Journée nationale de la vérité et de la réconciliation

UDEMNOUVELLES | LE 27 SEPTEMBRE 2021 | CHRISTINE FORTIER

# L'éducation à la réconciliation

Journée nationale de la vérité et de la réconciliation



#### Superconductivity in ultra-quantum matter: Part I

A.-M.S. Tremblay

RQMP 30 September 2021 10:30





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## **Atomic structure**





• Who ordered this?



Vishik, Rep. Prog. Phys. (2018)



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**Band structure for high Tc** 



#### "Universal" phase diagram



Public Domain, https://en.wikipedia.org/w/index.php?curid=21641300



#### **Mott Insulator : X-Ray absorption**



#### Meinders et al. PRB 48, 3916 (1993)

#### **Mott Insulator : X-Ray absorption**

#### Meinders et al. PRB 48, 3916 (1993)



#### Take home messages

- Most of the main features of the phase diagram follow from the Hubbard model.
- This physics is continuously connected to the Mott transition at halffilling
- We need to look beyond traditional tools of solid state physics to work this out.

## Minuterie

• 10 Minutes

## Outline

- Method
- One-band Hubbard model
  - Phase diagram
  - Pseudogap
  - d-wave superconductivity
  - A phase transition at the heart of the phase diagram
- Three-band Hubbard model : oxygen can probe the details
  - Pseudogap
  - d-wave superconductivity

# Method : The precursors

Hohenberg-Kohn : Exchange correlation Kohn-Sham : Basis set Density Functional Theory

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## Method

Metzner, Vollhardt PRL **62**, 324 (1989) Georges, Kotliar, PRB **45**, 6479 (1992) Jarrell PRL **69**, 168 (1992) Review: Georges, Kotliar, Krauth, Rozenberg, RMP **68**, 13 (1996)

**Dynamical Mean-Field Theory : DMFT** 





## For additionnal physical intuition: Compare with more analytical approaches

- Pseudogap
  - Wei Wu, Scheurer, Chatterjee, Sachdev, Georges, Ferrero PRX 8, 021048 (2018)
  - Scheurer, Chatterjee, Wu, Ferrero, Georges, Sachdev, PNAS 115, E3665 (2018).

#### Localized and delocalized pictures

Localized



Lichtenstein *et al.*,PRB 2000 Kotliar *et al.*, PRB 2000 M. Potthoff, EJP 2003

REVIEWS Maier, Jarrell et al., RMP. (2005) Kotliar *et al.* RMP (2006) AMST *et al.* LTP (2006)

$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$



$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

#### Localized and delocalized pictures





$$G_{ij}(\tilde{k}) = \left(\frac{1}{(i\omega_n + \mu)I - \varepsilon(\tilde{k}) - \Sigma}\right)_{ij}$$

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$$G_{ij}(\tilde{k}) = \left(\frac{1}{(i\omega_n + \mu)I - \varepsilon(\tilde{k}) - \Sigma}\right)_{ij} \longrightarrow G_{ij} = \int \frac{d^d \tilde{k}}{(2\pi)^d} G_{ij}(\tilde{k})$$

#### Localized and delocalized pictures C-DMFT





$$G_{ij} = \int \frac{d^d \tilde{k}}{(2\pi)^d} \left( \frac{1}{(i\omega_n + \mu)I - \varepsilon(\tilde{k}) - \Sigma} \right)_{ij}$$

$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

## **Dynamical cluster approximation (DCA)**



Hettler ...Jarrell...Krishnamurty PRB 58 (1998)

# **Impurity solvers**



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## Impurity solver (Exact diagonalisation)



Caffarel, Krauth, PRL 72 1545 (1994)

QCM David Sénéchal

Impurity solver : continuous-time quantum Monte Carlo

$$Z = \int \mathcal{D}[\psi^{\dagger}, \psi] \,\mathrm{e}^{-S_{c} - \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{\mathbf{K}} \psi_{\mathbf{K}}^{\dagger}(\tau) \Delta(\tau, \tau') \psi_{\mathbf{K}}(\tau')}_{\mathbf{K}}$$

Hybridization expansion :

Werner Millis PRB 74, 155107 (2006) Werner Millis B 75, 085108 (2007) Haule, PRB 75, 155113 (2007) Sémon, Sordi, AMST PRB 89, 165113 (2014) Sémon, Yee, Haule, AMST PRB 90, 075149 (2014)

#### LPSCoreCT-HYBiQISTComCTQMC

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Impurity solver : continuous-time quantum Monte Carlo

$$S = \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \sum_{\sigma=\uparrow,\downarrow} \xi^*_{\sigma}(\tau) \left[ g^{-1}_{0\sigma}(\tau - \tau') \right] \xi_{\sigma}(\tau') + U \int_0^\beta \mathrm{d}\tau \left( n_{\uparrow}(\tau) n_{\downarrow}(\tau) - \frac{n_{\uparrow}(\tau) + n_{\downarrow}(\tau)}{2} \right)$$

CT-AUX : Gull, Werner, Parcollet, Troyer, 2008, Europhys. Lett. 82, 57003 (2008) DCA++

Review of these methods

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner RMP 83, 349 (2011)

#### Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz),
    Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

# Critique



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#### + and -

- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath
- Included exactly:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations
  - Hence good when the corresponding correlation lengths are small

#### **Possible artefacts**



Verret, Roy, Foley, Charlebois, Sénéchal, A.-M.S.T, RPB 100, 224520 (2019)

STM Kohsaka, ... Davis, Nature (London) 454, 1072 (2008).

32

#### What to do

- Exact in the infinite size limit of the cluster
  - Compare different cluster sizes
  - Compare real-space (CDMFT) and momentum space (DCA) clusters

## Minuterie

- 10 Minutes
- 6 minutes = 16 minutes

# Back to our problem: Phase diagram



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Vishik, Rep. Prog. Phys. (2018)











Vishik, Rep. Prog. Phys. (2018)



#### A bird's eye overview of the T = 0 phase diagram

$$U = 8t, t' = -0.3t, t'' = 0.2t$$



A. Foley *et al.* Phys. Rev. B **99**, 184510 (2019)
S. S. Kancharla, *et al.* Phys. Rev. B **77**, 184516 (2008)
D. Sénéchal, *et al.* Phys. Rev. Lett. **94**, (2005)
M. Jarrell *et al.* EPL **56** 563, (2001)



A. Foley

S. Verret D. Sénéchal

CDMFT 4 sites

#### **Competing ground states**

#### PHYSICAL REVIEW X 10, 031016 (2020)

#### Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model

Mingpu Qin<sup>(b)</sup>,<sup>1,2,\*</sup> Chia-Min Chung<sup>(b)</sup>,<sup>3,4,\*</sup> Hao Shi,<sup>5</sup> Ettore Vitali,<sup>6,2</sup> Claudius Hubig<sup>(b)</sup>,<sup>7</sup> Ulrich Schollwöck<sup>(b)</sup>,<sup>3,4</sup> Steven R. White<sup>(b)</sup>,<sup>8</sup> and Shiwei Zhang<sup>(b)</sup>,<sup>5,2</sup>

PRL 113. 046402 (2014)	PHYSICAL	REVIEW	LETTERS	
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week ending 25 JULY 2014

#### Competing States in the *t-J* Model: Uniform *d*-Wave State versus Stripe State

Philippe Corboz,<sup>1,2</sup> T. M. Rice,<sup>1</sup> and Matthias Troyer<sup>1</sup>

### **Competing ground states**

#### ARTICLE OPEN

Stripe order from the perspective of the Hubbard model Edwin W. Huang<sup>13</sup>, Oxistian B. Mend<sup>2</sup>, Hung-Chen Jiang<sup>2</sup>, Bilan Motite<sup>3,2</sup> and Thomas P. Deveraux<sup>34</sup>





P. Mai, S. Karakuzu, S. Johnston & TAM, in preparation







J.-P. Faye Latyr



D. Sénéchal

Faye Sénéchal, PRB 95 (2017)

**43** 

# Minuterie

- 10 minutes
- 6 minutes
- 3 minutes = 19

# Minuterie

- 10 minutes
- 6 minutes
- 3 minutes
- 4 minutes
- 5 minutes = 28

# Pseudogap







Maxime Charlebois



Patrick Sémon



Marion Thénault

Reymbaut, *et al.* Phys. Rev. Research **1**, 023015 (2019)



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Zhao et al. Nat. Phys. 13, 250 (2017).



#### Knight shift (Q=0 spin susceptibility)



**Fig. 3** Temperature and doping dependence of the q = 0 spin susceptibility. At the smaller dopings (larger filling  $\langle n \rangle$ ),  $\chi_s(T)$  exhibits a peak in the temperature dependence indicating the opening of a PG

DCA 12 sites, *t*'=0, *U* = 7

T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

#### Comparison



**Fig. 3** Temperature and doping dependence of the q = 0 spin susceptibility. At the smaller dopings (larger filling  $\langle n \rangle$ ),  $\chi_s(T)$  exhibits a peak in the temperature dependence indicating the opening of a PG

**Knight shift** 



#### DCA 8 sites, U = 6, t' = -0.1t

Chen, LeBlanc, Gull, Nature Com. Apr. 2017 See also Jarrell *et al.* 2001, 2002

# Physical origin of the pseudogap

$$= \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$





#### **Spin susceptibility**



**Experiments and** *T*\* G.Sordi et al. Phys. Rev. B 87, 041101(R) (2013) YBCO 0.225 913 400 U=9= 00.200 812 0.175 710 300 (x) 200 0.150 609 507 T 406 T 0.125 0.100 0.075 304 100 0.050 203 0.025 101 0.05 0.1 0.15 0.2 0.25 0.3 0.000 0.5 0.2 0.1 0.3 0.4 δ

Cyr-Choinières et al. Phys. Rev. B 97, 064502

A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, Phys. Rev. Research **1**, 023015 (2019) W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018). Bragança, Sakai, Aguiar, Civelli, PRL **120**, 067002 (2018) **Experiments and** *T*\*



P. Sémon, AMT, Phys. Rev. Research 1, 023015 (2019)
 W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).
 Bragança, Sakai, Aguiar, Civelli, PRL 120, 067002 (2018)

**Entropy maximum** 





Tallon, Loram (2001) Physica C: Supercon 349(1):53–68. Tallon, *et al.* (2004) Physica C: Supercon. 415(1):9–14.

Fig. 14. (a) Entropy  $S(T_0)$  (in k<sub>B</sub>/CuO<sub>2</sub>) at fixed  $T = T_0$  vs p, reflecting spectral weight within fixed energy windows ~  $E_F \pm 2k_B T_0$  for LSCO and YBCO (0, 2, 7% Zn and 20% Ca). (b)  $\chi k_B T(T_0)$  (in  $\mu_B^2/CuO_2$ ) at fixed  $T = T_0$  vs p for LSCO and YBCO(0, 2, 7% Zn).

Fig. 2. False color contour plot of S(T)/T for (a) the real superconducting HTS system and (b) for the normal-state extrapolated to T = 0. The plots are a composite of Bi-2212 data for p > 0.13 and Y-123 data for p < 0.13. The crossover is marked by the vertical dashed line.

**Results : effect of** *t***'on** *T*\*



Doiron-Leyraud *et al.* Nature Comm. **8** 2044



 $p^* < p_{fs}$ 

Doiron-Leyraud *et al.* Nature Comm. **8** 2044

Effect of *t*'



A. Reymbaut *et al.* Phys. Rev. Research **1**, 023015 (2019)

Effect of *t*'



A. Reymbaut *et al.* Phys. Rev. Research **1**, 023015 (2019)

Effect of *t*'



A. Reymbaut *et al.* Phys. Rev. Research **1**, 023015 (2019)



**Results : effect of** *t***'on** *T*\*



#### **Results: van Hove singularity**



Doiron-Leyraud *et al.* Nature Comm. **8** 2044

A.Reymbaut, *et al.* Phys. Rev. Research 1, 023015 (2019) W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).

# Minuterie

- 10 minutes
- 6 minutes
- 3 minutes
- 4 minutes = 23

# d-wave superconductivity



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# Superconductivity











### **#1 Cooper pair, #2 Phase coherence**

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

$$E_{P} = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}^{*} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}^{*} \right\rangle$$

$$|\mathrm{BCS}(\theta)\rangle = \dots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \dots$$
**Cartoon « BCS » weak-coupling picture** 

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U(\mathbf{p} - \mathbf{p}') \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} (1 - 2n(E_{\mathbf{p}'}))$$

$$\mathbf{p}$$

$$\mathbf{p}$$
Exchange of spin waves?  
Kohn-Luttinger  
T<sub>c</sub> with pressure
$$\mathbf{p}$$
R. B. 34, 7716 (1986).  
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch  
P.R. B 34, 8190-8192 (1986).  
Kohn, Luttinger, P.R.L. 15, 524 (1965).

P.W. Anderson Science 317, 1705 (2007)

#### Exchange of spin waves, U = 4t doping 10%



Maier, Jarrell, Schulthess, Kent, White PRL 95, 237001 (2005)

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#### A cartoon strong correlation picture

$$J\sum_{\langle i,j\rangle} \mathbf{S}_{i} \cdot \mathbf{S}_{j} = J\sum_{\langle i,j\rangle} \left(\frac{1}{2}c_{i}^{\dagger}\vec{\sigma}c_{i}\right) \cdot \left(\frac{1}{2}c_{j}^{\dagger}\vec{\sigma}c_{j}\right)$$
$$d = \langle \hat{d} \rangle = 1/N\sum_{\vec{k}} (\cos k_{x} - \cos k_{y}) \langle c_{\vec{k},\uparrow}c_{-\vec{k},\downarrow} \rangle$$
$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^{\dagger} c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^{\dagger}) + F_{0}$$

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

P.W. Anderson ScienceMiyake, Schmitt–Rink, and Varma317, 1705 (2007)P.R. B 34, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

#### **Superconducting transition temperature**





T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

DCA, 8 sites, U/t = 6 and t'=0

DCA, 12 sites, U/t = 7 and t'/t = -0.15



#### d-wave in mean-field

Miyake, Schmitt–Rink et Varma, PRB **34**, 6554-6556 (1986) Anderson, Baskaran, Zou et Hsu, PRL **58**, 26 (1987)

#### $T_c$ controlled by J, CDMFT 2x2



Fratino et al. Sci. Rep. **6**, 22715

Some experiments that suggest  $T_c < T_{pair} < T^*$ T. Kondo *et al.* PRL **111** (2013) Kondo, Takeshi, et al. Kaminski Nature Physics 2011, **7**, 21-25 A. Pushp, Parker, ... A. Yazdani, Science **364**, 1689 (2009) Lee ...Tajima (Osaka) https://arxiv.org/pdf/1612.08830 Patrick M. Rourke, et al. Hussey Nature Physics **7**, 455–458 (2011) Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)



#### **Condensation energy**



#### **Condensation energy**

#### Fratino et al. Sci. Rep. **6**, 22715



Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014) Experiments: Bontemps, Santander-Syro Van der Marel ...

## Minuterie

- 10 minutes
- 6 minutes
- 3 minutes
- 4 minutes
- 5 minutes
- 9 minutes = 37



Kyung, Sénéchal, Tremblay, Phys. Rev. B **80**, 205109 (2009) Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013) A. Reymbaut *et al.* PRB **94** 155146 (2016)

# Im $\Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)



#### The glue CDMFT 2x2, T=0



#### The glue and neutrons



FIG. 3 (color online). **Q**-integrated dynamic structure factor  $S(\omega)$  which is derived from the wide-*H* integrated profiles for LBCO 1/8 (squares), LSCO x = 0.25 (diamonds; filled for  $E_i = 140$  meV, open for  $E_i = 80$  meV), and x = 0.30 (filled circles) plotted over  $S(\omega)$  for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO x = 0.25 and 0.30 are guides to the eyes.

Wakimoto ... Birgeneau PRL (2007); PRL (2004)



## Minuterie

- 10 minutes
- 6 minutes
- 3 minutes
- 4 minutes
- 5 minutes
- 9 minutes
- 3 minutes = 40



Giovanni Sordi



Patrick Sémon

# A phase transition at the heart of the phase diagram (and its relation to Mott)

G. Sordi, et al. Scientific Reports 2, 547 (2012)



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Kristjan Haule

#### Mott transition at half-filling, CDMFT 2 x 2



#### Change in potential energy due to large $\xi$



Fratino, Sémon, Charlebois, Sordi, AMST, PRB 95, 235109 (2017)

#### Mott and Sordi transition: CDMFT 2 x 2







G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
G.Sordi et al. Phys. Rev. B 87, 041101(R)/1-5 (2013)
P. Sémon, G. Sordi, *et al.*, Phys. Rev. B 89, 165113/1-6 (2014)

#### **Physics: Plaquette eigenstates**



U = 6.2; t' = 0

Sordi et al., Sci. Rep. 2 547 (2012);

See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges PRB **80**, 064501 (2009)



# Anisotropic triangular Downey lattice



Maxime Charlebois



Charles-David Hébert





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### Same Physics on the triangular lattice



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### Same Physics on the triangular lattice



### Same Physics on the triangular lattice



## **Triangular lattice with DCA, 6 patches**



100

#### **Some Physics on the triangular lattice**



# Mott and Sordi transition on the triangular lattice DCA, N=6



1.06

1.04

0.98

0.96



102

# (Topological) stability

Depends on - Cluster

Large
 changes in t'



# Another Fermi Surface Reconstruction without Symmetry Breaking

• Gazit, Assaad, Sachdev Phys. Rev. X 10, 041057

#### **Physics: Plaquette eigenstates**



U = 6.2; t' = 0

Sordi et al., Sci. Rep. 2 547 (2012);

See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges PRB **80**, 064501 (2009)

# Quantum Critical point Back to square lattice

Yang, ... Zaanen, and Jarrell PRL 106, 047004 (2011)

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#### Specific heat in the strange metal phase



B. Michon, C. Girod, Taillefer, Klein, Nature 567, 218 (2019)

107

#### Specific heat in the strange metal phase



A.Reymbaut, et al. Phys. Rev. Research 1, 023015 (2019)

See also for  $C_v$  Maximum: Sordi, Walsh, Sémon, and A.-M.S.T, PRB **100**, 121105(R) (2019) 108
## **Summary Conclusion**



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### Summary

- Intrinsic to the doped Mott insulator
  - Pseudogap
  - First-order transition QCP
  - d-wave superconductivity
    - Short-range spin fluctuations (J)
    - Role of charge-transfer gap and of oxygen-hole doping
- Other effects that have not been discussed V >> J
  - Reymbaut, Charlebois, Fellous Asiani, Fratino, Sémon, Sordi A.-M.S.T. PRB 94, 155146 (2016)
- Other experiment consistent with doped Mott picture
  - Frachet, ... Leboeuf, Julien Nat. Phys. 10.1038/s41567-020-0950-5

#### **Entanglement properties**

- Sharp variation in the entanglement-related properties and not broken symmetry phases characterizes the onset of the pseudogap phase at finite temperature.
  - Walsh, Sémon, Poulin, Sordi, A.-M.S.T. PRX QUANTUM 1, 020310 (2020)

#### Mammouth



CREATING KNOWLEDGE DRIVING INNOVATION BUILDING THE DIGITAL ECONOMY CRÉER LE SAVOIR ALIMENTER L'INNOVATION BÂTIR L'ÉCONOMIE NUMÉRIQUE

# Merci



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