# Lattice gauge theory treatment of electron correlation in Dirac semimetals

## ディラック半金属における電子相関と格子ゲージ理論

Yasufumi Araki [1,2]
荒木 康史
Kentaro Nomura [1]
野村 健太郎

[1] Institute for Materials Research, Tohoku Univ.
東北大学 金属材料研究所
[2] Frontier Research Institute for Interdisciplinary Sciences, Tohoku Univ.
東北大学 学際科学フロンティア研究所

*Paper in preparation*

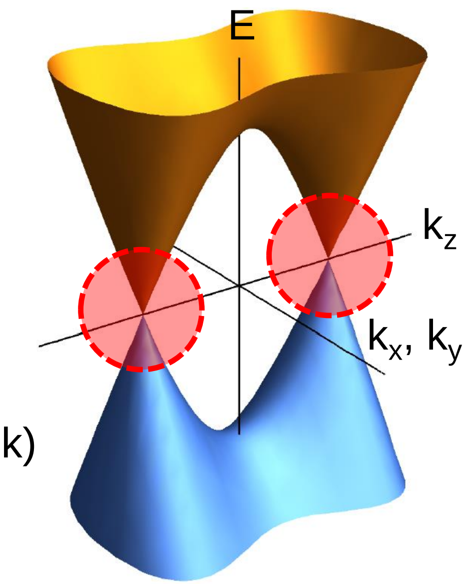
基研研究会「熱場の量子論とその応用」
京都大学 基礎物理学研究所 - Aug. 31, 2015

# IMR and FRIS


金属材料研究所 (IMR)

学際科学フロンティア研究所 (FRIS)

# Dirac semimetals




Dirac band structure realized in electronic spectrum:

- gapless, band touching at "Dirac points"
- protected by topology, crystalline symmetry, ...

**2D**

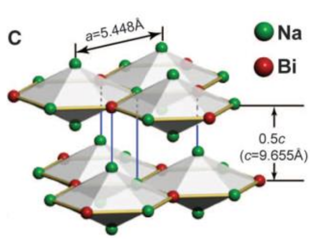
graphene (sheet of carbon atoms)
surface states of topological insulators (gapped in the bulk)

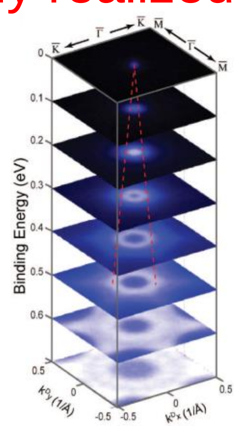
**3D counterpart...?** ("3D analogue of graphene")

Theoretical prediction: $BiO_2$ Young et al. PRL **108**, 140405 (2012)

⟹ Experimentally realized recently.

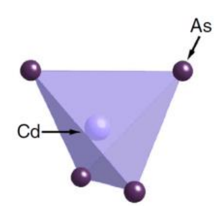
$Na_3Bi$

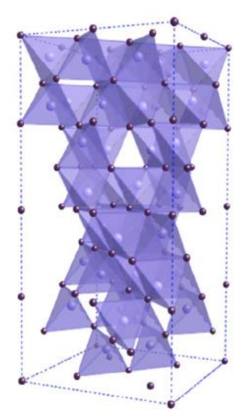


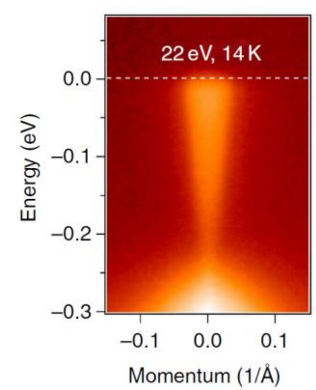




Liu et al. Science **343**, 864 (2014)

$Cd_3As_2$






Neupane et al. Nat. Commun. **5**, 3786 (2014)

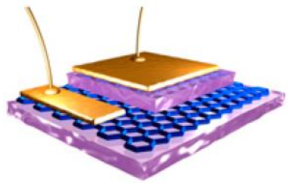
# Many-body effects?

- Electron-electron interaction

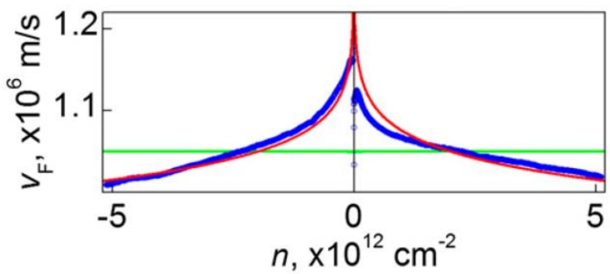
⇨ electron correlation can change the Dirac spctrum drastically...

- Dynamical mass generation (excitonic instability, chiSB)
- Renormalization of Fermi velocity (absence of Lorentz invariance)
- Dynamical screening

e.g.) graphene: $v_F$ renormalized at charge neutrality.



Yu et al. PNAS **110**, 3282 (2013)

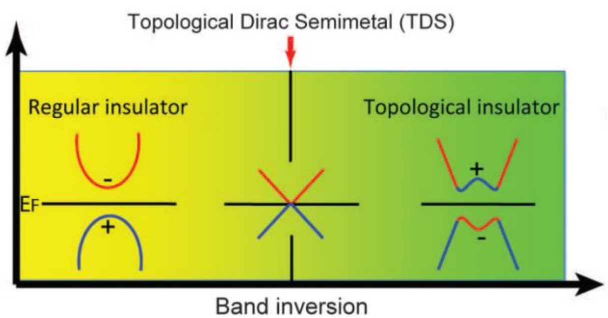



*Many-body effects in 3D Dirac semimetals?*

Change in the spectrum

⇨ turn into various phases...

e.g.) normal insulator, topological insulator,
Weyl semimetal, axionic insulator, ...




*Important as a platform for many novel states.*

Liu et al. Science **343**, 864 (2014)

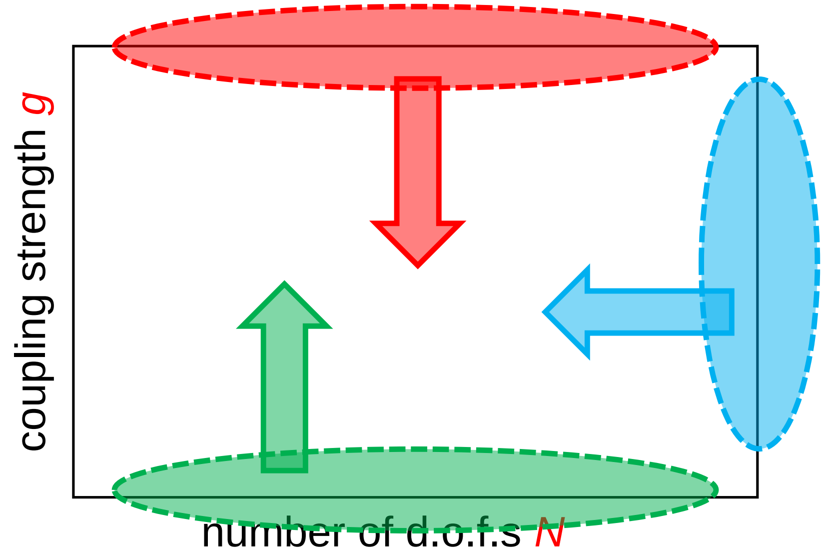
# Analysis on many-body effects

How to investigate many-body effects?

Choice of interaction:

- Lorentz non-invariant QED
- phenomenological potential

⇒ RG, self-consistent eqn., Lattice Monte Carlo, ... etc.




*In 3D Dirac semimetals...*

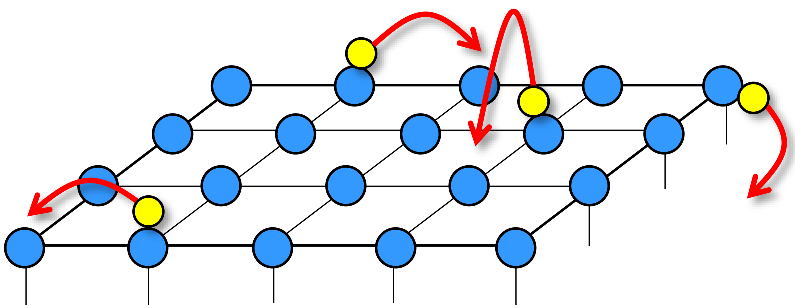
- RPA(large-$N$) analysis — Hofmann et al. PRB **92**, 045104 (2015)
- From weak coupling... self-consistent eqn. — Gonzalez, arXiv:1502.07640
  RG analysis — Throckmorton et al., arXiv:1505.05154
- From strong coupling... strong coupling expansion of lattice QED
  Sekine & Nomura, JPSJ **83**, 094710 (2014); PRB **90**, 075137 (2014)
  w/ hypothetical lattice models.

*Improve*

This work: Lattice QED analysis with realistic d.o.f.s/symmetries.
connect the analysis to continuum limit.

# Lattice action for fermions

- Lattice Hamiltonian:



$$\hat{H} \equiv \sum_s \hat{\psi}_s^\dagger \mathcal{H} \hat{\psi}_s - \mu_{\rm bg} \hat{b}^\dagger \hat{b}$$

tight-binding Hamiltonian

background charge

$(\mu_{\rm bg} \to \infty)$

Eigenvalue: $E(\mathbf{k}) \simeq v_F |\mathbf{k} - \mathbf{k}_D|$
around Dirac points $k_D$

- Path integral formalism:

Split the imaginary time $\beta$ into $N_\tau$ steps: $a_\tau$

⟹ Leave $a_\tau$ dependence ($a_\tau \to 0$ is required.)

$$S_F[\psi^\dagger, \psi; b^\dagger, b] = a_\tau \sum_\tau \left( \psi_s^\dagger \left[ \partial_\tau^{(+)} + \mathcal{H} \right] \psi_s + b^\dagger \left[ \partial_\tau^{(+)} - \mu_{\rm bg} \right] b \right)$$

with forward difference $\partial_\tau^{(+)} \psi(\tau) \equiv \dfrac{\psi(\tau + a_\tau) - \psi(\tau)}{a_\tau}$

cf.) A similar form appears in Astrakhantsev et al., arXiv:1506.00026

*Symmetries of the Hamiltonian [e.g. spin SU(2)] is preserved.*

e.g.) spin SU(2) is broken to U(1) in staggered fermion formalism.

# Coupling to gauge field

- Continuum:

  Scalar potential $A_0$: mediates 1/r Coulomb interaction.

  $v_F \ll c$: neglect the retardation ($A_{1,2,3}$) effect.

  e.g.) $Na_3Bi$: $v_F/c \sim 10^{-3}$

$$S_{\mathrm{int}} + S_{\mathrm{G}} = \int d^4x \left[ -iA_0 n + \frac{1}{2g^2}(\nabla A_0)^2 \right]$$

$n = \psi_s^\dagger \psi_s - b^\dagger b$ : local charge density

- Lattice:

  Define the gauge variable $U_0(\mathbf{r},\tau) = e^{i a_\tau A_0(\mathbf{r},\tau)}$ on each site.

  (not on the links)

$\Longrightarrow$ The total lattice action becomes

$$S_F[\psi^\dagger,\psi;b^\dagger,b;U_0] = a_\tau \sum_\tau \left( \psi_s^\dagger \left[ D_\tau^{(+)}[U_0] + \mathcal{H} \right] \psi_s + b^\dagger \left[ D_\tau^{(+)}[U_0^\dagger] - \mu_{\mathrm{bg}} \right] b \right)$$

$$S_G[U_0] = g_R^{-2} \sum_{\mathbf{r},\tau} \sum_{j=1,2,3} \mathrm{Re} \left[ 1 - U_0^\dagger(\mathbf{r},\tau) U_0(\mathbf{r}+a\hat{j},\tau) \right]$$

Take the "renormalized" coupling $g_R^{-2} = g^{-2} \dfrac{a}{a_\tau}$ as an expansion parameter.

# Strong coupling expansion

(i) Expand around the strong coupling limit $g_R^{-2}=0$

(ii) Integrate out the gauge degrees of freedom $U_0$

⟹ Derive the effective action for fermions: $S_{\rm eff}$

$$e^{-S_{\rm eff}[\psi^\dagger,\psi;b^\dagger,b]} = \int [dU_0] e^{-S_F[\psi^\dagger,\psi;b^\dagger,b;U_0]-S_G[U_0]}$$
$$\simeq \int [dU_0] e^{-S_F[\psi^\dagger,\psi;b^\dagger,b;U_0]} \left(1 - S_G[U_0] + \cdots\right)$$

---

- Strong coupling limit [$g_R^{-2}=0$]:

  Propagation of "photon" is suppressed.

  ⟹ Correlates charge density at the same site. $n \equiv \psi_s^\dagger \psi_s - b^\dagger b$

$$S_{\rm eff}^{(0)} = S_F[U_0 = 1] + \frac{1}{4}\sum_{\mathbf{r},\tau} n^2(\mathbf{r},\tau)$$

- NLO correction [$O(g_R^{-2})$]:

  $S_G$ carries "photon" to a neighboring site.

  ⟹ Correlates charge densities between nearest neighboring sites.

$$S_{\rm eff}^{(1)} = g_R^{-2} \sum_{\langle \mathbf{r},\mathbf{r}'\rangle,\tau} \left[1 + \left(\frac{n(\mathbf{r},\tau)}{2} + \frac{n^3(\mathbf{r},\tau)}{16}\right)\left(\frac{n(\mathbf{r}',\tau)}{2} + \frac{n^3(\mathbf{r}',\tau)}{16}\right)\right] \simeq g_R^{-2} \sum_{\langle \mathbf{r},\mathbf{r}'\rangle,\tau} \left[1 + \frac{1}{4} n(\mathbf{r},\tau) n(\mathbf{r}',\tau)\right]$$

# Strong coupling limit

On-site repulsion is generated in the strong coupling limit:

$$S_{\rm eff}^{(0)}[\psi^\dagger,\psi;b^\dagger,b] = a_\tau \sum_\tau \left[ \psi_s^\dagger \left[\partial_\tau^{(+)} + \mathcal{H}\right] \psi_s + b^\dagger \left[\partial_\tau^{(+)} - \mu_{\rm bg}\right] b + \frac{1}{4a_\tau} \sum_{\mathbf{r},\tau} n^2(\mathbf{r},\tau) \right]$$

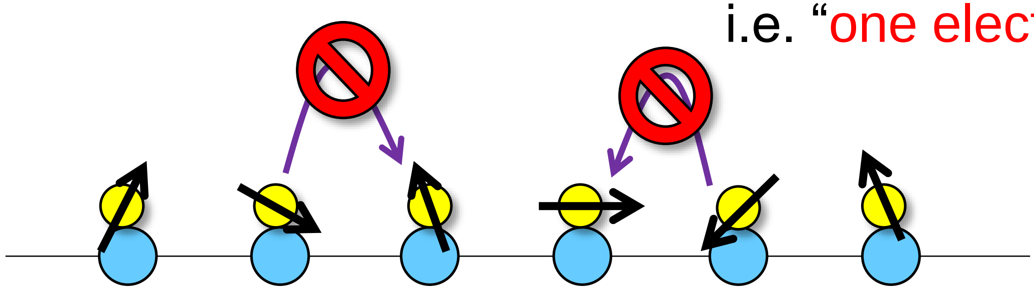
Going back to Hamiltonian formalism:

$$\hat{H} = \hat{\psi}_s^\dagger \mathcal{H} \hat{\psi}_s - \mu_{\rm bg} \hat{b}^\dagger \hat{b} + \boxed{\frac{1}{4a_\tau} \sum_{\mathbf{r}} \hat{n}^2(\mathbf{r})}$$

Repulsive Hubbard interaction: $U = 1/4a_\tau \to \infty$ in the continuum limit.

⟹ requires local charge neutrality: $\langle \hat{n}(\mathbf{r}) \rangle = \langle \hat{\psi}_s^\dagger \hat{\psi}_s \rangle(\mathbf{r}) - \langle \hat{b}^\dagger \hat{b} \rangle(\mathbf{r}) \overset{!}{=} 0$

i.e. "one electron per one site"



⟹ The system becomes Mott insulator in the continuum limit ($a_\tau \to 0$).

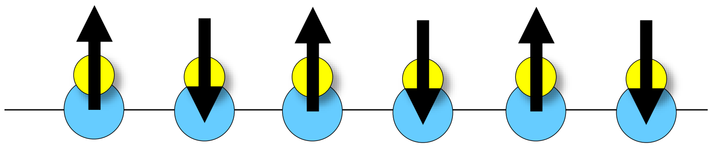
# Mean-field analysis

On-site repulsion: $\frac{1}{4}n^2 = \frac{1}{4}(\psi_\uparrow^\dagger\psi_\uparrow + \psi_\downarrow^\dagger\psi_\downarrow - 1)^2$

Introduce bosonic field $\vec{\phi} \sim \langle\psi^\dagger\vec{\sigma}\psi\rangle$ (local spin polarization)

(Hubbard-Stratonovich)

$$\frac{1}{12}|\vec{\phi}|^2 - \frac{1}{6}\psi^\dagger(\vec{\sigma}\cdot\vec{\phi})\psi$$



Mean field: antiferromagnetic (Neel) order $\vec{\phi}(\mathbf{r},\tau) \equiv (-1)^{(x+y+z)/a}\vec{\phi}$

---

e.g.) On the cubic lattice:

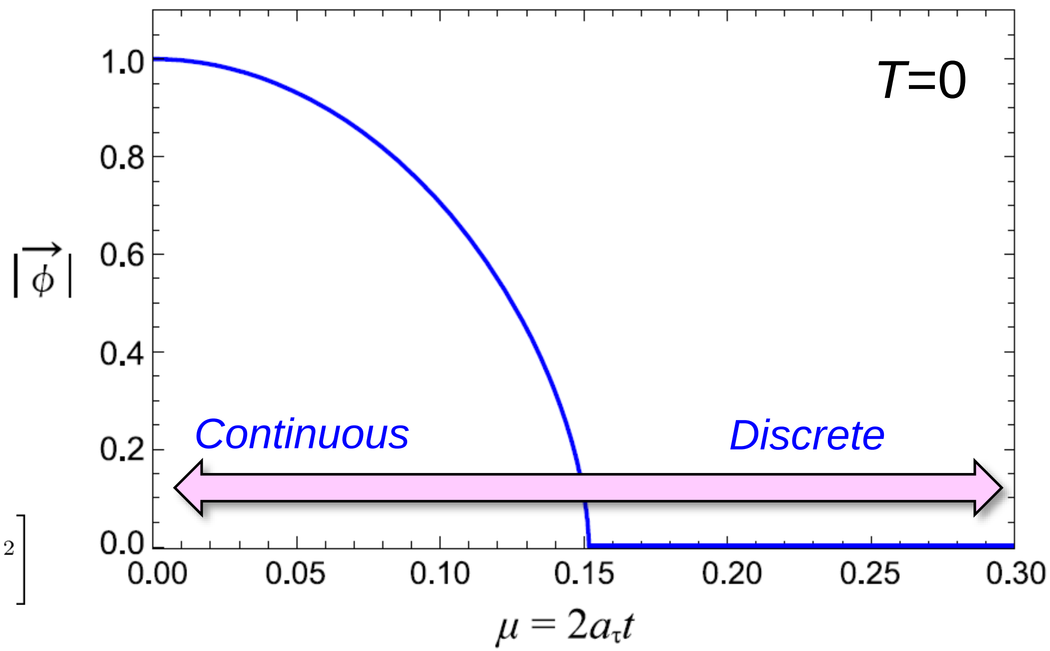
$$E(\mathbf{k}) = 2t\sqrt{\sum_j \cos^2(ak_j)}$$

($t$: hopping amplitude)

Integrate out the fermionic d.o.f.s:

$$F_{\text{eff}}(\vec{\phi}) = -\frac{1}{N_\tau N^3}\ln Z(\vec{\phi})$$

$$= \frac{1}{12}|\vec{\phi}|^2 - \frac{1}{N_\tau N^3}\sum_{\omega_n,\mathbf{k}}\ln\left[\frac{|\vec{\phi}|^2}{36} + a_\tau^2E^2(\mathbf{k}) - (e^{-ia_\tau\omega_n} - 1)^2\right]$$




$\Rightarrow$ $a_\tau \to 0$: Mott insulator (Dirac mass generation)

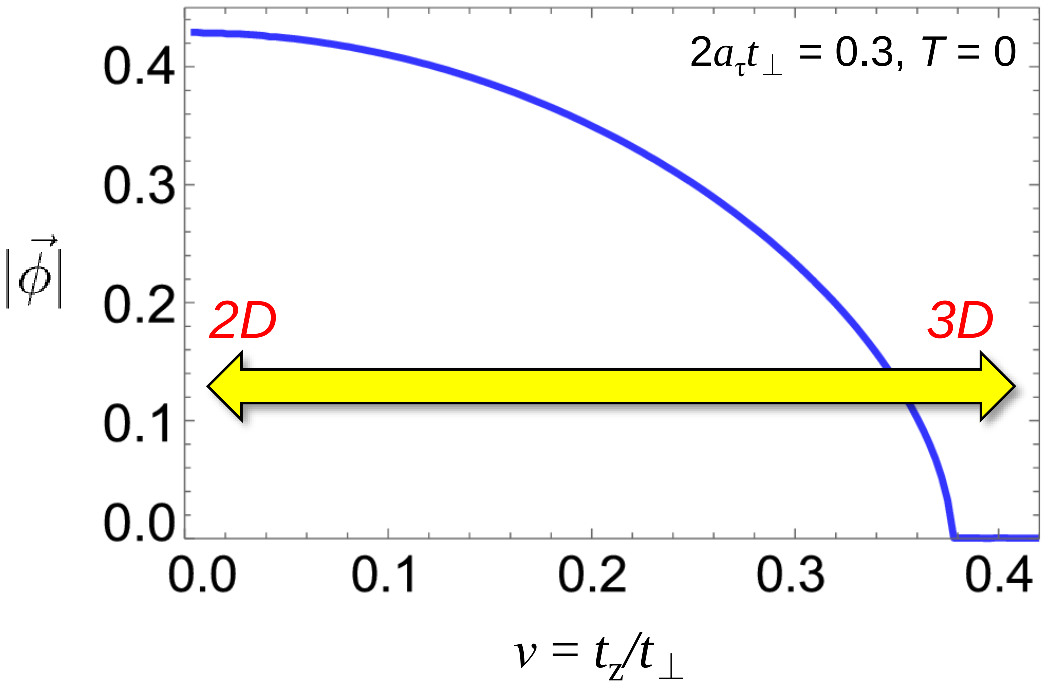
# Dimensionality dependence

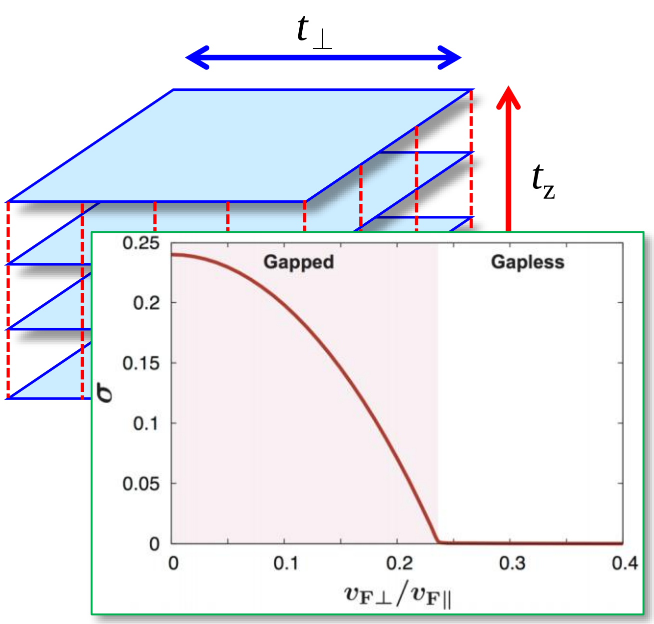
Introduce anisotropy in the hopping amplitude: $t_z/t_\perp = \nu$

$\begin{cases} \nu = 1\text{: 3D cubic symmetry} \\ \nu = 0\text{: stacked 2D (e.g. graphene)} \end{cases}$

e.g.) $Na_3Bi$: $\nu \sim 0.25$

⇨ Observe the 3D-2D crossover at finite $a_\tau \sim O(a)$.

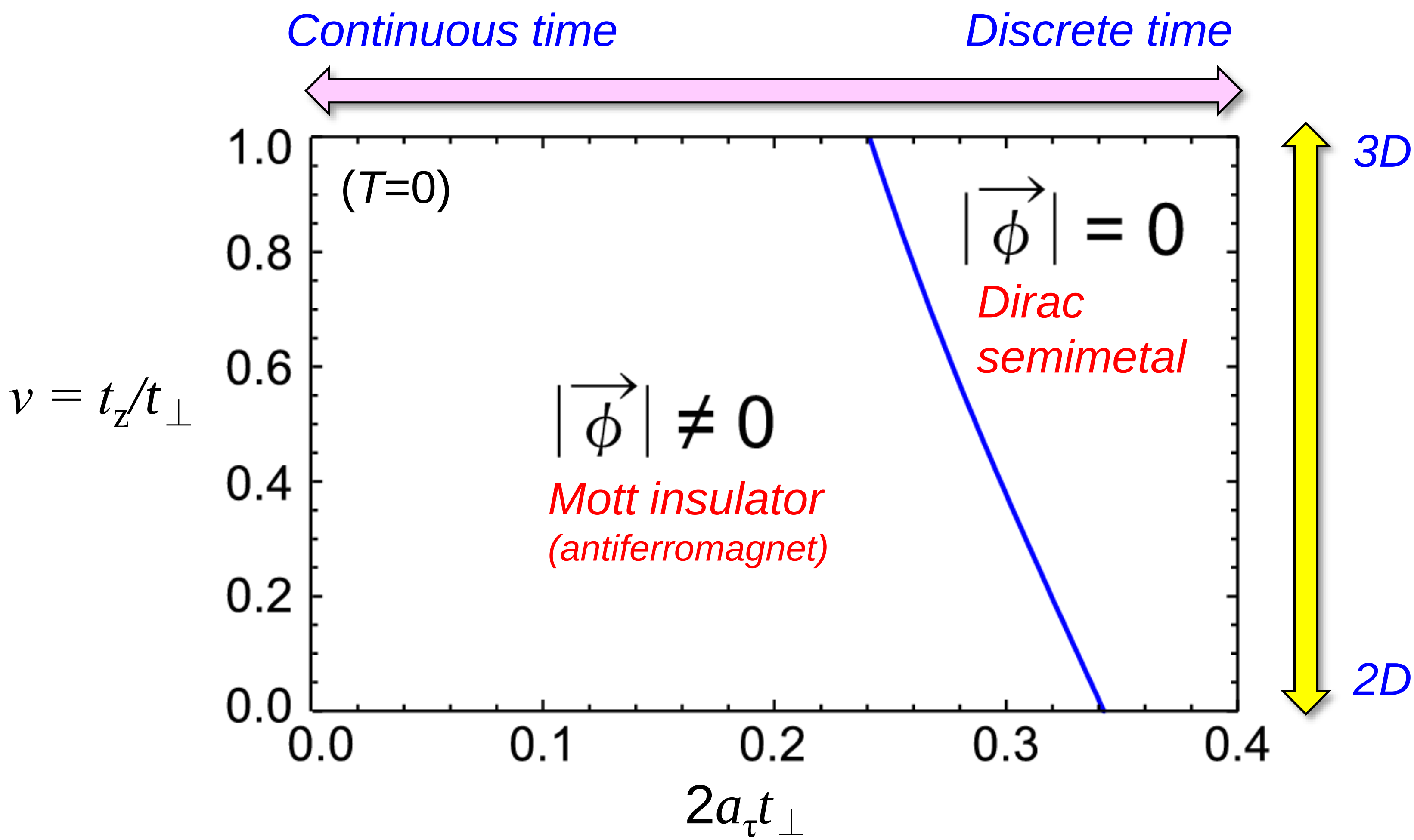



Consistent with previous calculation with hypothetical staggered fermion.

Sekine & Nomura, PRB **90**, 075137 (2014)

# "Phase diagram"




Finite $a_\tau \sim O(a)$: consistent with the "staggered fermion" results.

$a_\tau \to 0$ limit: local charge neutrality (Mott insulator) is required.

- connected by $a_\tau$-dependent formalism.

# Away from strong coupling limit

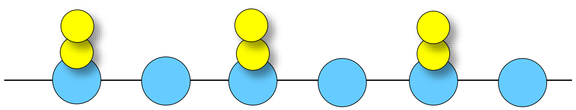
Nearest-neighbor repulsion is generated in the next-to-leading order:

$$S_{\text{eff}}^{(1)}[\psi^\dagger,\psi;b^\dagger,b] \simeq g_R^{-2} \sum_{\langle \mathbf{r},\mathbf{r}'\rangle,\tau} \left[1 + \frac{1}{4} n(\mathbf{r},\tau) n(\mathbf{r}',\tau)\right]$$

(assume $n \sim 0$ : around local charge neutrality)

⟹ Contributes to

- new type of order: "charge density wave"
  not favorable around local charge neutrality...
- renormalization of NN hopping → Fermi velocity



► Mean-field description:

Introduce a mean field (Hubbard-Stratonovich) $z$.

NN hopping: $t_R = t\,(1 + z)$ ⟹ Fermi velocity: $v_{FR} = v_F\,(1 + z)$

- renormalization from the strong coupling limit.

Effective action: $$F_{\text{eff}}(\vec{\phi}, z) = \frac{6(2a_\tau t)^2}{g_R^{-2}} z^2 + F_{\text{eff}}^0(\vec{\phi})\Big|_{t \,\to\, t_R = t(1+z)}$$

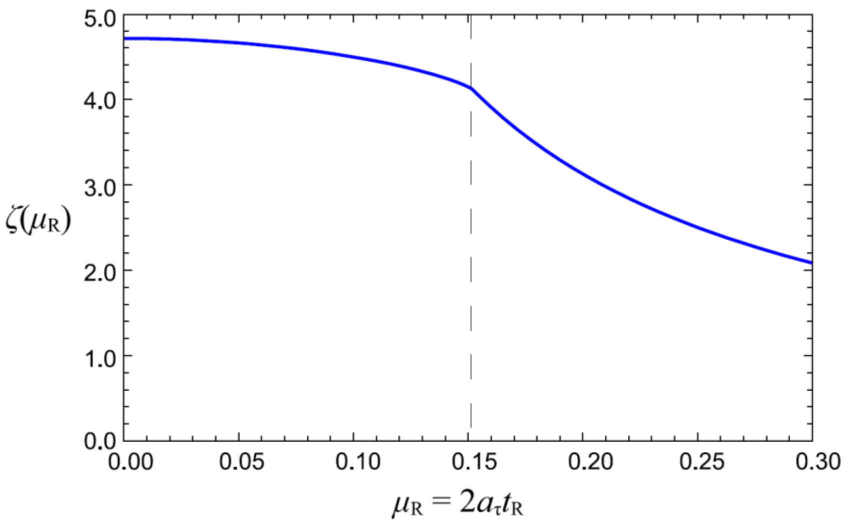
i.e. the behavior of $\phi$ can be obtained by replacing $t$ in the strong coupling limit with $t_R = t\,(1+z)$.

# Velocity renormalization and RG flow

Once the renormalized $t_{\mathrm{R}}$ at finite coupling $g_{\mathrm{R}}$ is chosen...

$$z \equiv g_R^{-2}\,\zeta(t_R) + O(g_R^{-4}) \Longrightarrow \frac{t_R}{1+z} = t \quad \text{(at strong coupling limit)}$$

- Coefficient $\zeta(t_{\mathrm{R}})$ is obtained from the self-consistent eqn.:



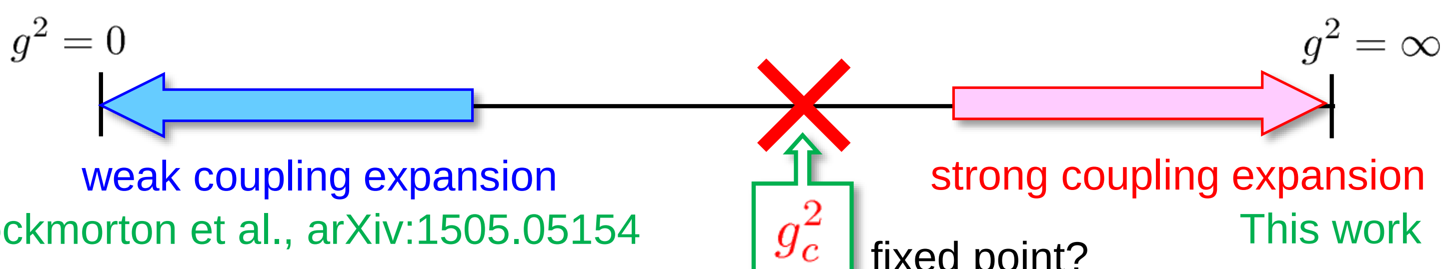

$$\boxed{\zeta > 0} \Longrightarrow t_R(g_R^2) > t(g_R^2 = \infty)$$

i.e. $v_F^R(g_R^2) > v_F(g_R^2 = \infty)$

The effect of EM field on carriers becomes smaller.

$\Longrightarrow$ AFM order gets suppressed.

- RG flow of effective coupling strength: $g_R^2 = g^2/v_F$




weak coupling expansion

Throckmorton et al., arXiv:1505.05154

fixed point?

strong coupling expansion

This work

# Summary

- Defined the lattice action for 3D Dirac semimetals,

  including $\left\{\begin{array}{l}\text{imaginary time discretization } a_\tau \\ \text{“background charge” field } b\end{array}\right.$

- In the strong coupling limit ($g_R^{-2} = 0$) of Coulomb interaction,

  infinitely large on-site (Hubbard) repulsion for $a_\tau \to 0$

  $\Longrightarrow$ Local charge neutrality is required. = Mott insulator.

  Necessary to connect finite $a_\tau$ analysis to $a_\tau \to 0$ limit.

- At the next-leading-order [$O(g_R^{-2})$] in strong coupling expansion:

  renormalization of Fermi velocity (NN hopping amplitude)

  $\Longrightarrow$ Opposite to the RG flow from weak coupling expansion.

---

- Include other novel topological phases...

  Weyl semimetal, topological insulator, axionic insulator, ...