Universität Regensburg

Study of negative magneto-resistivity in interacting model of Dirac semimetals

Pavel Buividovich, Matthias Puhr and Senia Valgushev
(University of Regensburg)

Condensed matter physics meets relativistic quantum field theory
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Negative Magneto-Resistivity in 3D Dirac semimetals

Three key steps:

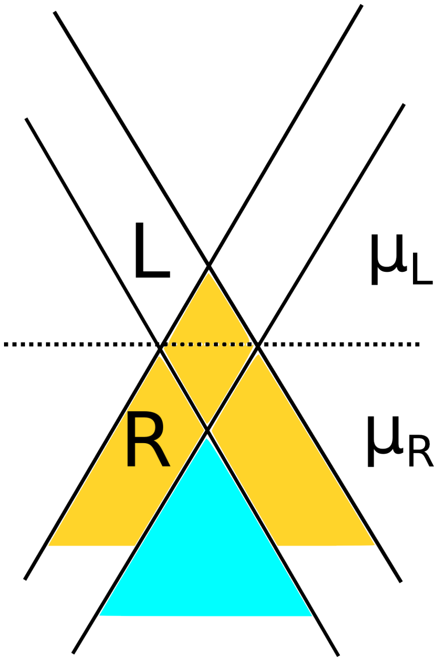
1. Quantum Chiral Anomaly + Scattering:

$$\frac{\mathrm{d}\rho_5}{\mathrm{d}t} = \frac{1}{4\pi^2}\vec{E}\cdot\vec{B} - \frac{\rho_5}{\tau} \qquad \rho_5 = \frac{\mu_5^3}{3\pi^2} + \frac{\mu_5}{3}\left(T^2 + \frac{\mu^2}{\pi^2}\right) \qquad \mu_5 = \frac{\mu_L - \mu_R}{2}$$

Steady state solution:

$$\mu_5 = \frac{3}{4\pi^2}\frac{\vec{E}\cdot\vec{B}}{T^2 + \frac{\mu^2}{\pi^2}}\tau$$

Turns Dirac semimetal into parity-breaking Weyl semimetal



2. Chiral Magnetic Effect (CME):

$$\vec{J}_{CME} = \frac{\mu_5}{2\pi^2}\vec{B}$$

3. Combining 1. and 2. we obtain: $\vec{J} = \frac{3}{8\pi^4}\frac{\tau B^2}{T^2 + \frac{\mu^2}{\pi^2}}\vec{E}$

Experimental observation: **D. Kharzeev et al, Nature Physics 12, 550–554 (2016)**

It seems that it can be observed even in systems with ill-defined chirality:

F. Arnold et al, Nature Communications 7, 11615

But how interactions modify this picture?

Derivation of mean-field approximation for interacting Dirac semimetal

We start with Wilson-Dirac Hamiltonian and add contact interactions, which serve as a simple model of screened Coulomb interactions:

$$H = \psi^\dagger h_{WD} \psi + H_{int} \qquad h_{WD} = -i v_f \sum_i \alpha_i \nabla_i[\vec{A}] + r\gamma_0 \Delta[\vec{A}]$$

$$H_{int} = V(\psi_x^\dagger \psi_x - 2)^2$$

For the partiton function we perform standard Suzuki-Trotter decomposition:

$$Z = \mathrm{Tr}(\exp(-H/T)) = \mathrm{Tr}(\exp(-\delta\tau H)\ldots) + O(\delta\tau^2) \qquad T = N\delta\tau$$

And perform Hubbard-Stratonovich transformation:

$$\exp(-V(\psi^\dagger\psi - 2)^2) = \int d\Phi \exp(-\frac{\mathrm{Tr}\Phi^2}{4V} + \psi^\dagger\Phi\psi + V\psi^\dagger\psi)$$

where matrices are said to correspond to different condensates in the mean-field approximation:

$$\Phi^0_{\alpha\beta} \sim < \psi^\dagger_\alpha \psi_\beta >$$

Derivation of mean-field approximation for interacting Dirac semimetal

First of all, let us study phase diagram of this model at zero external fields and vanishing bare chemical potential, so that particle-hole symmetry is intact:

$$\vec{A} = 0 \qquad \mu_0 = 0$$

To this end we find such values of Hubbard fields which minimize the free energy:

$$F = -T \log Z \qquad \partial F / \partial \Phi = 0|_{\Phi = \Phi^\star}$$

so that mean-field value is $$F = \sum_{\epsilon_i < 0} \epsilon_i + \sum_A \frac{\Phi_A^{\star 2}}{V}$$

It is interesting how interactions renormilize chiral chemical potential.

We add two bare parameters to the model: mass and chiral chemical potential:

$$H = H + m^{(0)} \gamma_0 + \mu_5^{(0)} \gamma_5$$

Finally we numerically minimize the free energy for different values of bare parameters.

The phase diagram

To make it more convinient we separate different matrix structures in Hubbard field:

$$\Phi_{\alpha\beta} = \sum_{A=1}^{16} \Phi_A \Gamma_{A,\alpha\beta}$$

where gamma-matrices form complete basis in the space of Hermitian matrices.

What have we found?

1) All condensates appear to be homogeneous in space.

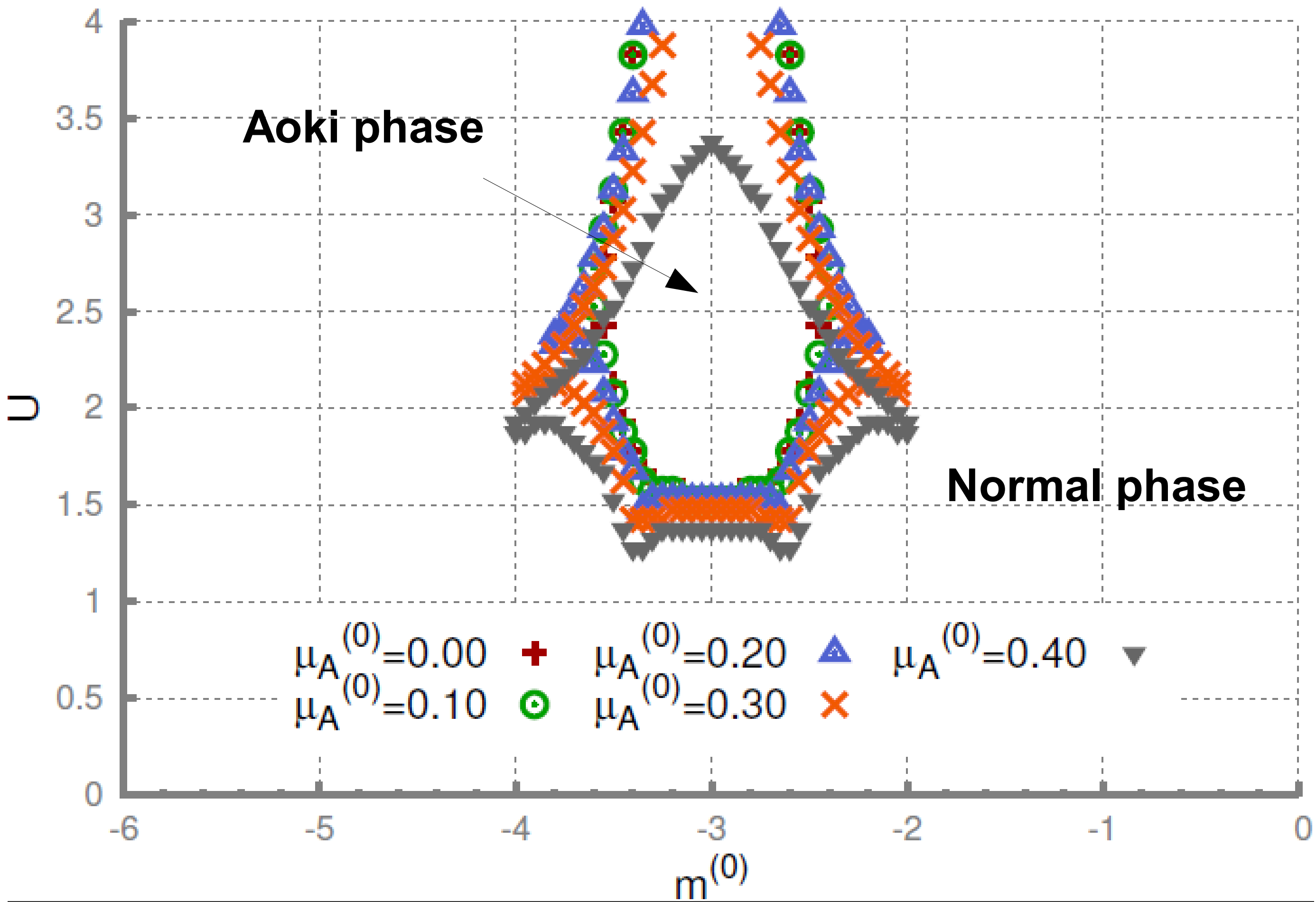
2) Non-zero condensates are:

Chiral condensate:	$m\gamma_0$
CP-breaking mass:	$-im_5\gamma_0\gamma_5$
Chiral chemical potential:	$\mu_5\gamma_5$

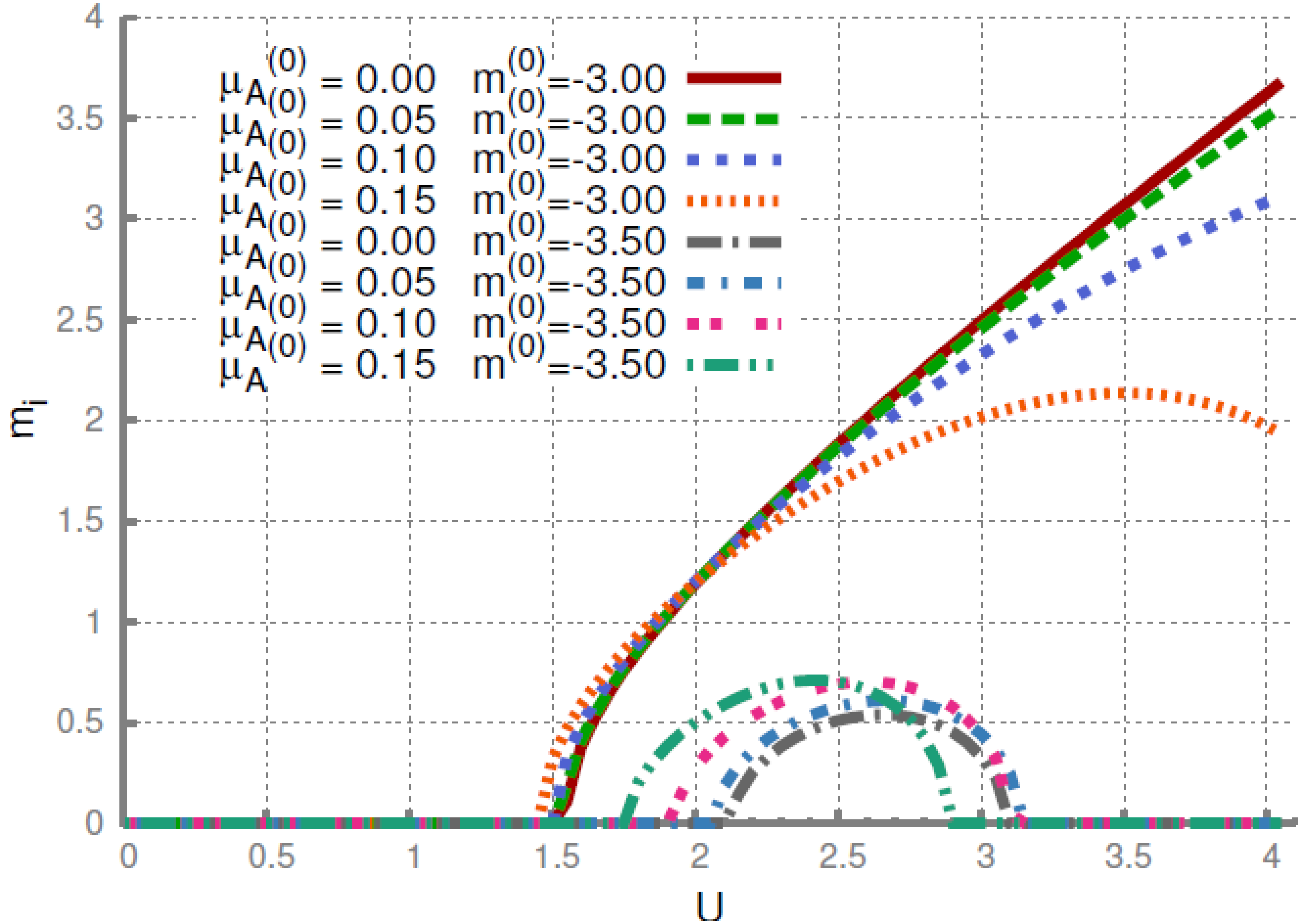
The phase diagram

There are two phases: normal (as well as topological insulator) when $m_5 = 0$

and so-called Aoki phase (Axionic insulator phase) when $m_5 \neq 0$ **.**

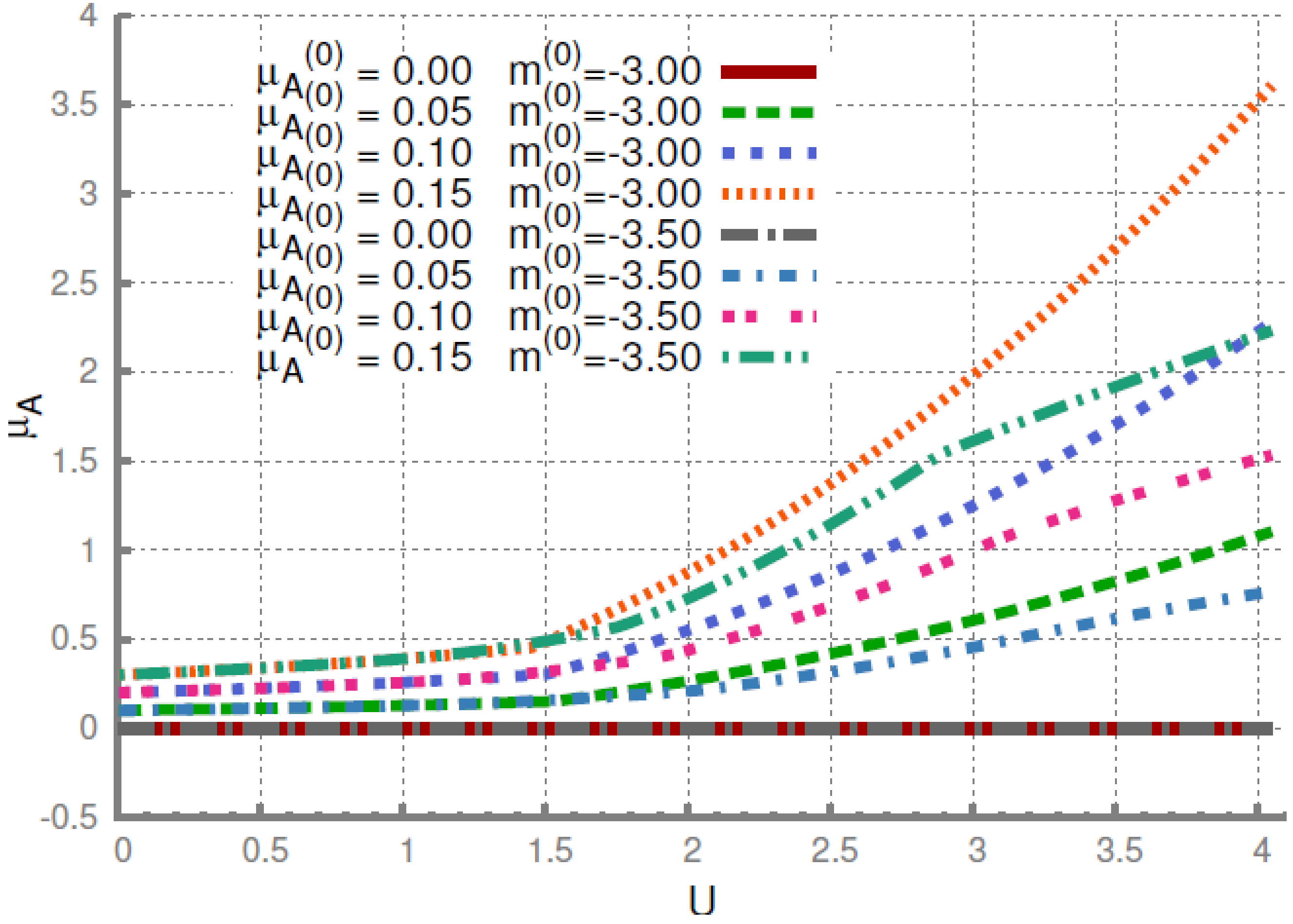


The phase diagram



Dependance of CP-breaking mass on interaction strength.

The phase diagram



Chiral chemical potential is strongly enhanced by interactions,

especially in the Aoki phase

CME conductivity

But at the end of the day, we can not measure chiral chemical potential.

Let us study something which can be related to measurable in experiment quantities, the CME conductivy:

$$J_{CME} = \sigma_{CME} B$$

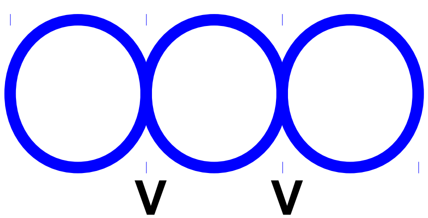
Naively, we could say that since chiral chemical potential is enhanced, then this conductivity is enchanced, too.

But there are also loop corrections:

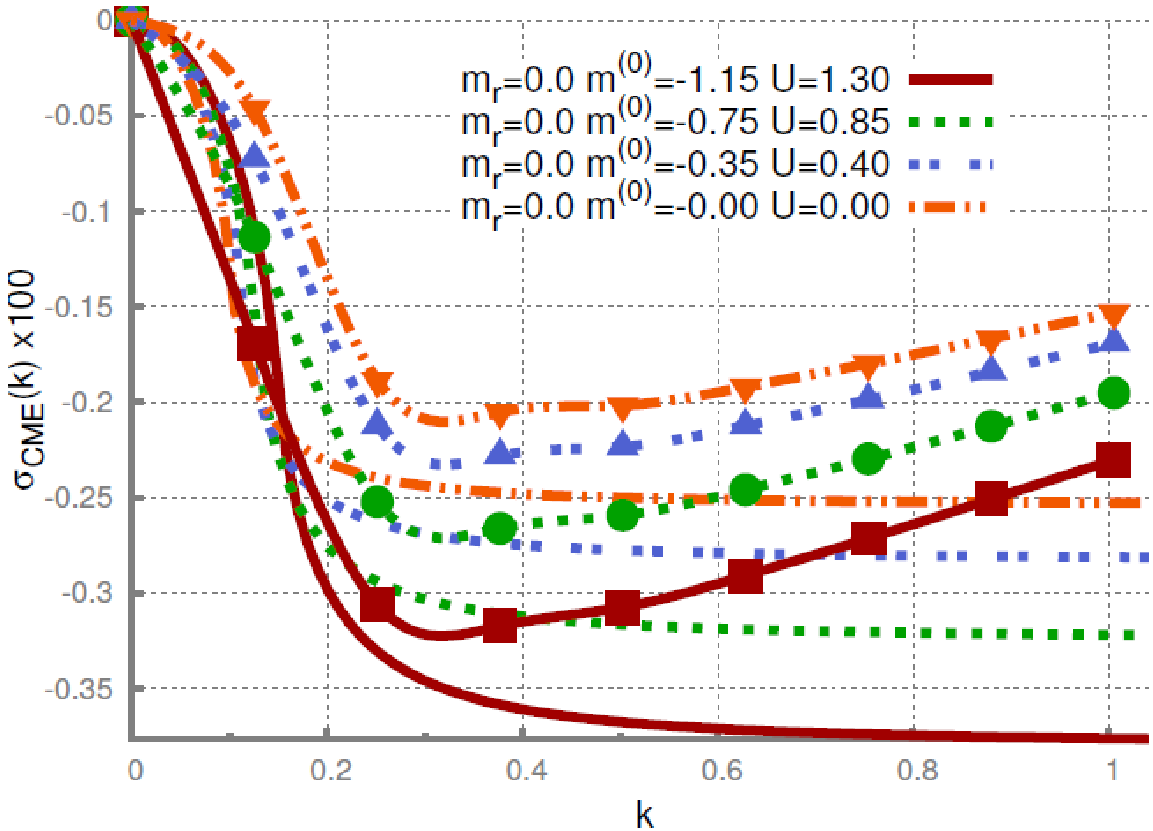
$$\langle j_{x,k} \rangle = \sum_{y,l} \frac{\delta^2 \mathcal{F}[A_{x,k}]}{\delta A_{x,k}\, \delta A_{y,l}} \bigg|_{A=0} A_{y,l}$$

$$\frac{\delta^2 \mathcal{F}[\Phi_x^\star, A_{x,k}]}{\delta A_{x,i}\, \delta A_{y,j}} = \frac{\partial^2 \mathcal{F}[\Phi_x^\star, A_{x,k}]}{\partial A_{x,i}\, \partial A_{y,j}} - $$

$$- \sum_{z,A,t,B} G_{z,A;t,B} \frac{\partial^2 \mathcal{F}[\Phi_x, A_{x,k}]}{\partial A_{x,i}\, \partial \Phi_{z,A}} \frac{\partial^2 \mathcal{F}[\Phi_x, A_{x,k}]}{\partial A_{y,j}\, \partial \Phi_{t,B}} \bigg|_{\Phi_x^\star}$$

… +  + …

CME conductivity



Lines without markers represent analytical formula with appropriate parameters:

$$\sigma_{CME}(k) = \frac{1}{(2\pi)^2}\left(\mu_5 + \frac{\mu_5^2 - k^2/4}{|k|}\log\left|\frac{2\mu_5 - |k|}{2\mu_5 + |k|}\right|\right)$$

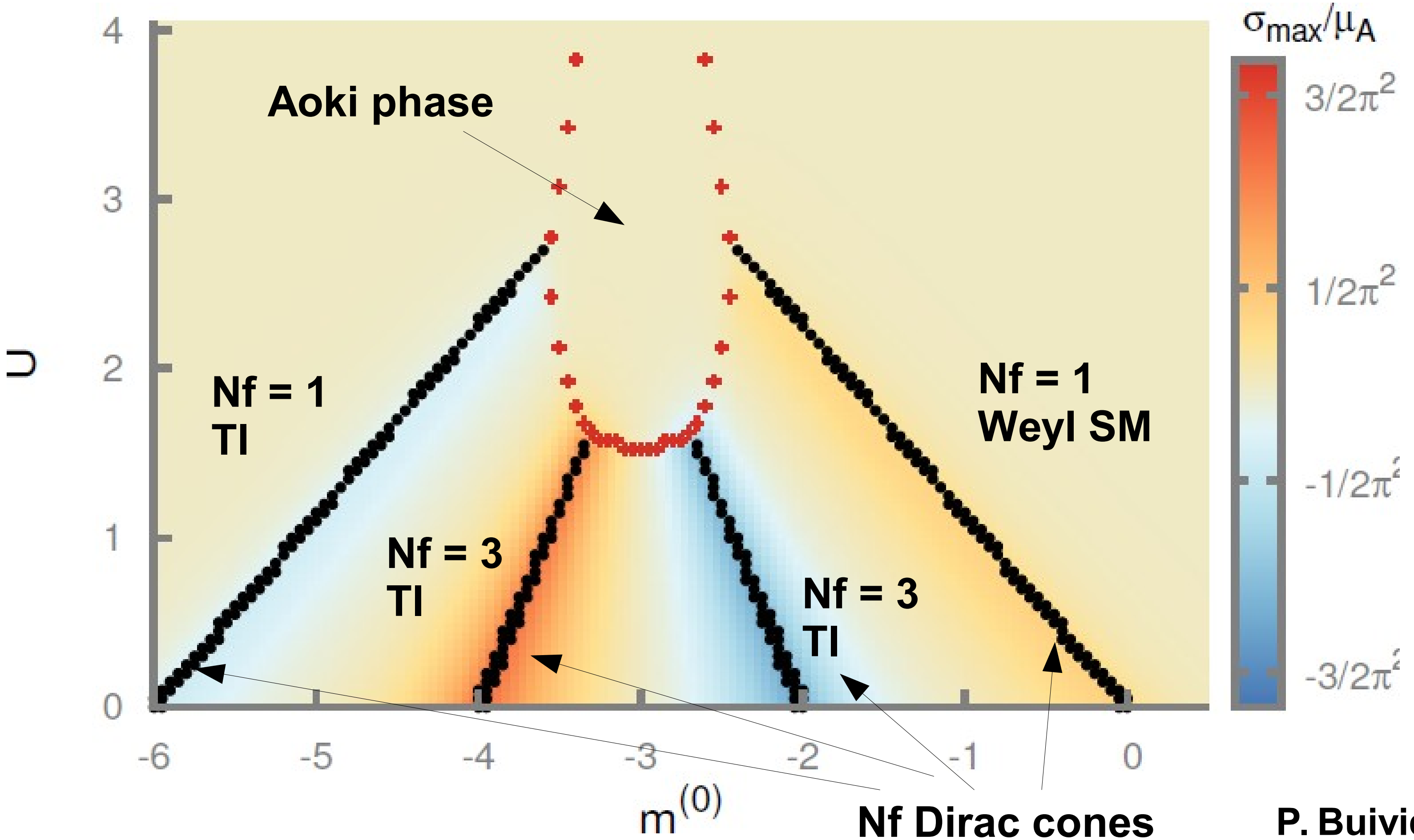
Note: on the lattice static CME conductivity is zero at k = 0!

See also for absence of CME in equilibrium:

N. Yamamoto, Phys. Rev. D 92, 085011 (2015)

M. Zubkov, Phys.Rev. D93 (2016) no.10, 105036

CME conductivity



Values of CME conductivity on the phase digram

Dr. Pavel Buividovich

Matthias Puhr

P. Buividovich, M. Puhr, S. Valgushev, Phys. Rev. B 92, 205122 (2015)

1) Never exceeds naive result for CME conductivity with renormilized chiral chemical potential

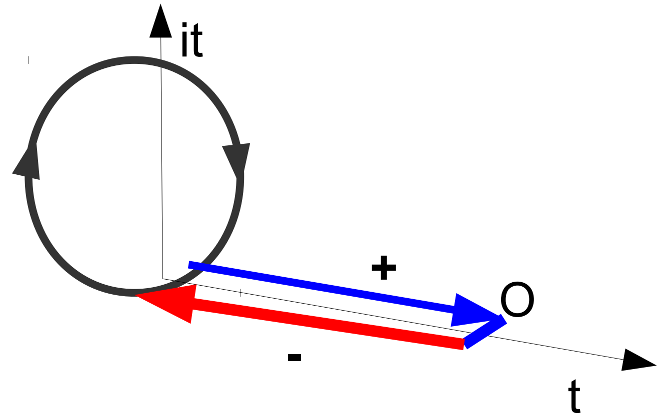
2) Effect of the mass is strong — always supresses conductivity

3) When there is a Dirac cone in the spectrum loop corrections are very small

Step towards out-of-equlibrium dynamics

Can we generilize mean-field approach in order to study non-euilibrium dynamics?

We can use Keldysh formalism:



$$< O(t) >= \mathrm{Tr}(\rho_0 U_+(0,t) O U_-(t,0))$$

$$U_\pm(0,t) = \mathcal{T} \exp(\pm i \int_0^t d\tau H_\pm(\tau))$$

Next we perform Hubbard-Stratonovich transformation again for each part of Keldysh contour and parametrise fields along forward and backward branches as:

$$\Phi_\pm = \Phi_{cl} \pm \frac{1}{2}\Phi_q$$

where we separate «classical» fields and «quantum» fluctuations, integrate out fermions and obtain path-integral representation for observable:

$$< O(t) >= \int d\Phi_E \Phi_{cl} \Phi_q \exp(-\beta \frac{\mathrm{Tr}\Phi_E^2}{4V}) \times$$
$$\times \exp(-i \left[\mathrm{tr} \ln(1 + U_+(0,t) U_E U_-(t,0)) + \int dt \frac{\Phi_{cl}(t)\Phi_q(t)}{2V} \right]$$
$$\times \mathrm{tr} \left[\left(1 + U_+^{-1}(0,t) U_E^{-1} U_-^{-1}(t,0) \right) O \right]$$

Step towards out-of-equlibrium dynamics

$$< O(t) >= \int d\Phi_E \Phi_{cl} \Phi_q \exp(-\beta \frac{\mathrm{Tr}\Phi_E^2}{4V}) \times$$

$$\times \exp(-i \left[\mathrm{tr} \ln(1+U_+(0,t)U_E U_-(t,0)) + \int dt \frac{\Phi_{cl}(t)\Phi_q(t)}{2V} \right]$$

$$\times \mathrm{tr} \left[\left(1 + U_+^{-1}(0,t) U_E^{-1} U_-^{-1}(t,0) \right) O \right]$$

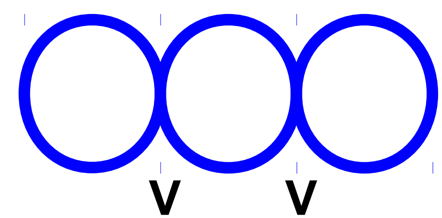
Linear in quantum fields

Neglect Φ_q

Expand to first order of quantum fields

Integrating out quantum fields we formulate the following self-consistent equations of motion:

$$\begin{cases} \partial_t \Phi_A(t) = -i\frac{V}{2} \sum_n \psi_n^\dagger(t)[H(t), \Gamma_A]\psi_n(t) \\ \partial_t \psi_n(t) = -iH(t)\psi_n(t) \end{cases}$$

… +  **+ …**

with time-dependent mean-field Hamiltonian:

$$H(t) = -iv_f \sum_i \alpha_i \nabla_i [\vec{A}(t)] + r\gamma_0 \Delta[\vec{A}(t)] + \sum_A \Phi_A \Gamma_A + V + m^{(0)}\gamma_0$$

Step towards out-of-equlibrium dynamics

$$
\begin{cases}
\partial_t \Phi_A(t) = -i\frac{V}{2}\sum_n \psi_n^\dagger(t)[H(t),\Gamma_A]\psi_n(t) \\
\partial_t \psi_n(t) = -iH(t)\psi_n(t)
\end{cases}
$$

Partialy digonalized Hamiltonian!

$$
\begin{aligned}
H(t) = & -iv_f\alpha_x\nabla_x + r\gamma_0\Delta + V + m^{(0)}\gamma_0 + \sum_A \Phi_A(t)\Gamma_A \\
& + v_f\alpha_y \sin(k_y + Bx) + 2r\gamma_0\sin^2((k_y+Bx)/2) \\
& + v_f\alpha_z \sin(k_z + A_z(t)) + 2r\gamma_0\sin^2((k_z+A_z(t))/2)
\end{aligned}
$$

Essentialy classical dynamics of Hubbard field + fully quantum dynamics of fermions in the background of classical fields (external gauge fields and dynamical Hubbard fields)

We can numerically solve these differential equations with appropriate initial values.

Physical setup:

1) Let's impose static homogeneous background magnetic field: $A_y^{ext}(x) = Bx$
so that magnetic field points in the z diection.

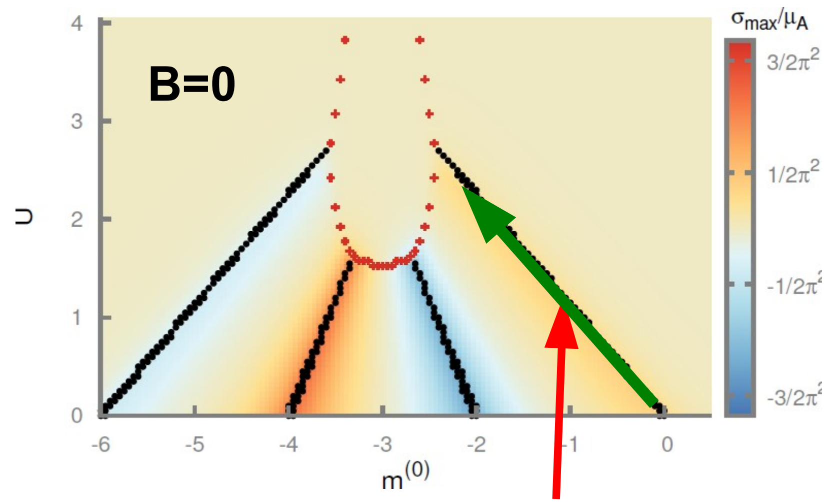
2) For simplicity we study dynamics only at T = 0.

3) Lattice is periodic, therefore flux of magnetic field is quatized: $B = 2\pi n/L$

Phase diagram in the magnetic field

We study the line of constant physics where there is only one Dirac cone in the spectrum

Zero bare chiral chemical potential: $\mu_5^{(0)} = 0$



Line of constant physics with Nf=1 Dirac cone

After numerical minimization we find that:

1) All condensates are again homogeneous in space.

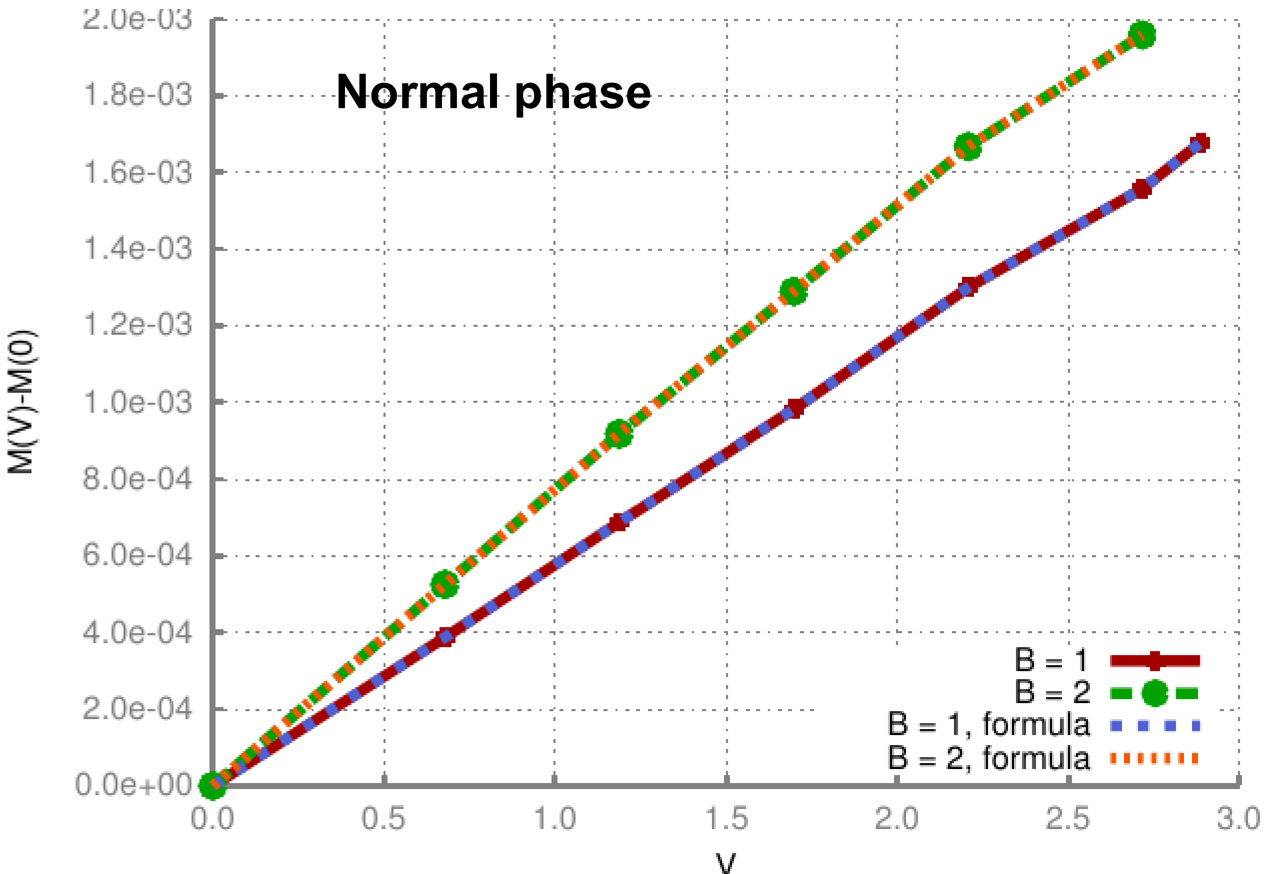
2) Non-zero condensates are:

Chiral condensate:	$m\gamma_0$
CP-breaking mass:	$-im_5\gamma_0\gamma_5$
Anomolous magnetic moment:	$\eta\gamma_3\gamma_5$
Chiral anomalous magnetic moment:	$-i\eta_5\gamma_3$

Anomalous magnetic moment induce Zeeman splitting: $\varepsilon_n(k_z) = \pm\sqrt{p_z^2 + (\sqrt{m^2 + 2Bn} \pm \eta)^2}$

(Formula is given for continuum fermions)

Phase diagram in the magnetic field



L=100

Renormalization of the mass of electrons in normal phase by interactions at different values of magnetic field and comparison to the formula:

$$M = \sqrt{(m-\eta)^2 + (m_5 - \eta_5)^2}$$

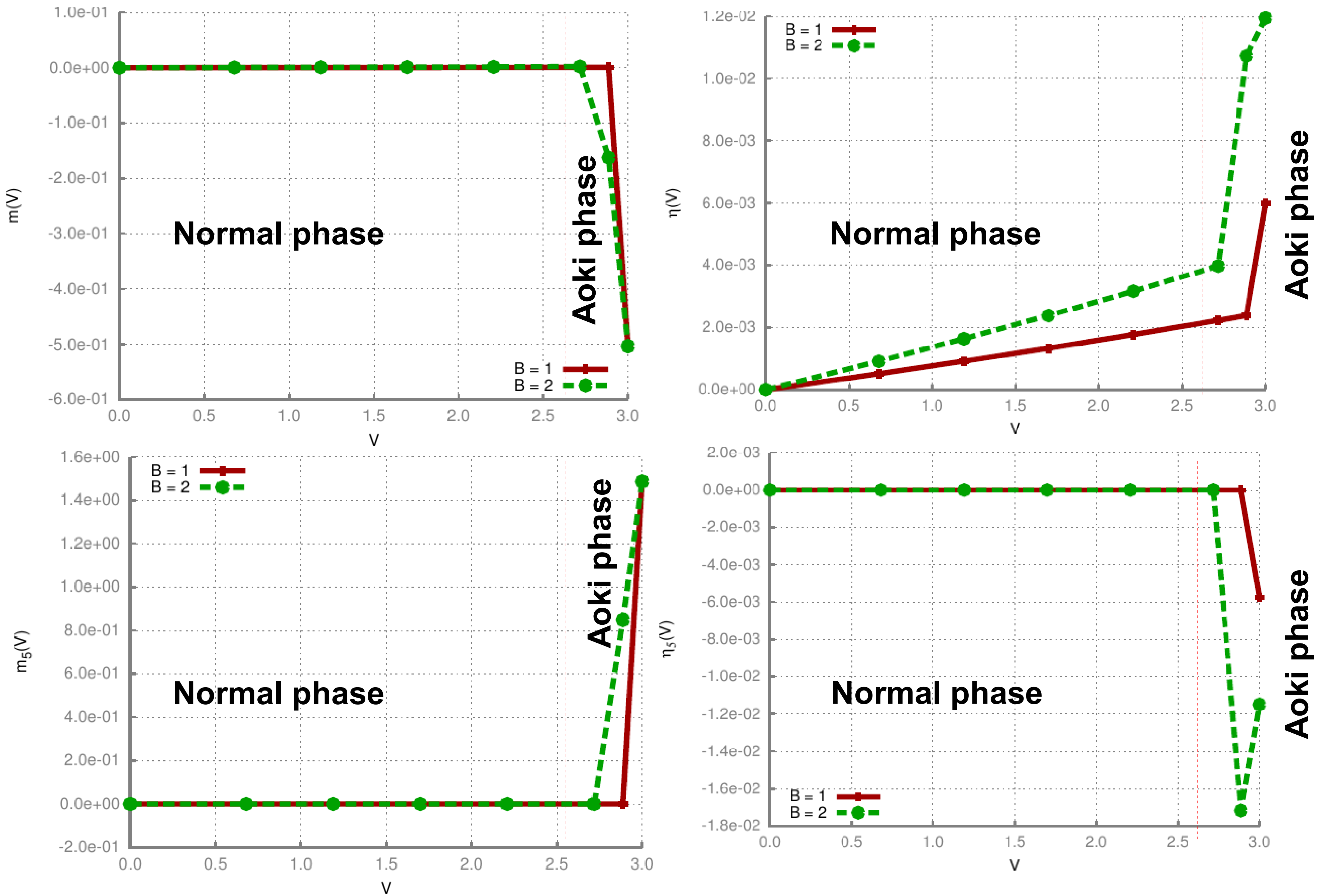
(Derived for LLL in continuum)

Our magnetic field B = 1 corresponds to physical magnetic field B ~ 1T for reasonable size of lattice step a ~ 0.1 nm.

Renormalization is very weak in normal phase

L=100

Phase diagram in the magnetic field



Real-time simulations: setup

$$\begin{cases} \partial_t \Phi_A(t) = -i\frac{V}{2}\sum_n \psi_n^\dagger(t)[H(t),\Gamma_A]\psi_n(t) \\ \partial_t \psi_n(t) = -iH(t)\psi_n(t) \end{cases}$$

$$H(t) = -iv_f\alpha_x\nabla_x + r\gamma_0\Delta + V + m^{(0)}\gamma_0 + \sum_A \Phi_A(t)\Gamma_A$$
$$+v_f\alpha_y \sin(k_y + Bx) + 2r\gamma_0\sin^2((k_y+Bx)/2)$$
$$+v_f\alpha_z \sin(k_z + A_z(t)) + 2r\gamma_0\sin^2((k_z+A_z(t))/2)$$

Since initial ground state is completely homogeneous in space, we can greatly speed up numerical calculations — by a factor of L.

Let us illustrate the idea in continuum theory, however the same holds also for lattice.

In magnetic field states are described by wave-functions of quantum oscillator which obey: $\psi_n(x, p_y) \equiv \psi_n(p_y + Bx)$

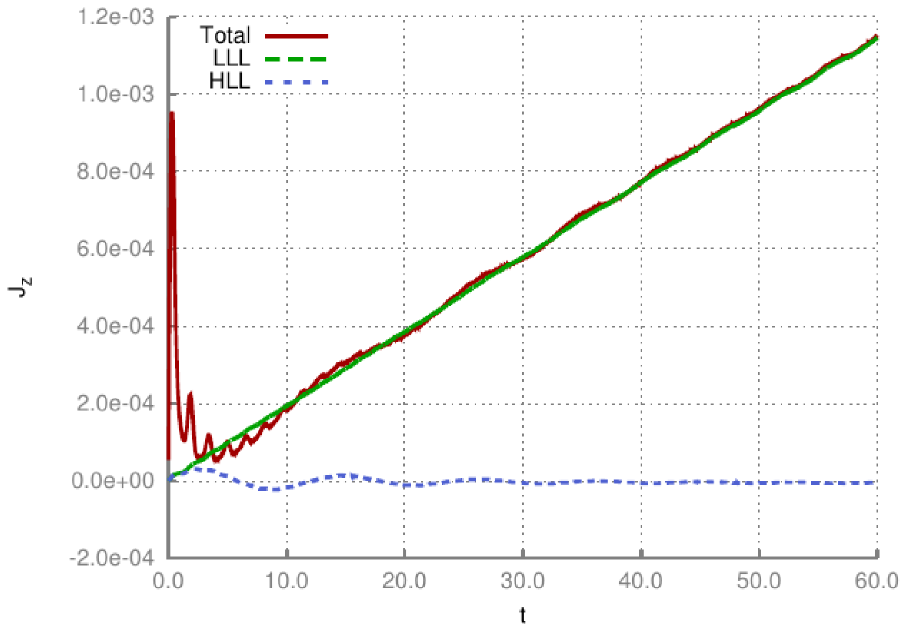
It is possible to show that because of this if initial state is homogeneous, then this homogeneouty will be preserved by evolution.

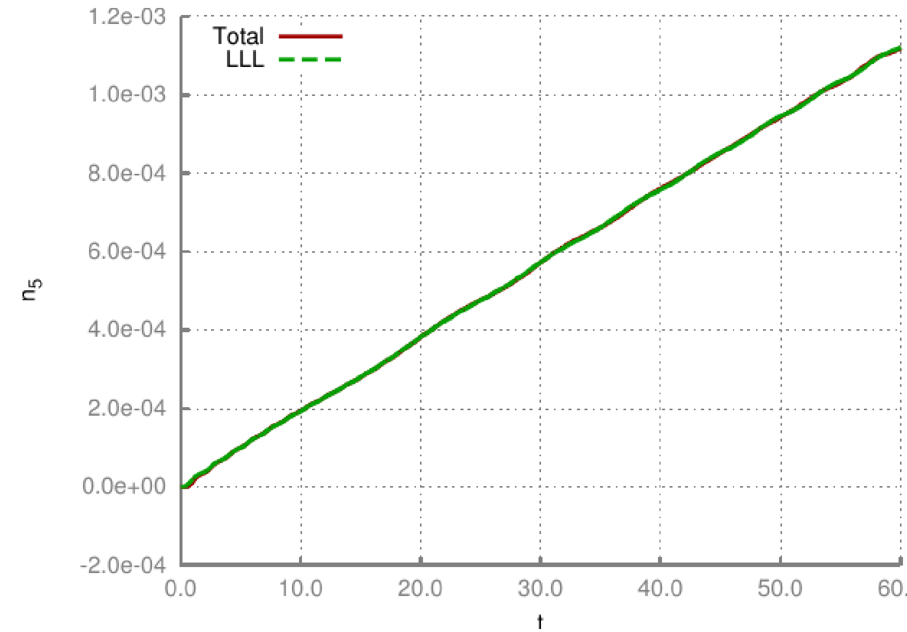
We can use this in order to simulate all quantities at a single point:

$$\Phi_A(\cancel{x})$$

Vector current and anomaly in constant electric field

We apply constant electric field E||B to the free sysytem (V = 0)





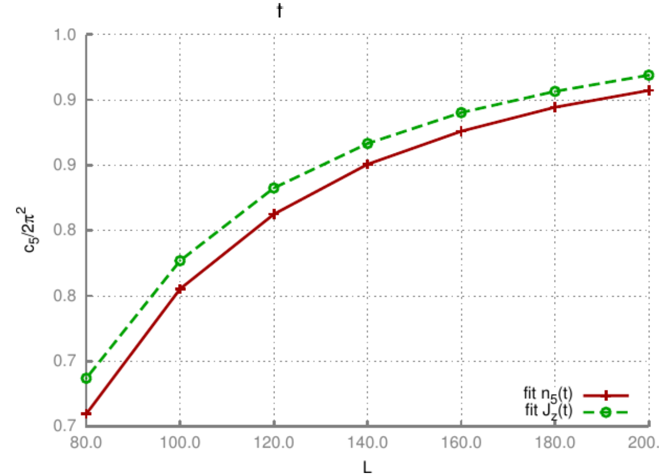
The current and axial density are saturated by contrubution of lowest Landau level.

In limit of infinite lattice size we reproduce chiral anomaly and Nielsen-Ninomia static magnetoconductivity:

$$\frac{dn_5}{dt} = \frac{1}{2\pi^2} BE$$

$$\boxed{\sigma = \frac{B}{2\pi^2}}$$

**Nielsen, Ninomiya,
Phys. Lett. B 130 (1983) 389**

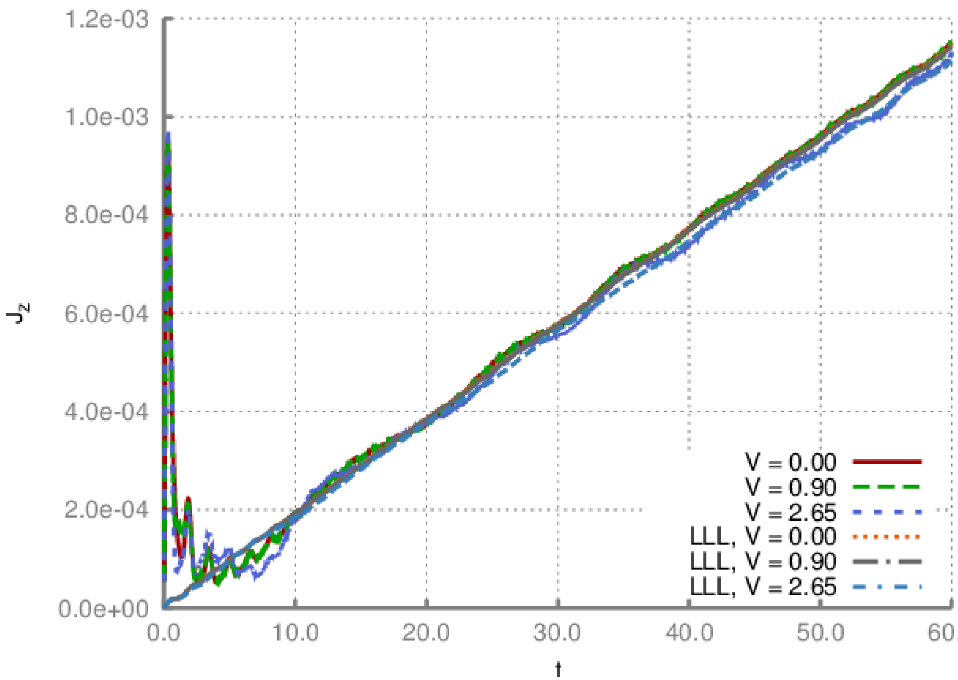


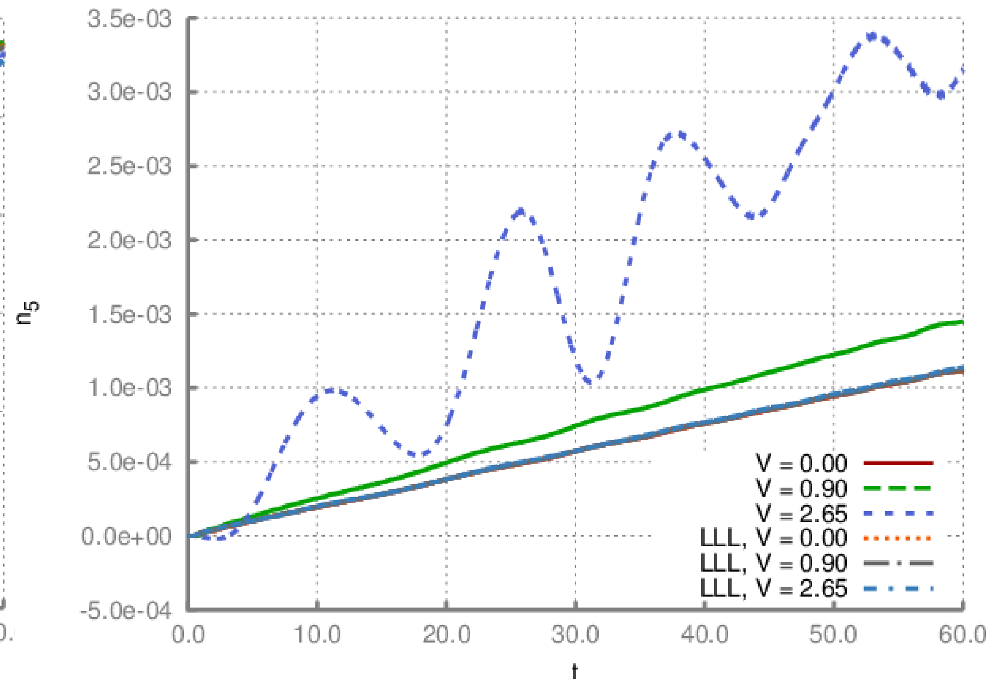
Scaling of anomaly coefficient with the volume

For real time evolution of free Weyl SM see also **B. Rosenstein, M. Lewkowicz Phys. Rev. B 88, 045108**

Vector current and anomaly in constant electric field

Now we switch on iteractions:





Although naive «chiral density» production rate is greatly increased, the DC conductivity is almost insensitive to interactions!

It is also interesting to test the result obtained by M. Zubkov and R.A. Abramchuk:

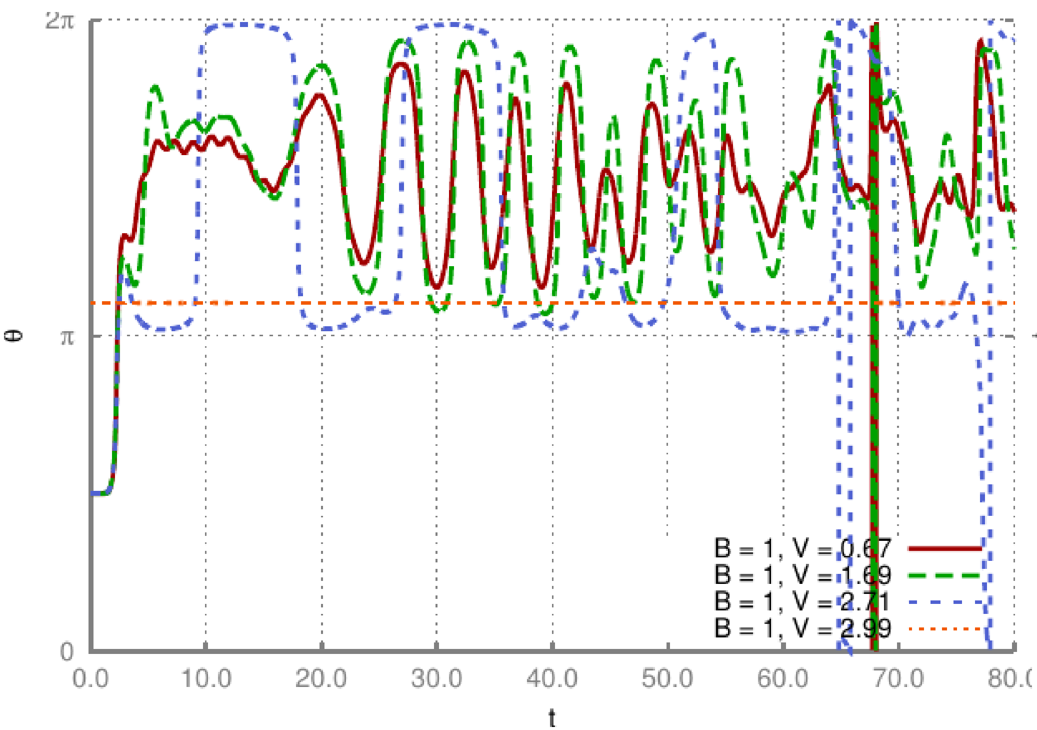
$$J_z(t) = \frac{BE}{2\pi^2} \coth\left(\frac{\pi B}{E}\right) t$$

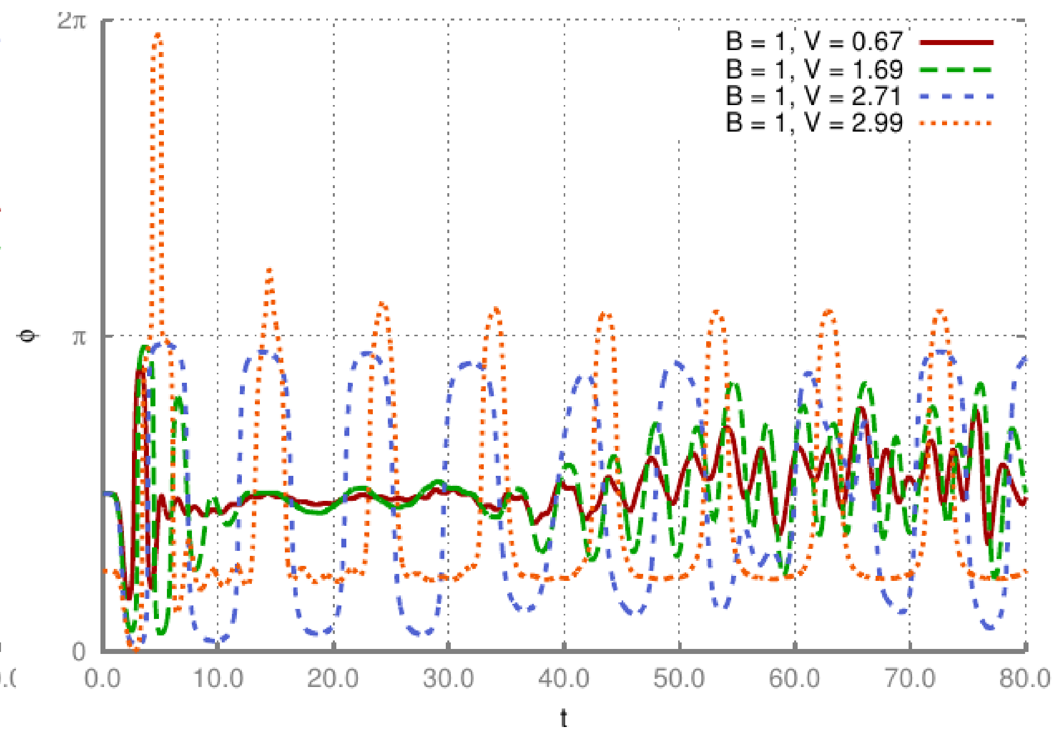
arXiv:1605.02379

But with present data we cannot see such corrections since our parameters correspond to asymtotic region $B \to \infty$. This gives an important direction for future work.

Dynamics of condensates: Axion(s)

$$m\gamma_0 + \eta\gamma_3\gamma_5 - im_5\gamma_0\gamma_5 - i\eta_5\gamma_3 = |M|\gamma_0 e^{-i\theta\gamma_5} + |N|\gamma_3\gamma_5 e^{-i\phi\gamma_5}$$

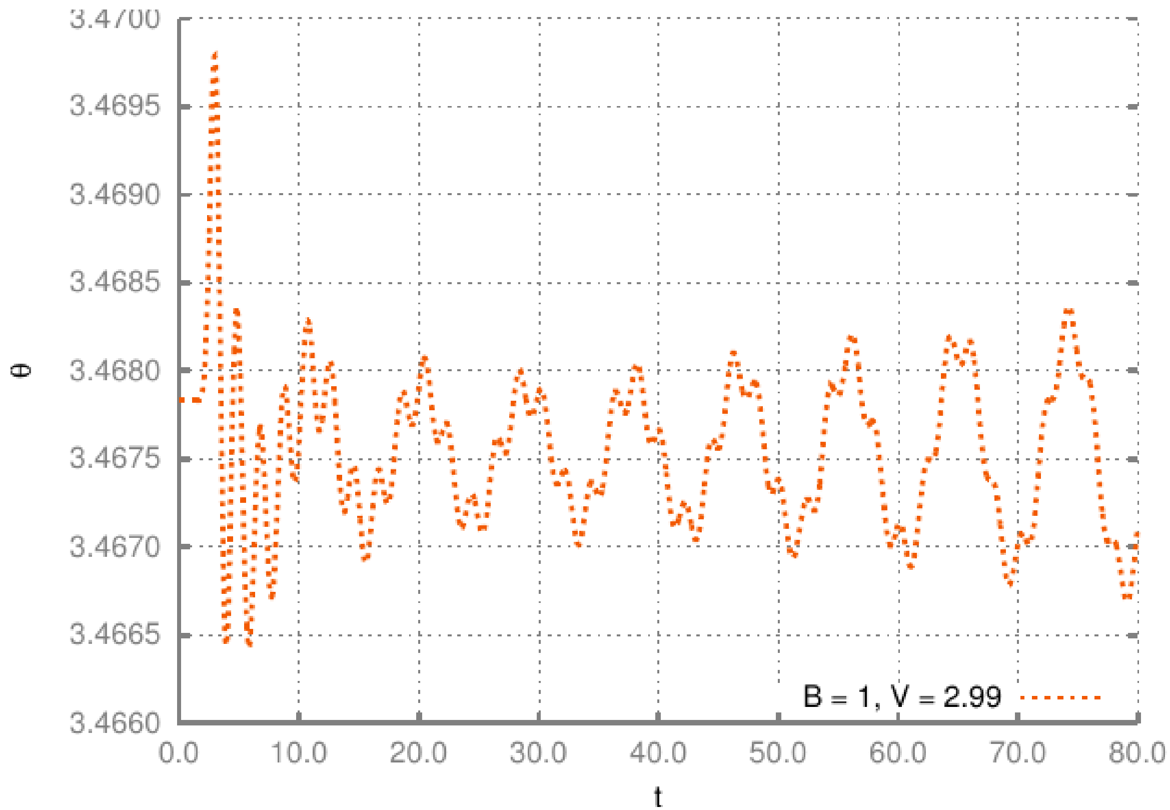




Are there any signatures of axion dynamics in the vector current?

Dynamics of condensates: Axion(s)

$$m\gamma_0 + \eta\gamma_3\gamma_5 - im_5\gamma_0\gamma_5 - i\eta_5\gamma_3 = |M|\gamma_0 e^{-i\theta\gamma_5} + |N|\gamma_3\gamma_5 e^{-i\phi\gamma_5}$$

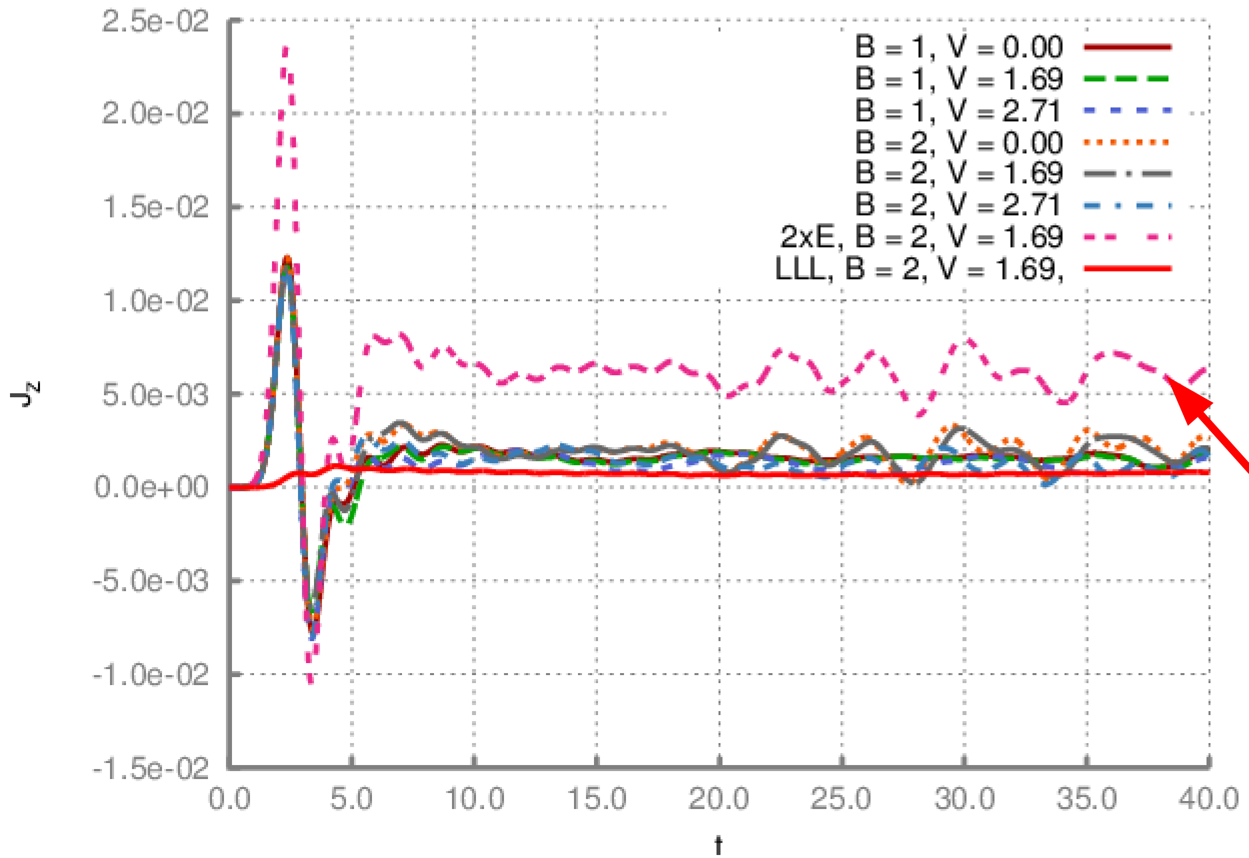


Zoomed in fluctuations of axion in the Aoki phase

Are there any signatures of axion dynamics in the vector current?

AC conductivity

We can also study a response to a short pulse of electric field parallel to magnetic field:



An induced steady («CME») current is again insensitive to interactions!

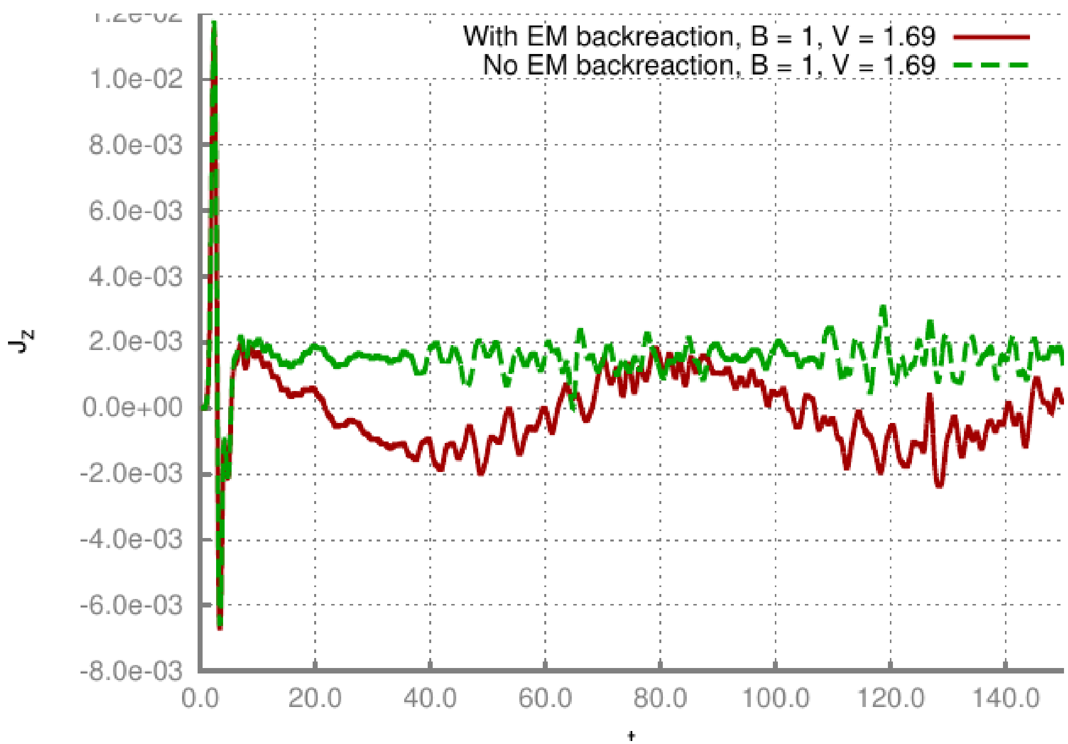
This current is a sum of ordinary Ohmic conductivity and CME, and depending on the time length of the pulse either Ohmic conductivity dominates or CME.

AC conductivity

But we miss important ingredient — namely, backreaction of electric field!

Let us supplement our equations with Maxwell eqautions for homogeneous in space and static magnetic field and homogeneous electric field:

$$\begin{cases} \partial_t A_z(t) = -E_z(t) \\ \partial_t E_z(t) = -< J_z(t) > \end{cases}$$

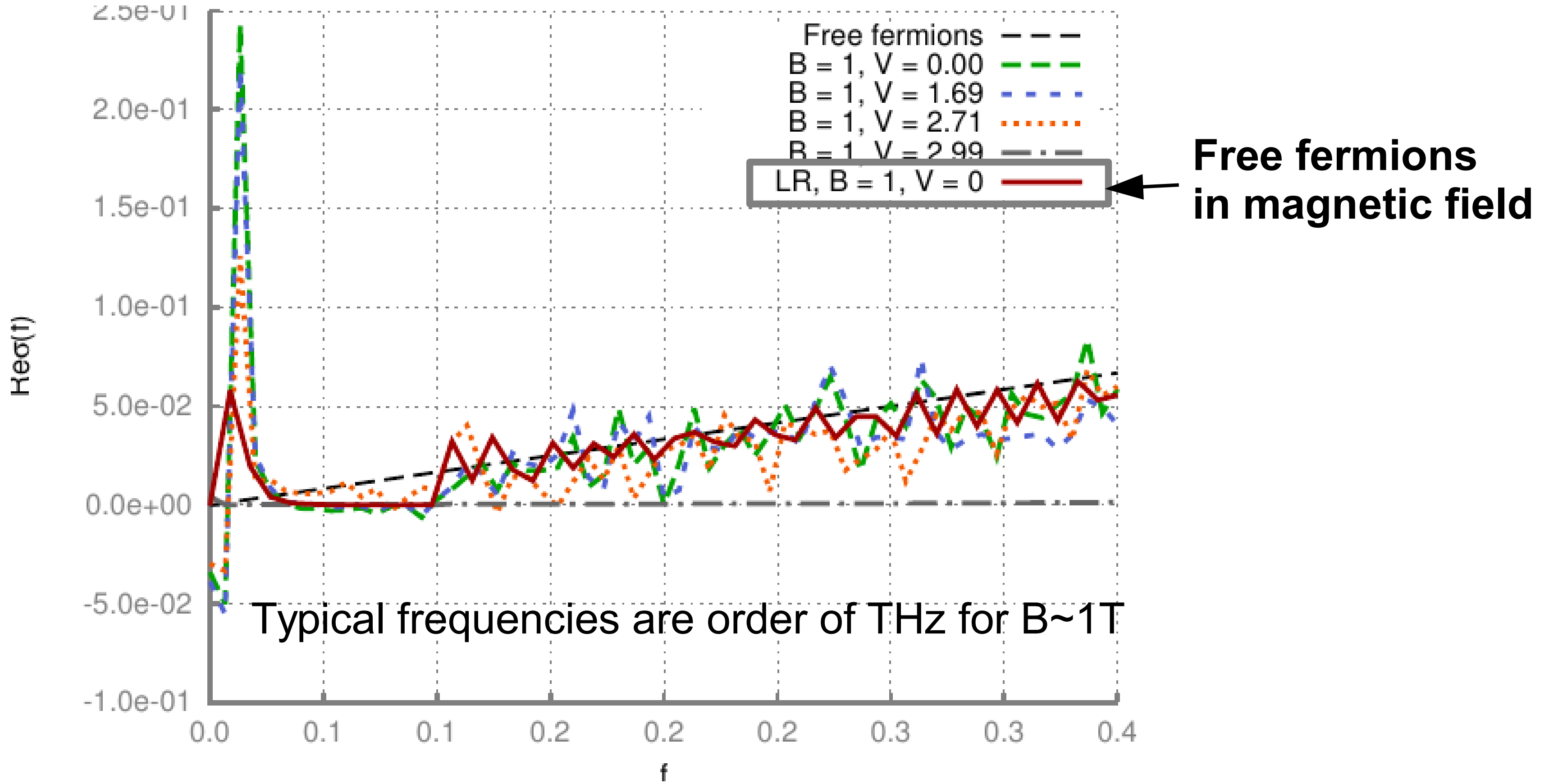


Plasma oscillations emerge as a consequence of backreaction of electric field

Doesn't significantly affect on dynamics of axion

AC conductivity

Knowing electric field and the response, one can use defenition of optical conductivity in order to estimate it:



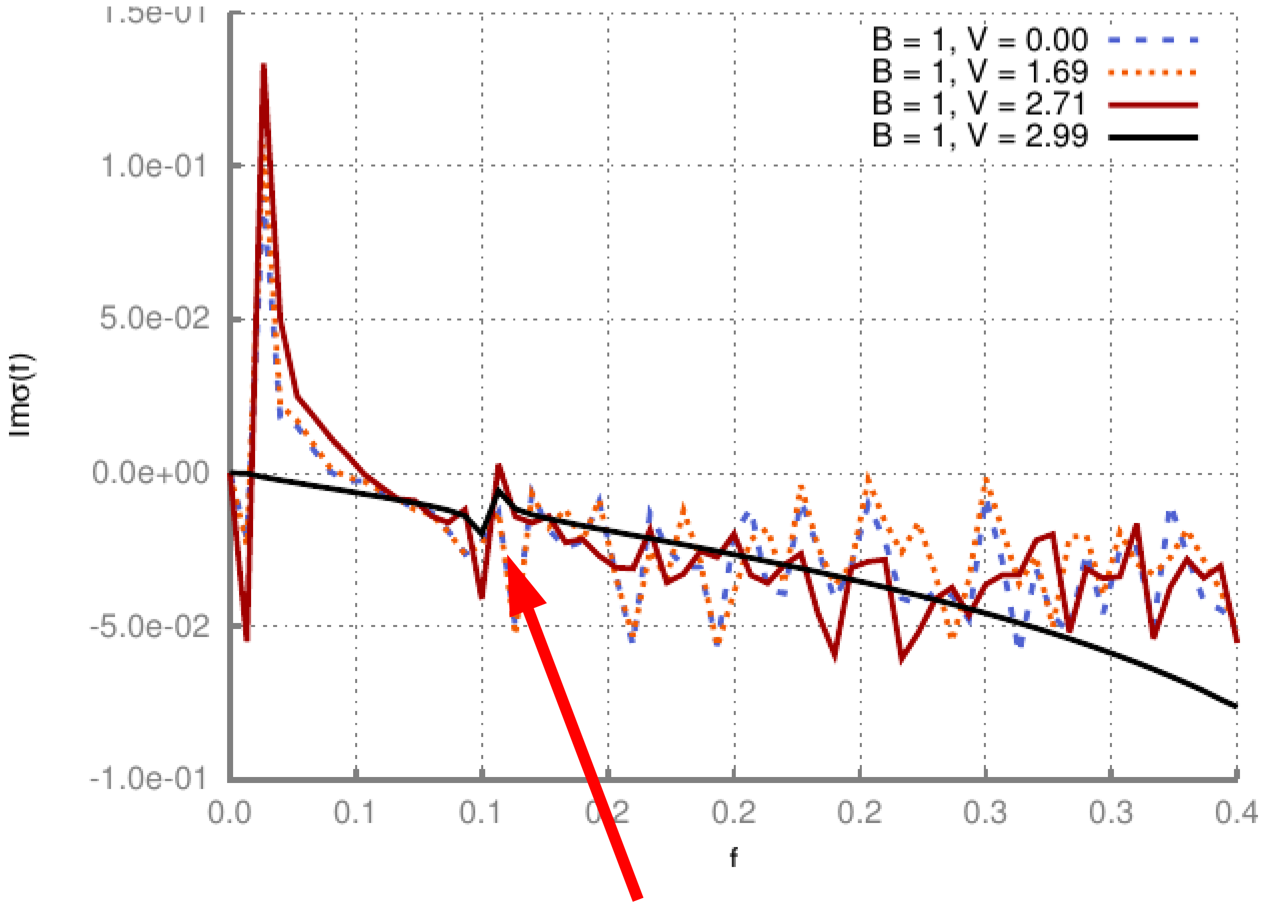
Preliminary conclusions:

1) It seems that optical response is very similar to response of free fermions in magnetic field (in normal phase) and effects of interactions are presumably small

2) No evident signatures of axion (probably poorely visible..)

AC conductivity

Imaginary part of conductivity:



In Aoki phase some interesting resonanse emerges at frequency f~0.1

Period of oscillations of axion is an agreement with this observations: T~10

Position of the resonanse is almost insensitive to external fields!

Conclusions

1) We have studied model of interacting Dirac semimetal using Wilson-Dirac fermions with contact interaction term both in equlibrium and in out-of-equlibrium setups.

2) In equlibrium we explored the phase diagram and observed enchancement of chiral chemical potential by interactions.

3) However, calculated value of CME conductivity was enhanced primarily due to enchancement of chiral chemical potential, while loop corrections were quiet small and always decreased the conductivity, so that conductivity never exceeded naive value with renormilized chiral chemical potential.

4) In out-of-equlibrium setup we studied process of formation of chiral imbalance in parallel magnetic and electric fields and found that effect of interactions is quiet small.

5) Effects of interactions in the normal phase are turned out to be very small in both DC and AC conductivity.

6) Although there is a dynamical axion field, we were not able to detect any observable signatures of it in the response of vector current in normal phase.

7) As one of possible directions of future development it is interesting to simulate different types of chiral waves:

M. Chernodub, JHEP 1601 (2016) 100