma^+(e, \xi) = (\xi e, \xi)$, $\sigma^-(e, \xi) = (\bar{\xi} e, \xi)$; that is, the fiber over a point of T^*X is multiplied by the complex number corresponding to this cotangent vector in the case σ^+, and on the conjugate to this complex number in the case σ^-.

The composition $\sigma^+ \sigma^-: \pi_* E \to \pi_* E$, $\sigma^+ \sigma^-(e, \xi) = (|\xi|^2 e, \xi)$ coincides with the identity id$: \pi_* E \to \pi_* E$ on the unit sphere subbundle of T^*X. So $[\sigma^+] + [\sigma^-] = 0$, where $[\sigma]$ is the class of σ in the group $K(T^*X)$, where K denotes K-theory with compact supports (a description of this variant of K-theory is contained in Ref. 15).

Applying "topological index," that is, homomorphism index$: K(T^*X) \to \mathbb{Z}$ constructed by Atiyah and Singer,[15] to this equality, we get

$$\text{index}[\sigma^+] + \text{index}[\sigma^-] = 0.$$

The operators $P_s^\pm: H_s(E) \to H_{s-1}(E)$ are Fredholm since symbols $\sigma^\pm$ are invertible outside the zero section of T^*X (Ref. 15). The value index$P_s^\pm \triangleq \dim \text{Ker } P_s^\pm - \dim \text{Coker } P_s^\pm$ depends only on $[\sigma^\pm]$ and is independent of the choice of $s \leq 2$ and the connection field A (but of course they depend on $N(E)$, which defines the isomorphism class of E): index $P_s^\pm$ =index$[\sigma^\pm]$ (Ref. 15).

Note that at $s \geq 1$ for $u, v \in H_s(E)$, we have $u\bar{v} \in H_s(1_X)$. So $\int_X (u\bar{v})_x dx dy = \int_X (u\bar{v})_y dx dy = 0$, and $\langle P_1^+ u, v \rangle_0 + \langle u, P_1^- v \rangle_0 = 0$ for any $u, v \in H_1(E)$. Identifying Coker $P_1^\pm$ with the orthogonal complement of Im $P_1^\pm$ in $H_0(E)$, we obtain

$$\text{Ker } P_1^- = (\text{Coker } P_1^+) \cap H_1(E),$$

$$\text{Ker } P_1^+ = (\text{Coker } P_1^-) \cap H_1(E).$$

Hence,

$$\text{index} P_1^+ \leq \dim \text{Ker } P_1^+ - \dim \text{Ker } P_1^-,$$

$$\text{index} P_1^- \leq \dim \text{Ker } P_1^- - \dim \text{Ker } P_1^+,$$

where each of these inequalities becomes an equality if and only if the cokernel of the corresponding operator is contained in $H_1(E)$. However, $\text{index} P_1^+ + \text{index} P_1^- = \text{index}[\sigma^+] + \text{index}[\sigma^-] = 0$, so both inequalities should be equalities, and we obtain $\text{Coker } P_1^\pm \subset H_1(E)$ and $\text{Ker } P_1^\pm \cong \text{Coker } P_1^\mp$. Hence,

$$\dim \text{Ker } P_1^+ - \dim \text{Ker } P_1^- = \text{index} P_1^+ = \text{index}[\sigma^+].$$
$$(A3)$$

Repeating this consideration almost literally for the operators $Q_2^\pm = (\nabla_x \pm i\nabla_y)^2 = P_1^\pm P_2^\pm$ acting from $H_2(E)$ to $H_0(E)$, and using the fact that the index of the composition of Fredholm operators is equal to the sum of their indices,[33] we have

$$\text{Coker } Q_2^\pm \subset H_2(E), \quad \text{Ker } Q_2^\pm \cong \text{Coker } Q_2^\mp,$$

$$\dim \text{Ker } Q_2^+ - \dim \text{Ker } Q_2^- = \text{index} Q_2^+ = \text{index}(P_1^+ P_2^+)$$
$$= \text{index} P_1^+ + \text{index} P_2^+$$
$$= 2 \text{ index}[\sigma^+]. \quad (A4)$$

We present below an explicit calculation of the value of $\text{index}[\sigma^+]$ based on one famous theorem from algebraic geometry, but for more clarity we start with a simple reasoning showing the proportionality of $\text{index}[\sigma^+]$ to $N(E)$.

Let us see, on the construction of complex bundles over X. Let F be a $U(n)$-vector bundle over X. Cut out the disk B^2 from the torus X. Since the disk is contractible, the restriction of F to B^2 is trivial. $X - B^2$ is homotopically equivalent to the wedge product of two circles, and $U(n)$ is connected, so the restriction of F to $X - B^2$ is trivial too. Thus, the isomorphism class of the bundle F is uniquely defined by its dimension n and by the homotopical class of the map $\varphi: S^1 = \partial B^2 \rightarrow U(n)$ gluing together these trivial bundles. This homotopical class is defined by the degree of the map $\det \varphi: S^1 \rightarrow U(1)$, where $\det: U(n) \rightarrow U(1)$ is the determinant homomorphism. The sum of degrees corresponds to the Whitney sum of bundles over X, so $K(X) = \mathbb{Z} \oplus \mathbb{Z}$. Here, $K(X)$ is an Abelian group generated by elements $[F]$ with relations $[F \oplus F'] = [F] + [F']$ for all complex bundles F, F' over X; a detailed description of K-theory is contained in Ref. 35.

Particularly, the isomorphism class of a linear bundle E is defined by the integer $N(E) = \deg(\det \cdot \varphi) = (2\pi)^{-1} \int_X dA$, and for the class $[E]$ of E in $K(X)$ we have

$$[E] - 1 = N(E)([E_1] - 1), \quad (A5)$$

where E_1 is a linear bundle over X for which $N(E_1) = 1$.

If E is trivial, then choosing a trivial connection we obtain that $\text{Ker } P^+$ is the space of holomorphic functions on torus and $\text{Ker } P^-$ is the space of antiholomorphic functions on torus. Both these spaces contain only constants and are one-dimensional, so $\text{index} P^+ = 0$ in this case. Taking into account that σ^+ is the image of $[E] \in K(X)$ at the Thom isomorphism $K(X) \rightarrow K(X \times \mathbb{C})$ (the description of this isomorphism can be seen in Ref. 15), from Eq. (A5) we obtain that $\text{index}[\sigma^+]$ is proportional to $N(E)$.

To calculate the coefficient of this proportionality, moreover, to calculate the value of $\text{index}[\sigma^+]$, let us replace E by the other bundle of the same class in $K(X)$, and replace P_s^+ by the other operator of the same symbol class in $K(T^*X)$ (the index of the operator does not change at such a replacement).

Consider the torus X as an algebraic curve, with local complex coordinate $z = x + iy$. Choose holomorphic line bundle F over X isomorphic to E in the smooth category; that is, such that $N(F) = N(E)$ [for example, we can take the divisor on X consisting of a point $z_0 \in X$ of the multiplicity $N(E)$, and turn from the divisor to a corresponding holomorphic line bundle in the way described in Ref. 36].

Consider now the differential operator $\bar{\partial}: C^\infty(\mathcal{F}^{0,0}) \rightarrow C^\infty(\mathcal{F}^{0,1})$, $\bar{\partial} = \frac{\partial}{\partial \bar{z}} = \frac{\partial}{\partial x} + i\frac{\partial}{\partial y}$, where $\mathcal{F}^{0,k}$ is the bundle of differential forms on X of type $(0, k)$ with coefficients in F. Since the complex cotangent bundle of X is trivial and linear, we have $\mathcal{F}^{0,0} \cong \mathcal{F}^{0,1} \cong F$, so the symbol of the operator $\bar{\partial}$ coincides with σ^+. Hence $\text{index}[\sigma^+] = \text{index}\bar{\partial}$. However, $\text{index}\bar{\partial}$ is equal to the Euler characteristic $\chi(X, F)$ of the sheaf of germs of holomorphic sections of F. We can compute $\chi(X, F)$ using the Riemann-Roch-Hirzebruch theorem.[37] For a curve X and linear bundle F this theorem yields $\chi(X, F) = c_1(F)[X] + 1 - g$, where g is the genus of the curve X and $c_1(F) \in H^2(X; \mathbb{Z})$ is the first Chern class of the bundle F. In our case $g = 1$, $c_1(F)[X] = c_1(E)[X] = (2\pi)^{-1}\int_X dA = N(E)$, so we obtain the final formula

$$\text{index}[\sigma^+] = N(E). \quad (A6)$$

Substituting Eq. (A6) into Eqs. (A3) and (A4), we obtain the assertion of the Theorem.

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*M.Katsnelson@science.ru.nl

†pmf@imm.uran.ru

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