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Boundary states and edge currents for free fermions

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Abstract

We calculate the ground state current densities for $(2+1)$-dimensional free fermion theories with local, translationally invariant boundary states. Deformations of the bulk wave functions close to the edge and boundary states both may cause edge current divergencies, which have to cancel in realistic systems. This yields restrictions on the parameters of quantum field theories which can arise as low-energy limits of solid-state systems. Some degree of Lorentz invariance for boosts parallel to the boundary can be recovered, when the cutoff is removed.

1 Introduction

The prediction of a relativistically invariant quantum field theory in $2+1$ dimensions as low-energy limit of a solid-state system [1] was confirmed by investigation of graphene [3]. Modification of the graphene structure may allow to obtain more general quantum field theories [2]. Since solid state systems typically have edges, the study of quantum field theories with boundaries acquired additional interest. An important tool in this context is the bulk-boundary operator product expansion (OPE). In particular, some of its singularities yield divergent observables and constitute obstructions to

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any experimental realization. The coefficient function of the identity in such an OPE is just the corresponding vacuum expectation value in the presence of the boundary. Integrated expectation values of current operators can be interpreted as measurable charge or spin currents and should remain finite in realistic systems. Here, we study this obstruction in the simplest case of free fermions, where vacuum expectation values can be interpreted as integrated contributions of the particles in the Dirac sea.

It is of course well known that such effects can prevent the lifting of a quantum mechanical system to a quantum field theory, even without the presence of a boundary. In our case the Dirac sea of a single fermion yields a half-integral value of the Hall conductivity [4–6]. Consequently one needs an even number of fermions, although some of them may be shifted to infinite mass, which results in a Chern–Simons term instead. For boundary states we shall find more intricate obstructions, which depend on the numerical parameters of the boundary state.

2 Boundary conditions from self-adjoint extensions

We consider spinor fields ψ acted upon by the Dirac operator

$$H := -\mathrm{i}\sigma_1 \frac{\partial}{\partial x} - \mathrm{i}\sigma_2 \frac{\partial}{\partial y} + m\sigma_3, \tag{2.1}$$

on the open half-plane $\{\mathbf{x} = (x, y) \in \mathbb{R}^2 |\, x > 0\}$, as in [7]. This operator is a closable symmetric operator on the domain $\mathcal{D}(H) = C_0^\infty(\mathbb{R}_+ \times \mathbb{R}, \mathbb{C}^2)$ of smooth functions with compact support vanishing in a neighbourhood of $x = 0$. The possible boundary conditions are classified by its self-adjoint extensions. The latter can be obtained by the standard von Neumann theory. Here we give a modification, which is less general but better adapted to the present problem. Since $\mathcal{D}(H)$ is dense in the Hilbert space $\mathcal{H} := L^2(\mathbb{R}_+ \times \mathbb{R}) \otimes \mathbb{C}^2$, the image of an arbitrary vector $\psi \in \mathcal{H}$ in the domain of a self-adjoint extension is uniquely determined by the unextended operator, so the problem is reduced to the determination of such domains. Let $\bar{H}$ and H^* be the closure and the adjoint, respectively, of H. By the von Neumann theory, every self-adjoint extension of H corresponds 1–1 to an isometry $V : N_+ \to N_-$ between the defect spaces

$$N_\pm = \{\psi \in \mathcal{D}(H^*) |\, H^*\psi = \pm\mathrm{i}\mu\psi\},$$

where μ is a fixed but arbitrary positive number. Indeed, V gives rise to the self-adjoint extension H_V with domain

$$\mathcal{D}(H_V) = \mathcal{D}(\bar{H}) + (I - V)\, N_+. \tag{2.2}$$

The choice $\mu = 1$ is standard, but we shall see that the limit of large μ allows a more direct physical interpretation. Applied to (2.1), $N_\pm$ is given by k integrals over elements of the one-dimensional spaces

$$N_\pm(k) = \mathbb{C}\,\mathrm{e}^{-\lambda x + \mathrm{i}ky} \begin{pmatrix} 1 \\ s_k^\pm \end{pmatrix} (1 + O(\mu^{-1})),$$

where

$$s_k^\pm = \frac{\mathrm{i}(k+\lambda)}{m \pm \mathrm{i}\mu} \quad \text{and} \quad \lambda = \sqrt{\mu^2 + k^2 + m^2}.$$

For $\mu \to \infty$ the defect spaces consist of wave functions which become supported on an arbitrarily small neighbourhood of the boundary and factorize in a universal term $\exp(-\mu x)$ and a spinor of the form

$$g(y) \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}, \quad \text{with } g \in L^2(\mathbb{R}).$$

Thus isometries $N_+ \to N_-$ become tensor products of a unitary map $V : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ with the map between one dimensional subspaces of $\mathbb{C}^2$ which takes $(1, -1)$ to $(1, 1)$. From (2.2) we read off that any $\psi \in \mathcal{D}(H_V)$ satisfies

$$\begin{aligned} \psi_1|_{x=0} &= (1 - V)g, \\ \psi_2|_{x=0} &= (1 + V)g. \end{aligned}$$

If 1 is not an eigenvalue of V, then

$$\psi_2|_{x=0} = \mathrm{i}\Gamma\, \psi_1|_{x=0}, \tag{2.3}$$

where Γ is the self-adjoint operator

$$\Gamma = -\mathrm{i}(1 + V)(1 - V)^{-1}.$$

The physical necessity of such a boundary condition can be understood as follows. Consider the conserved current densities

$$j^\mu(\mathbf{x}) = \lim_{\mathbf{x}' \to \mathbf{x}} \psi(\mathbf{x}')^\dagger\, \sigma^\mu\, \psi(\mathbf{x}).$$

One needs a boundary condition which implies $\int j^1(0, y)\, dy = 0$, and this indeed follows from (2.3).

We only study local boundary conditions for which $j^1(0, y)$ vanishes identically and also impose translational invariance. Thus Γ has to commute with d/dy and with multiplication by functions of y. This implies that it is a real constant γ, and we obtain the boundary condition

$$\psi_2(0,y) = \mathrm{i}\gamma\,\psi_1(0,y),$$

which we shall use in the sequel. To include the case $V = 1$, we consider γ as an element of the projective real line, including the value $\gamma = \infty$.

For any γ the Hamiltonian commutes with the PT transformation $\psi(x,y) \mapsto \sigma_3\psi^*(x,-y)$. The space reflection $(x,y) \mapsto (x,-y)$ lifts by $\psi(x,y) \mapsto \sigma_1\psi(x,-y)$ to a map between systems with parameters (m,γ) and $(-m,-\gamma^{-1})$. Because of this duality we only need to consider positive m. Arbitrary values of m will only be considered at the very end of the calculation. It turns out that the results allow a continuous extension to $m = 0$, which is the case relevant for graphene.

The CPT map (simultaneous reflection in charge, space and time) $\psi(x,y) \mapsto \sigma_2\psi(x,-y)$ relates the positive energy states for (m,γ) to the negative energy states for (m,γ^{-1}). A different type of duality is given by $\psi(x,y) \mapsto \sigma_2\psi(-x,y)$, $(m,\gamma) \mapsto (-m,\gamma^{-1})$, which relates boundary states of complementary half-planes.

3 Eigenfunctions

The Dirac operator commutes with $-\mathrm{i}\partial/\partial y$ and consequently with

$$(\mathrm{i}\partial/\partial x)^2 = H^2 + (\partial/\partial y)^2 - m^2.$$

We denote the real eigenvalues of these Hermitean operators by k and l^2, respectively. We take $l \in \mathbb{R}^+$ for positive l^2 and $l = i\lambda$ with $\lambda \in \mathbb{R}^+$ for negative l^2. The corresponding eigenvalues E of H satisfy $E^2 = k^2 + l^2 + m^2$.

According to the sign of l^2 the spectrum of H has two parts, which will be referred to as bulk and edge. Bulk eigenfunctions u_{lk} with given k, l^2 have the form

$$u_{lk}(x,y) = \exp(\mathrm{i}lx + \mathrm{i}ky)\chi_+ + \exp(-\mathrm{i}lx + \mathrm{i}ky)\chi_-$$

with constant spinors $\chi_\pm$. The equation $Hu_{lk} = Eu_{lk}$ and the boundary condition reduce to $(m - E,\, \pm l - ik)\chi_\pm = 0$ and $(\chi_+ + \chi_-)_2 = i\gamma(\chi_+ + \chi_-)_1$. For each $l > 0$ there is a unique solution up to normalization, such that for the bulk part we just recover the spectrum of the Dirac operator on the whole plane, with a gap $\Delta = (-m, m)$. We normalize these eigenfunctions with respect to the measure $dk\, dl/(2\pi^2)$ and choose phases such that

$$u_{lk}(x,y) = \left(\mathrm{e}^{\mathrm{i}\phi(l,k)} \begin{pmatrix} \mathrm{i}\rho_{lk} \\ 1 \end{pmatrix} \mathrm{e}^{\mathrm{i}lx+\mathrm{i}ky} - \begin{pmatrix} \mathrm{i}\rho_{lk}^* \\ 1 \end{pmatrix} \mathrm{e}^{-\mathrm{i}lx+\mathrm{i}ky} \right) \sqrt{\frac{E-m}{4E}},$$

where

$$\mathrm{e}^{\mathrm{i}\phi(l,k)} = \frac{1+\gamma\rho_{lk}^*}{1+\gamma\rho_{lk}} \tag{3.1}$$

with

$$\rho_{lk} := \frac{k+\mathrm{i}l}{m-E}. \tag{3.2}$$

Edge eigenfunctions [7] have the form $U_k = \exp(-\lambda x + \mathrm{i}ky)\chi$. We normalize them with respect to the measure dk/π and choose phases such that

$$U_k(x,y) = \sqrt{\frac{\lambda}{1+\gamma^2}} \begin{pmatrix} \mathrm{i} \\ -\gamma \end{pmatrix} \mathrm{e}^{-\lambda x+\mathrm{i}ky}.$$

The equation $HU_k = EU_k$ yields

$$E = \frac{2\gamma}{1+\gamma^2}k + \frac{1-\gamma^2}{1+\gamma^2}m$$

and

$$\lambda = \frac{\gamma^2-1}{\gamma^2+1}k + \frac{2\gamma}{\gamma^2+1}m.$$

Thus E, λ are one-valued functions of k, and for any k one has a unique edge state whenever $\lambda > 0$ and no edge state otherwise. The latter inequality restricts the possible values of k and E. The limiting values for $\lambda = 0$ lie on the mass shell. When we put

$$\eta = \operatorname{sgn}\frac{1-\gamma}{1+\gamma},$$

then the positive energy half of the mass shell is touched for $m\eta = 1$ and the negative energy half for $m\eta = -1$. One finds energies within the spectral gap Δ of the bulk iff $m\gamma > 0$.

The linear dispersion relation implies that edge states travel at the fixed velocity

$$v_{\text{edge}} = \frac{2\gamma}{1+\gamma^2}.$$

Note that v_{edge} determines γ up to the replacement of γ by γ^{-1}, which is the one induced by CPT. The latter transformation changes the signature η. Altogether, the boundary condition can be characterized by v_{edge} and η, except for the fact that η is undefined in the limiting cases $\gamma = \pm 1$. One observes that

1. for vanishing edge velocity, i.e., for $\gamma = 0$ and $\gamma = \infty$, edge states have $E = m$ and $E = -m$, respectively, independently of k. This case is probably unphysical, since all edge states have the same energy and the thermodynamic partition function diverges for a system of infinite width. Since the width of the edge excitation increases linearly with k, the thermodynamic properties of a finite system would depend on the sample size.
2. The edge velocity is equal to the maximal bulk velocity for the CPT invariant boundary conditions $\gamma = \pm 1$. These yield $E = \gamma k$ and $\lambda = \gamma m$ independently of k. For $\gamma m < 0$ there are no edge states, for $\gamma m > 0$ all edge states have the same dependence on x. This yields particular divergences, so we will tacitly exclude $\gamma = \pm 1$ in most of the subsequent calculations.

In (k, E)-space the half-line of edge states is tangent to the half-hyperboloid given by $l \geq 0$ and $E^2 = k^2 + m^2 + l^2$ at $l = \lambda = 0$. For $\gamma^2 < 1$, this happens at positive energy and for $\gamma^2 > 1$ at negative energy. The tangency has consequences for the behaviour at large distance from the boundary, as we shall see later.

The portion of edge energies within Δ gives rise to a current parallel to the boundary, with conductivity equal to (in units of $\frac{e^2}{h}$) [7]

$$\sigma^{\text{edge}} = \begin{cases} \operatorname{sgn}(m), & \text{if } m\gamma > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{3.3}$$

This applies whenever some subinterval of the gap is actually occupied, independently of the size of this subinterval.

4 Current densities

When no boundary exists, Fermi energies within the gap Δ obviously yield the same theory. This means that any pair (γ, E_{F}) with $E_{\text{F}} \in \Delta$ yields a boundary state of the standard Lorentz invariant free fermion theory. We want to calculate the corresponding expectation values of the current densities. The bulk contribution does not depend on the choice of E_{F} and edge contributions for energies within Δ are finite and were calculated in [7]. Thus it suffices to consider $E_{\mathrm{F}} = -m$.

The required vacuum expectation values are

$$\langle j^\mu \rangle = j^\mu_{\mathrm{bulk}} + j^\mu_{\mathrm{edge}},$$

where

$$j^\mu_{\mathrm{bulk}} = \int j^\mu_{lk}|_{\mathrm{bulk}} \frac{dl\,dk}{2\pi^2},$$
$$j^\mu_{\mathrm{edge}} = \int \Theta(-m-E)\, j^\mu_k|_{\mathrm{edge}} \frac{dk}{\pi},$$

and

$$j^\mu_{lk}(\mathbf{x})|_{\mathrm{bulk}} = u^\dagger_{lk}(\mathbf{x})\,\sigma^\mu\, u_{lk}(\mathbf{x}),$$
$$j^\mu_k(\mathbf{x})|_{\mathrm{edge}} = U^\dagger_k(\mathbf{x})\,\sigma^\mu\, U_k(\mathbf{x}).$$

Here the variable E in u_{lk} is the negative roots of $k^2+l^2+m^2$.

Note that $j^1_{lk}|_{\mathrm{bulk}}$ and $j^1_k|_{\mathrm{edge}}$ vanish identically. On the other hand equations (3.1) and (3.2) yield

$$j^2_{lk}(\mathbf{x})|_{\mathrm{bulk}} = \frac{k}{E} - \frac{1}{E}\Re\left(\frac{f}{g}\,\mathrm{e}^{-2\mathrm{i}lx}\right), \tag{4.1}$$

where

$$g = m - E + \gamma(k - \mathrm{i}l),$$
$$f = (k-\mathrm{i}l)g^*.$$

The first term on the r.h.s. of equation (4.1) is an odd function of k, so that its contribution to the vacuum expectation value of j^2 vanishes for any symmetric regularization. For the second term, we also will find a partial cancellation.

We substitute $k \in (-\infty,\infty)$ by $v = \mathrm{e}^{\operatorname{arcsinh}(k/a)} \in (0,\infty)$, which yields for negative E

$$-\frac{dk}{E} = \frac{dv}{v}. \tag{4.2}$$

Moreover,

$$-\frac{f}{g}\frac{dk}{E} = \left(\frac{a^2}{4}(v-v^{-1})^2 + l^2\right)(D_1^{-1} + D_2^{-1})\,dv.$$

Here

$$D_1 = \frac{a}{2}(\gamma + 1)(v - v_3)(v - v_4),$$
$$D_2 = \frac{a}{2}(\gamma^{-1} + 1)(v - v_3)(v + v_4),$$

where

$$a = \sqrt{l^2 + m^2}$$

and

$$v_3 = \frac{\mathrm{i}l + m}{\sqrt{l^2 + m^2}} \frac{\gamma - 1}{\gamma + 1},$$
$$v_4 = \frac{-\mathrm{i}l + m}{\sqrt{l^2 + m^2}}.$$

The two denominators D_1 and D_2 are formally related by a reflection across the boundary, with $(m, \gamma) \mapsto (-m, \gamma^{-1})$.

One obtains a partial fraction expansion

$$-\frac{f}{g} \frac{dk}{E} = \{P_1(v) + P_2(v) + P_3(v) + P_4(v)\}\, dv$$

with

$$P_1(v) = \frac{a}{2},$$
$$P_2(v) = -\frac{a}{2} v^{-2}.$$

In order to regularize the momentum integrals we have to introduce a cutoff. In a solid state context the underlying physics selects a stationary Lorentz frame, in which a symmetric cutoff in k is natural. For this cutoff the dv integrals of these two terms cancel against each other due to the symmetry $k \mapsto -k$, $v \mapsto 1/v$. The remaining terms are

$$P_3(v) = \mathrm{i}l \frac{\gamma + 1}{\gamma - 1} v^{-1},$$
$$P_4(v) = -\mathrm{i}l \frac{4\gamma}{\gamma^2 - 1} (v - v_3)^{-1}.$$

For a symmetric cutoff Λ of the v-integration one finds

$$\int \Re(P_3(v) \mathrm{e}^{-2\mathrm{i}lx}) \frac{dl dv}{2\pi^2} = -\frac{1}{2\pi} \frac{\gamma + 1}{\gamma - 1} \delta'(x) \ln \Lambda.$$

In order to calculate the P_4 integral we need

$$\int \left(v - \frac{\mathrm{i}l + m}{\sqrt{l^2+m^2}}\frac{\gamma-1}{\gamma+1}\right)^{-1} dv = \ln(\Lambda) - \ln\left(\frac{1+\gamma}{1-\gamma}\sqrt{\frac{m+\mathrm{i}l}{m-\mathrm{i}l}}\right),$$

where the principal value of the logarithm has to be taken, so that

$$\ln\left(\frac{1+\gamma}{1-\gamma}\sqrt{\frac{m+\mathrm{i}l}{m-\mathrm{i}l}}\right) = \ln\left(\sqrt{\frac{m+\mathrm{i}l}{m-\mathrm{i}l}}\right) + \ln\left|\frac{1+\gamma}{1-\gamma}\right| - \pi\mathrm{i}\,\Theta(\gamma^2-1).$$

In order to calculate the dl integral over the logarithmic part, we use

$$2\int_0^\infty \mathrm{i}l \ln\left(\sqrt{\frac{m+\mathrm{i}l}{m-\mathrm{i}l}}\right)\cos(2lx)\, dl = \int_{-\infty}^{\infty} \mathrm{i}l\ln\left(\sqrt{\frac{m+\mathrm{i}l}{m-\mathrm{i}l}}\right) \mathrm{e}^{2\mathrm{i}lx}\, dl.$$

The argument of ln has branching points at $l = \pm\mathrm{i}m$. We may move the integration path towards the cut with branching point $l = \mathrm{i}m$. Since the discontinuity of the logarithm is $\mathrm{i}\pi$, this yields an elementary integral. Altogether we obtain

$$\begin{aligned} j^2(\mathbf{x})_{\mathrm{bulk}} = &-\frac{1}{2\pi}\frac{\gamma^2+1}{\gamma^2-1}\delta'(x)\,\ln\Lambda + \frac{\gamma}{\pi(\gamma^2-1)}\ln\left|\frac{1+\gamma}{1-\gamma}\right|\,\delta'(x) \\ &+ \frac{\gamma}{2\pi(\gamma^2-1)}\left(\frac{1}{2x^2}+\frac{m}{x}\right)\mathrm{e}^{-2mx} \\ &- \frac{\gamma}{\pi(\gamma^2-1)}\frac{1}{2x^2}\,\Theta(\gamma^2-1). \end{aligned} \tag{4.3}$$

For the contribution from the edge functions, we have

$$dk\,\frac{\gamma^2-1}{\gamma^2+1} = d\lambda.$$

We have to integrate over those λ for which $\lambda > 0$ and $E < -m$. This yields

$$j^2(\mathbf{x})_{\mathrm{edge}} = \frac{\gamma}{\pi(\gamma^2-1)}\left[\frac{1}{2x^2}\Theta(\gamma^2-1) - \left(\frac{1}{2x^2}+\frac{m}{\gamma x}\right)\mathrm{e}^{-2mx/\gamma}\Theta(\gamma)\right].$$

Note that j^2_{edge} vanishes for $\gamma \in (-1,0)$ and is non-singular for $\gamma > 1$.

For $\gamma^2 > 1$ both the bulk and the edge current densities decay algebraically at large distance from the boundary. In their sum these terms cancel, an interesting effect which reflects the tangency of the edge state and bulk state manifolds in (k, E) space, which was discussed in the previous section.

In all cases the singular part of the vacuum expectation value has the form

$$\langle j^2(\mathbf{x})\rangle_{\text{singular}} = -\frac{1}{2\pi}\frac{\gamma^2+1}{\gamma^2-1}\delta'(x)\ln\Lambda - \frac{|\gamma|}{4\pi(\gamma^2-1)}\frac{1}{x^2}.$$

Remarkably, this equation is invariant under y reflection together with $\gamma \mapsto -\gamma^{-1}$, such that it remains true for $m < 0$ and is in fact independent of m. The regular part of the expectation value is continuous in m and vanishes for $m = 0$. For infinite m the contribution becomes localized at the boundary and is given by the δ' terms in (4.3). It may be interesting to rederive this result from a Chern-Simons Lagrangian.

5 Conclusion

A single free fermion yields a divergent edge current on a half plane. For N fermions with boundary conditions γ_n the cut-off dependent edge current vanishes for

$$\sum_{n=1}^{N}\frac{\gamma_n^2+1}{\gamma_n^2-1} = 0.$$

One still has a dipolar edge current

$$\sum_{n=1}^{N}\frac{\gamma_n}{\pi(\gamma_n^2-1)}\ln\left|\frac{1+\gamma_n}{1-\gamma_n}\right|\delta'(x),$$

which in general does not vanish. In addition there is a $1/x^2$ singularity, which yields an unphysical divergent particle transport in the neighbourhood of the edge, unless

$$\sum_{n=1}^{N}\frac{|\gamma_n|}{\gamma_n^2-1} = 0.$$

Since the bulk system and the boundary at $x = 0$ are Lorentz invariant under boosts in the y direction, one should be able to act with Lorentz transformations on the boundary conditions. In the context of relativistic quantum mechanics this is straightforward. The action on the parameters γ_n can be determined from the dispersion relation, according to which boundary states are characterized by a Lorentz invariant signature η_n and their fixed travel velocity

$$v_n = \frac{2\gamma_n}{1+\gamma_n^2}.$$

This translates into a rapidity θ_n given by $\tanh\theta_n = v_n$, or equivalently by

$$\eta_n \exp\theta_n = \frac{1+\gamma_n}{1-\gamma_n},$$

to which the rapidity of the Lorentz boost is added. When one moves from one-particle states to field theory, control of divergencies requires a cutoff which breaks Lorentz invariance. It may or may not be restored, when this cutoff is taken to infinity. One would expect that a restoration of Lorentz invariance implies CPT invariance. Due to the unbroken PT invariance this should yield invariance under charge conjugation and consequently an absence of net boundary currents. In our case we will find an unexpected subtlety, however. In terms of edge velocities and signatures the two divergency cancellation conditions can be rewritten as

$$\sum_{n=1}^{N} \eta_n \exp(\epsilon_n\theta_n) = 0 = \sum_{n=1}^{N} \eta_n \exp(-\epsilon_n\theta_n),$$

where

$$\epsilon_n = \mathrm{sgn} v_n.$$

For $N=1$, there is no solution, in agreement with the restriction to an even N coming from the bulk physics. For $N=2$ one needs $\gamma_2 = -\gamma_1^{-1}$, thus invariance under charge conjugation. More generally, pairs of edge states related by charge conjugation do not contribute to the breaking of Lorentz invariance or to net boundary currents, as expected. There is an unexpected remainder of Lorentz invariance in more general situation, however. When all v_n of the remaining states have the same sign, the cancellation conditions are invariant under sufficiently small boosts which do not change the sign of edge velocities. When v_n of different signs occurs, no aspect of Lorentz invariance is recovered when the cutoff is removed. In any case, breaking of Lorentz invariance by edge states does not seem to be an argument against the realization of such systems in solid state physics, where this invariance is only a low-energy phenomenon.

It will be interesting to see to what extent the γ values can be controlled experimentally. Systems without time-reversal invariance would be particularly interesting, but are certainly very difficult to realize.

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