Oct. 27th. 2021

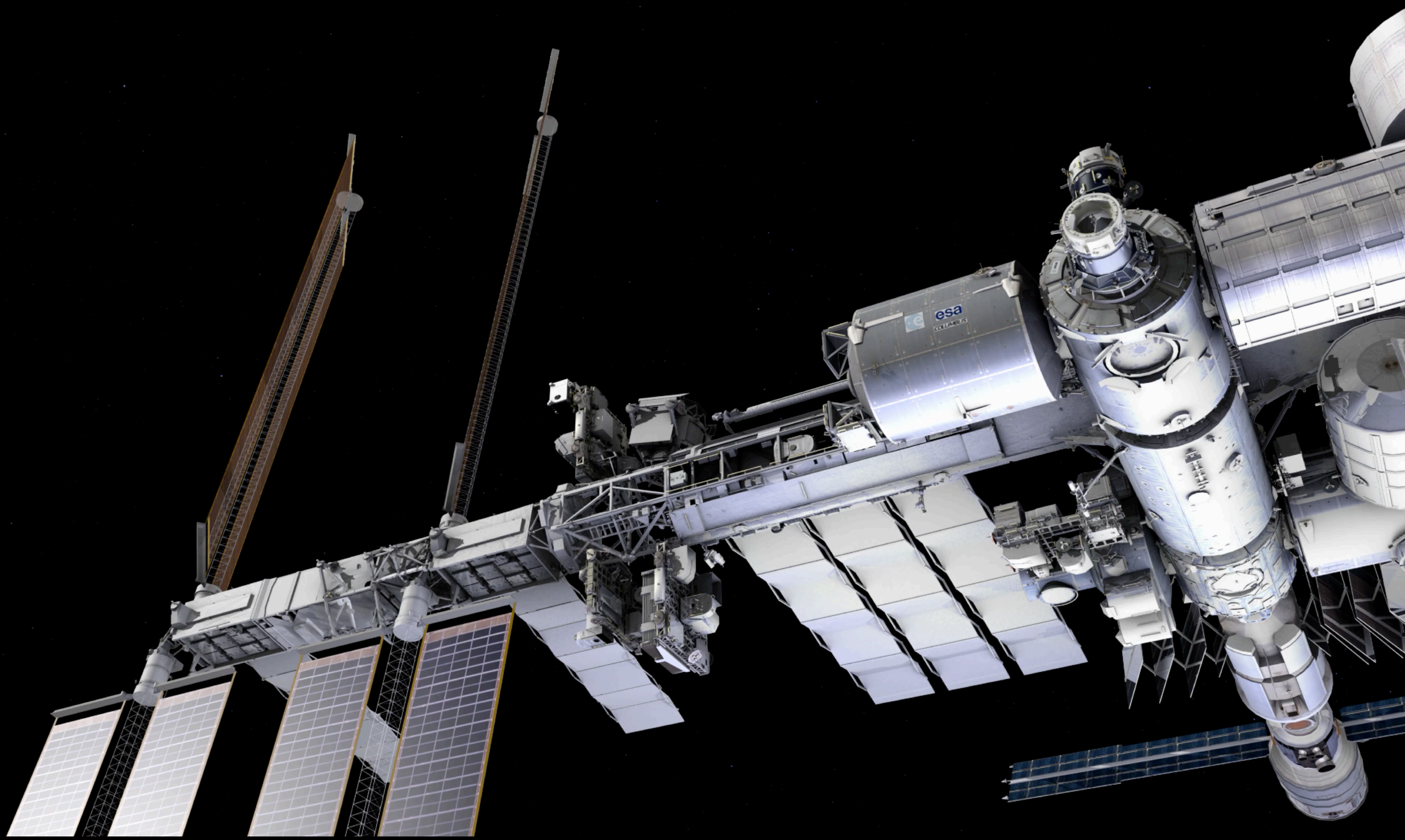
Equation of State from Color Molecular dynamics

Nobutoshi Yasutake (Chiba Inst. Tech./JAEA)

Color-molecular dynamics
Y. Mukobara,(Tokyo Inst. Tech.), T. Maruyama(JAEA), T.Hatsuda(RIKEN)

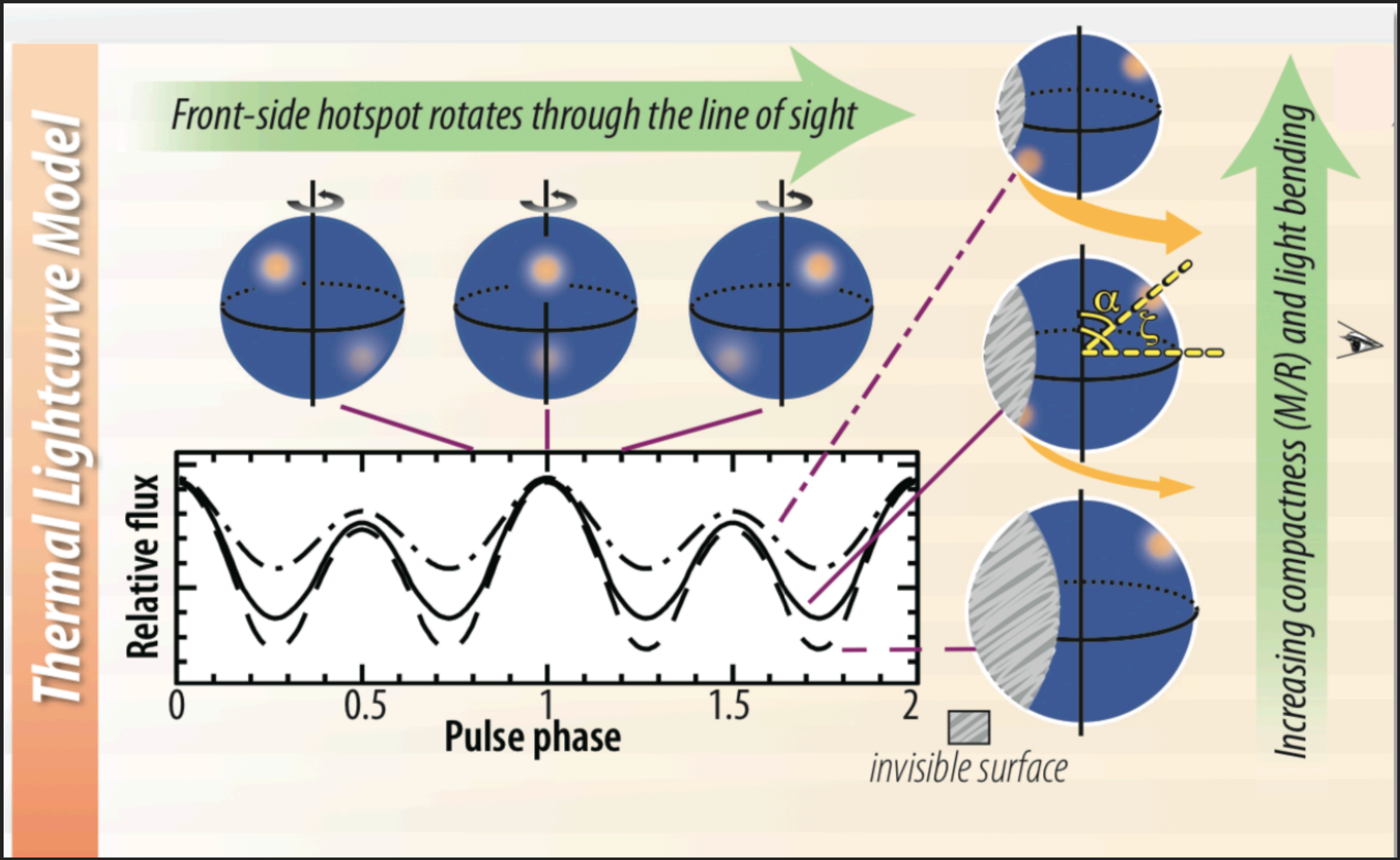
VR/3D Graphic movies
H.Tanihisa, J. Hakozaki(CIT)


(c)NASA
NICER • SEXTANT
MIT • MOOG • DTU
NASA • GSFC • ISS
PULSU STELLARUM, SCIENTIA ET VIA CAELESTIS
Since launch , June 3rd. 2017
NICER
NEUTRON STAR INTERIOR COMPOSITION EXPLORER




(c)NASA

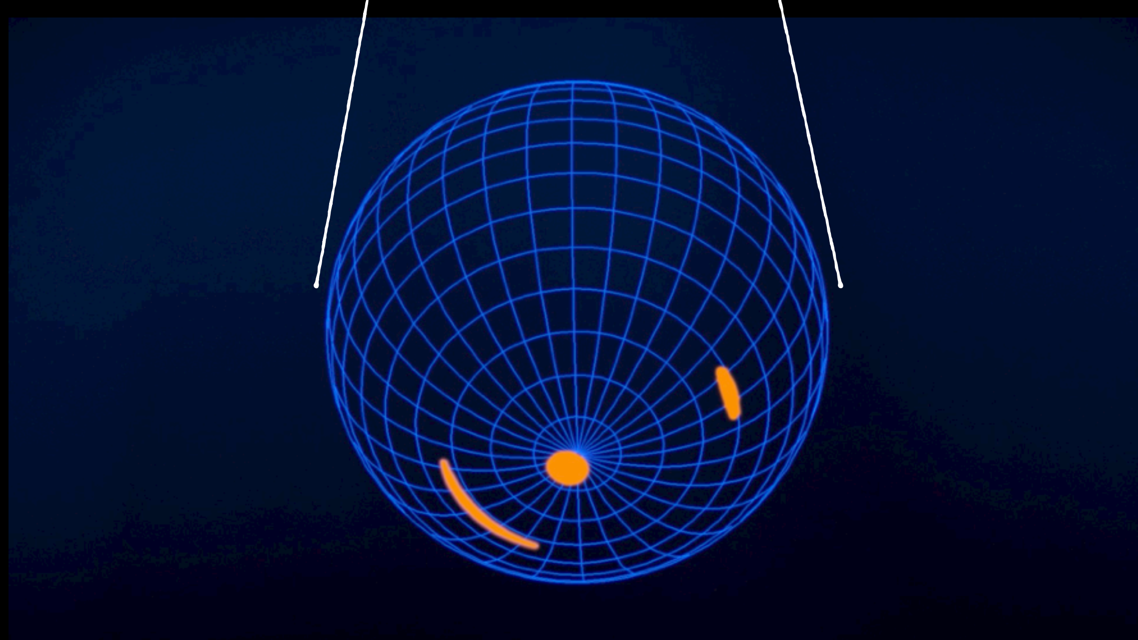
COMPACTNESS BY NICER



Dec. 2019

(c)NASA

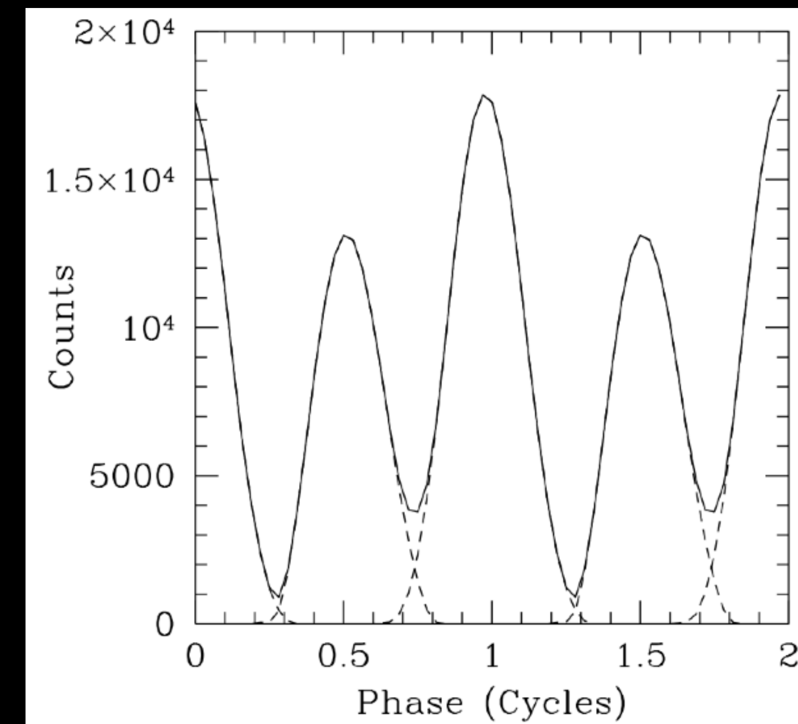
PSR J0030+0451



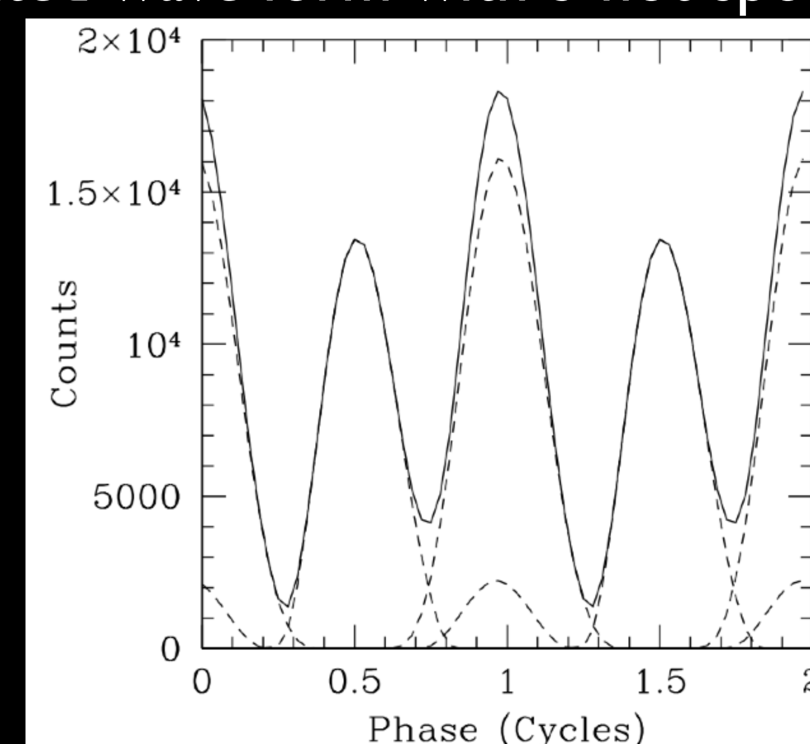
2 or 3 hot spots in the southern hemisphere

Not dipole → We need 3D simulations to understand.

Best fitted wave form with 2 hot spots

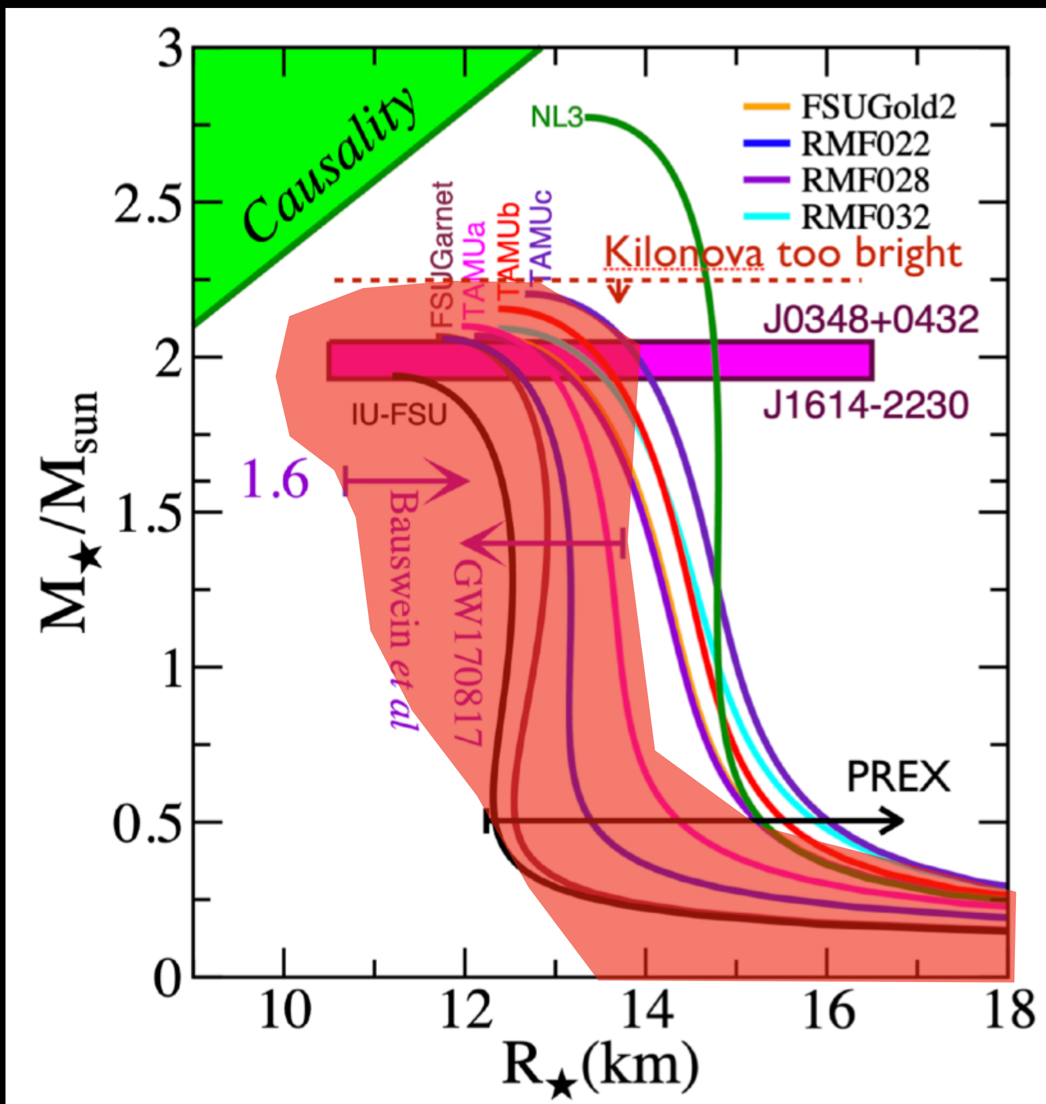


Best fitted wave form with 3 hot spots



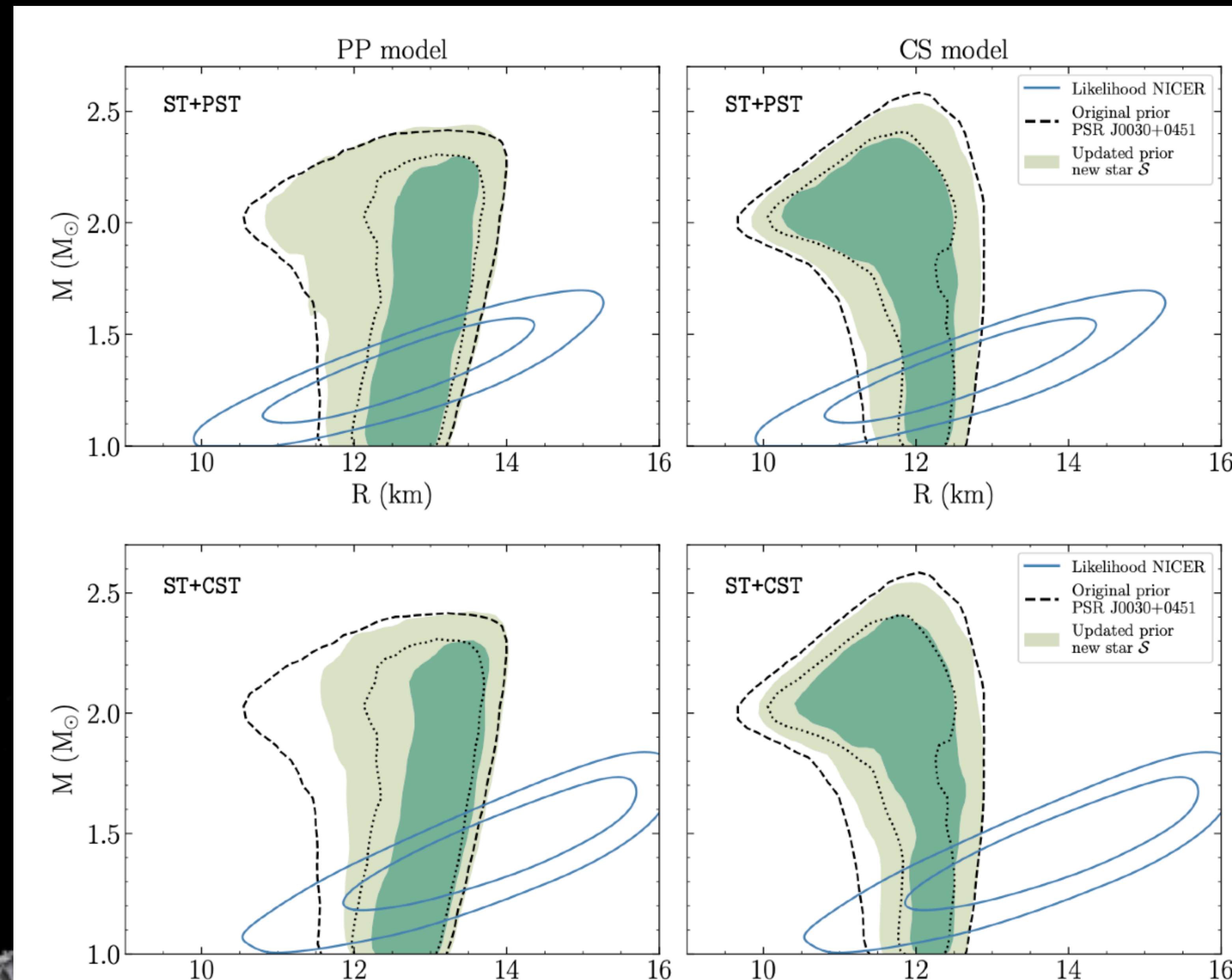
MR relation

before NICER



Horowitz (arXiv:1911.00411)

with “a” NICER constraint



Raajimakers et al. 2021

PSR J0030+0451

MASS-RADIUS RELATION

Targets & Exposures by Working Group

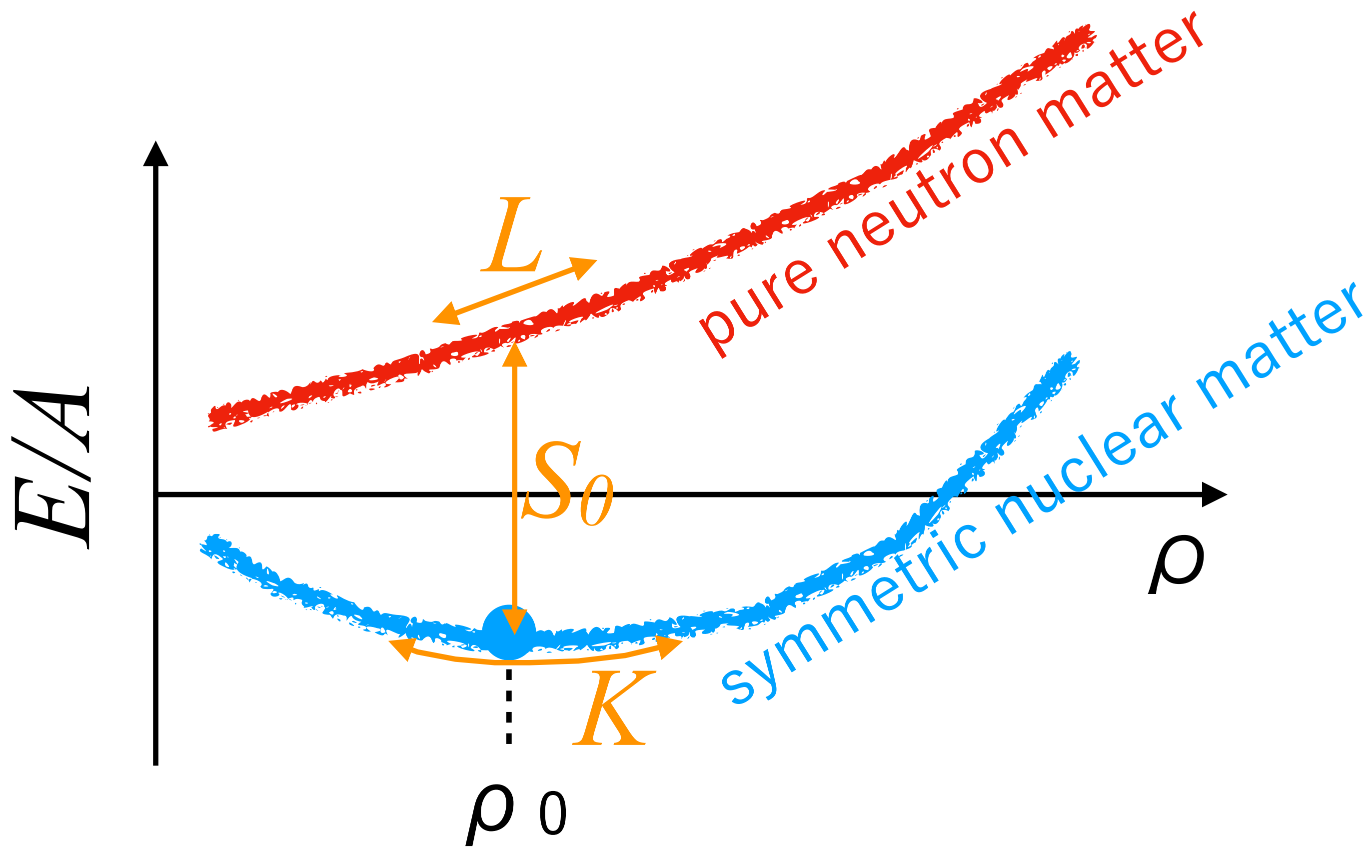
https://heasarc.gsfc.nasa.gov/docs/nicer/proposals/science_team_investigations/

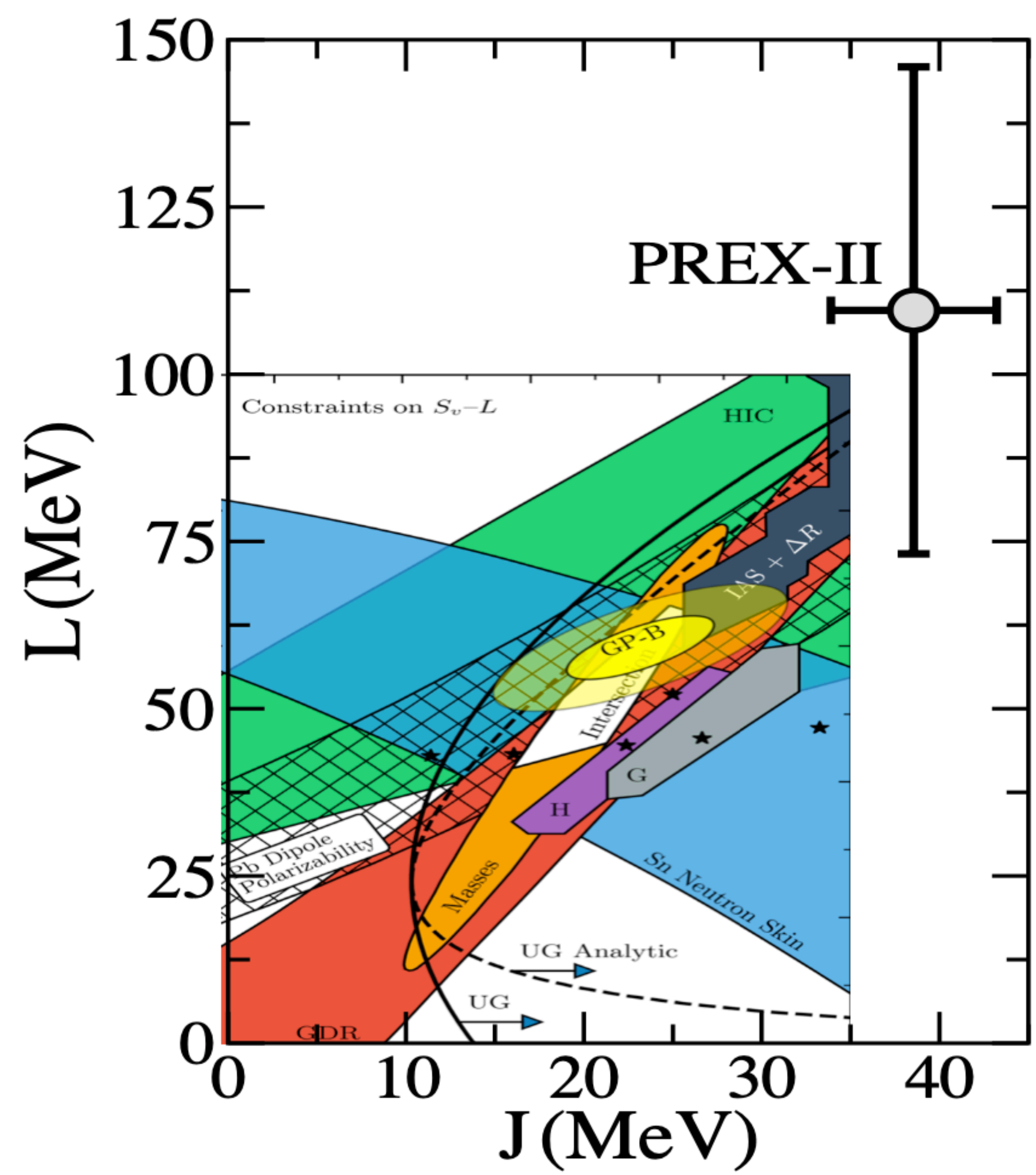
Target Name	Contact	Exposure (ksec)		Legacy	Purpose
		Plan	To date		
✔ PSR J0030+0451	S. Bogdanov	1,600	1,936	Y	Radius, mass constraints from energy-dependent lightcurve modeling
PSR J0437-4715	S. Bogdanov	1,000	951	Y	Same
PSR J0740+6220	Z. Arzoumanian	1,600	75	Y	Same
PSR J1231-1411	P. Ray	1,600	1356	Y	Same
PSR J2124-3358	S. Bogdanov	1,600	1051	Y	Same
PSR J1614-2230	M. Wolff	500	400	Y	Radius lower limit from lightcurve modeling

Constraints from PREX II
around saturation density

Reed et al. PRL 126,172503 (2021)

$$E/A = J + \frac{L(\rho - \rho_0)}{3\rho_0} + \frac{K_{sym}(\rho - \rho_0)^2}{18\rho_0}$$

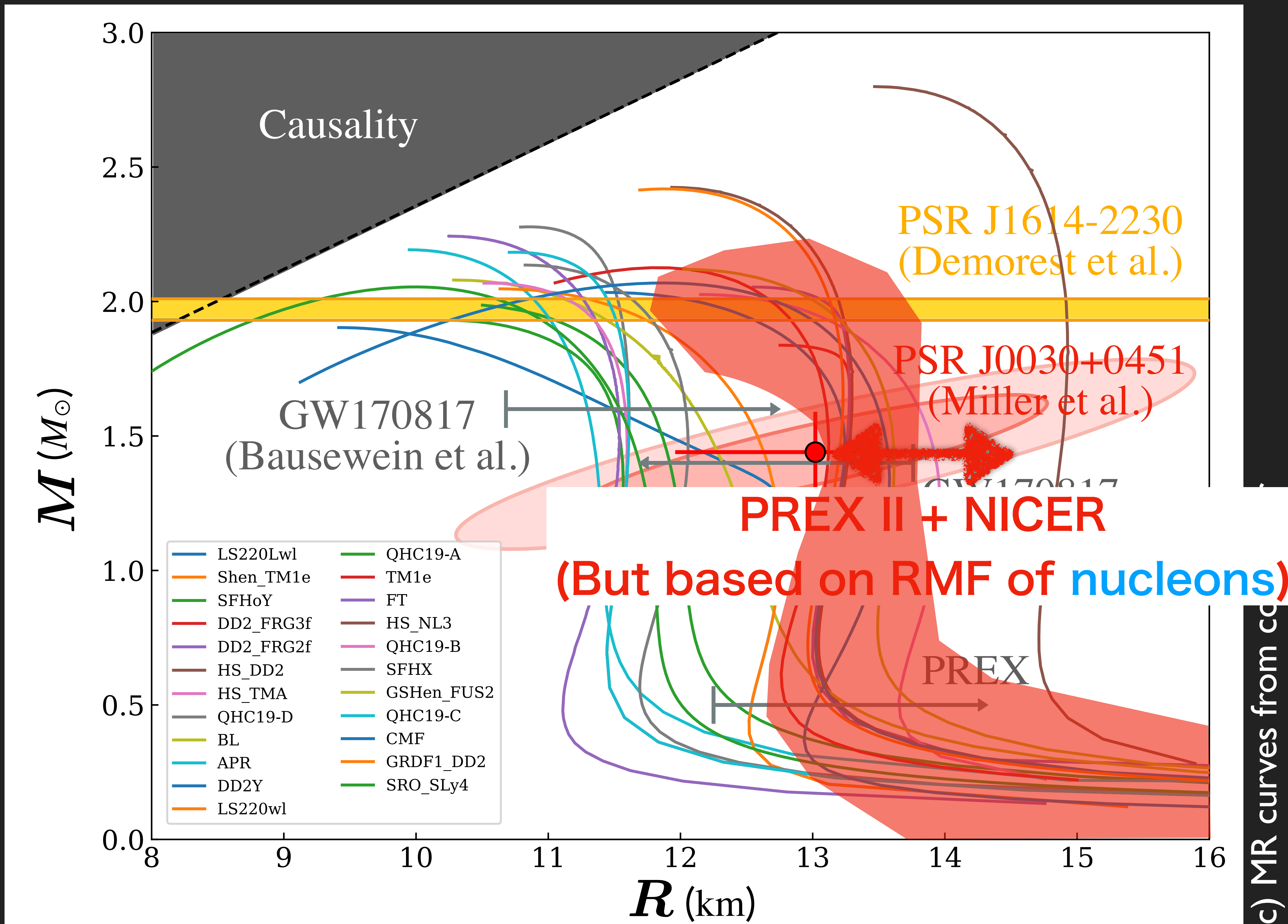




$$E/A = E/A(\rho_0) + \frac{K(\rho - \rho_0)^2}{18\rho_0^2}$$

- But it depends on the analysis methods? (Reinhard et al. arXiv:2105.15050)
- CREX results suggest ordinary L values, not large as PREX-II (preliminary result).

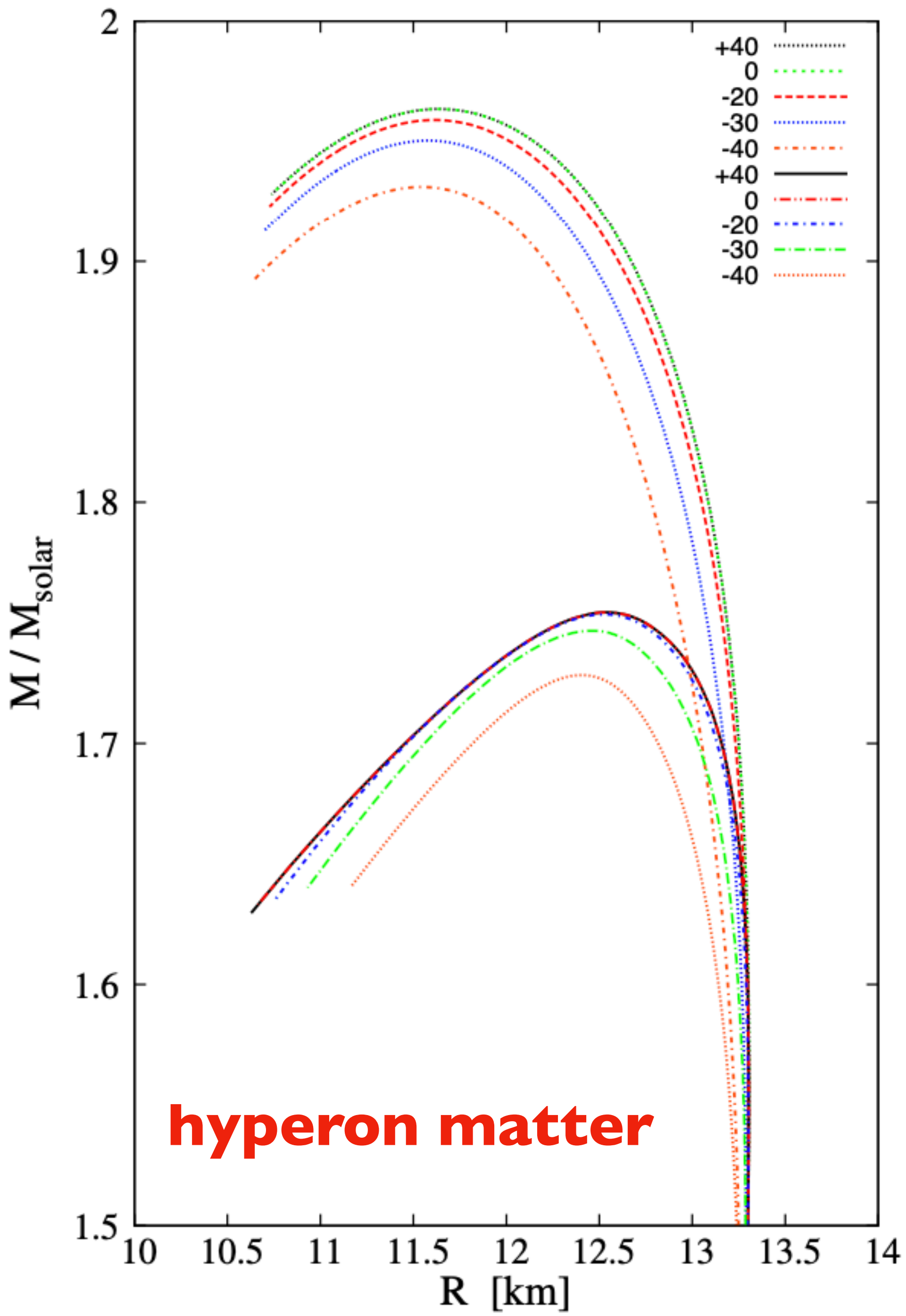
PREX II & NICER



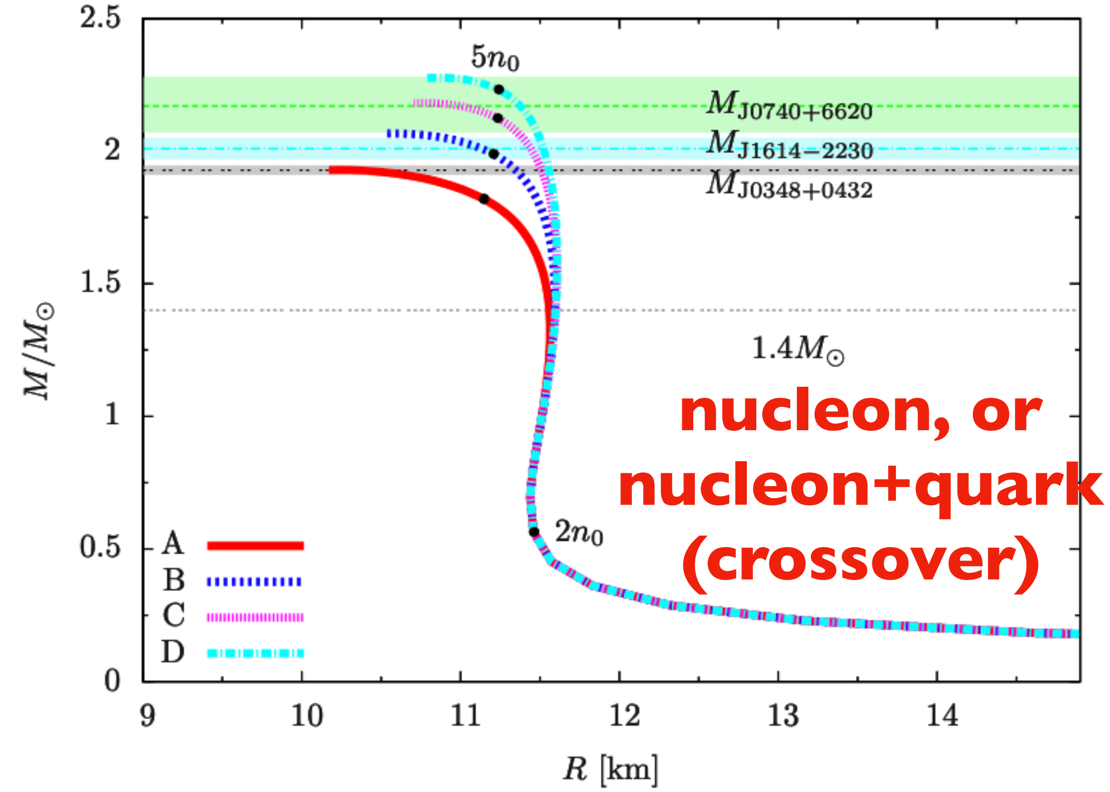
(c) MR curves from co

Quiz: What is the component?

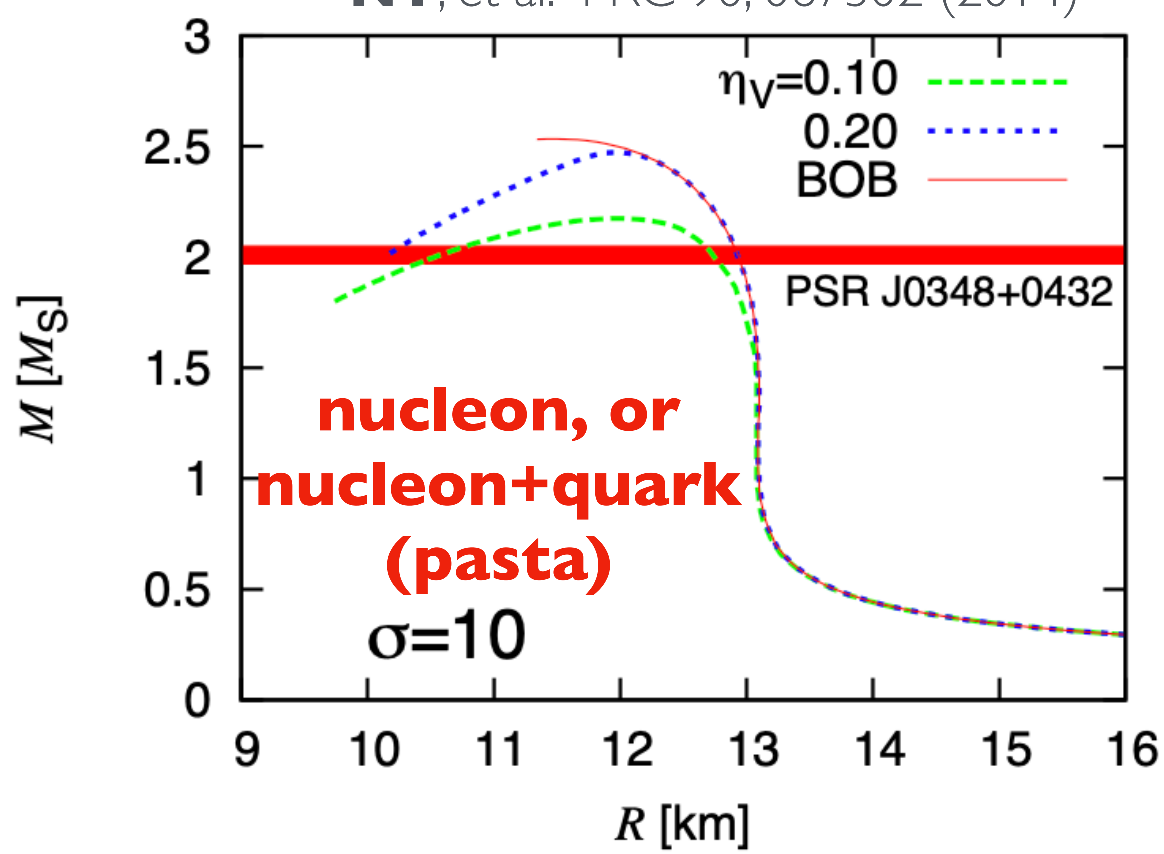
S. Weissenborn, et al. PRC 85, 065802 (2012)



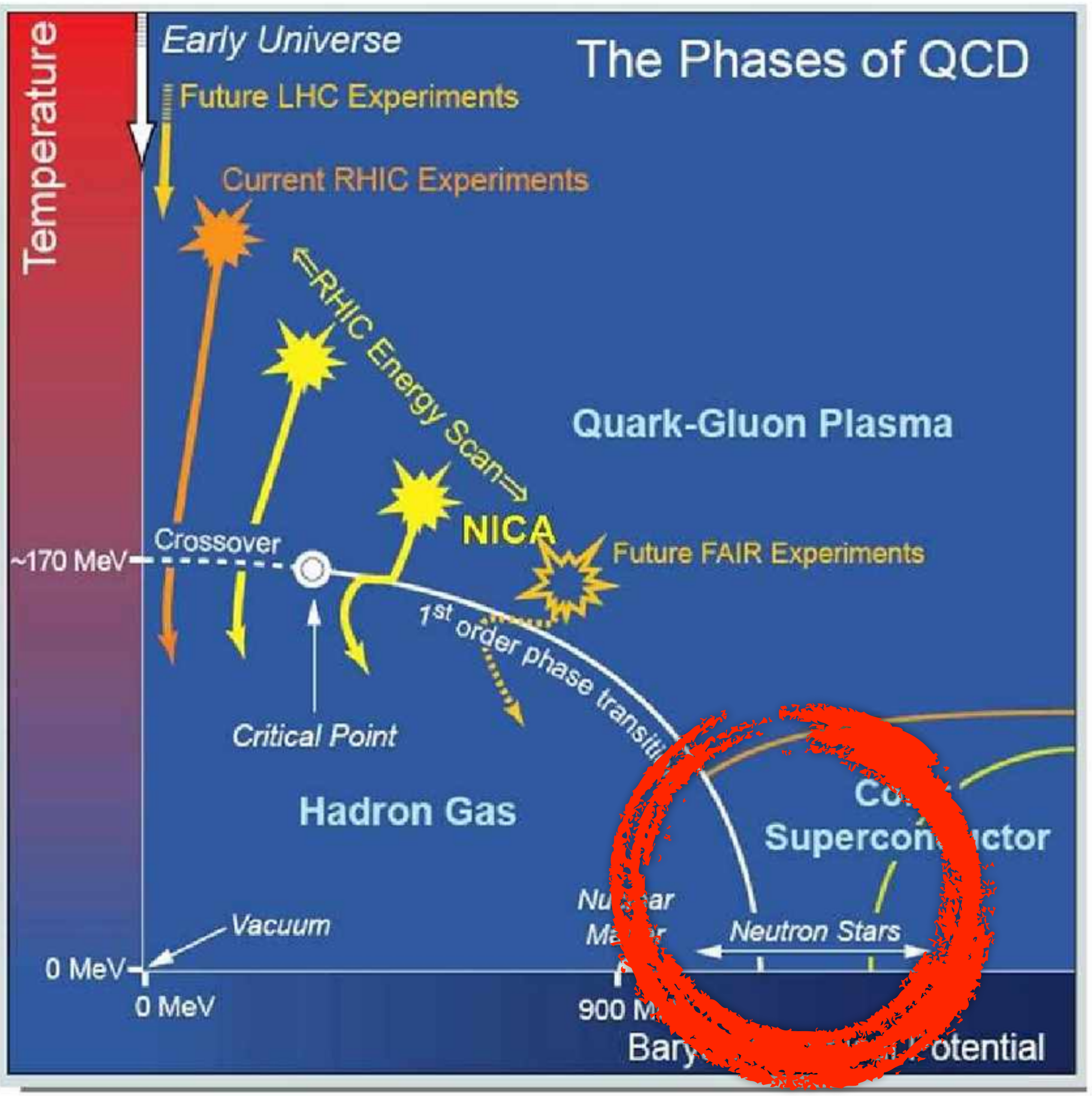
G. Baym, et al. ApJ 885, 42 (2019)



NY, et al. PRC 90, 067302 (2014)



Other properties?



Progress of the NICA project (2009)

- We will obtain “MR relation”.
- But what kind of material?

↓

✔ Pressure(energy) vs density.
△ Other physical properties.

e.g. thermal conductivity,
heat capacity…

Lattice QCD
(sign problem)

\+ Color Molecular dynamics

Other physical property

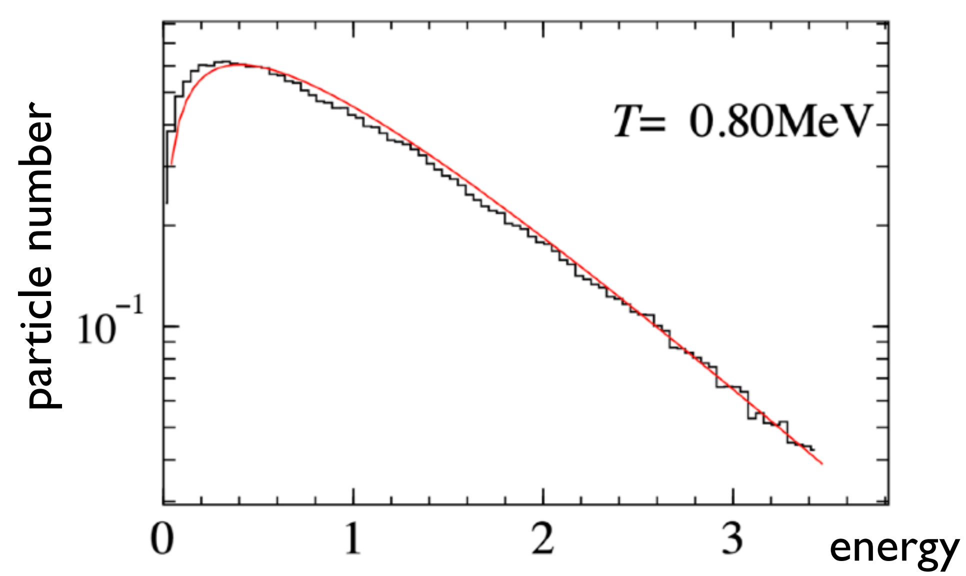
We can obtain physical quantities by Green-Kubo formula.

$$\alpha = \int_0^\infty \left\langle \dot{U}(t)\dot{U}(0) \right\rangle dt.$$

e.g. thermal conductivity λ

$$\begin{aligned} \alpha &= VT^2\lambda, \\ U_x(t) &= \sum_{i=1}^{N} x_i(t)E_i(t), \\ \dot{U}_x(t) &= \frac{d}{dt}\sum_{i=1}^{N} x_i(t)E_i(t). \end{aligned}$$

Statistical temperature from CMD is consistent with theoretical distribution.



COOLING OF NEUTRON STARS

Cooling…

→many physical properties

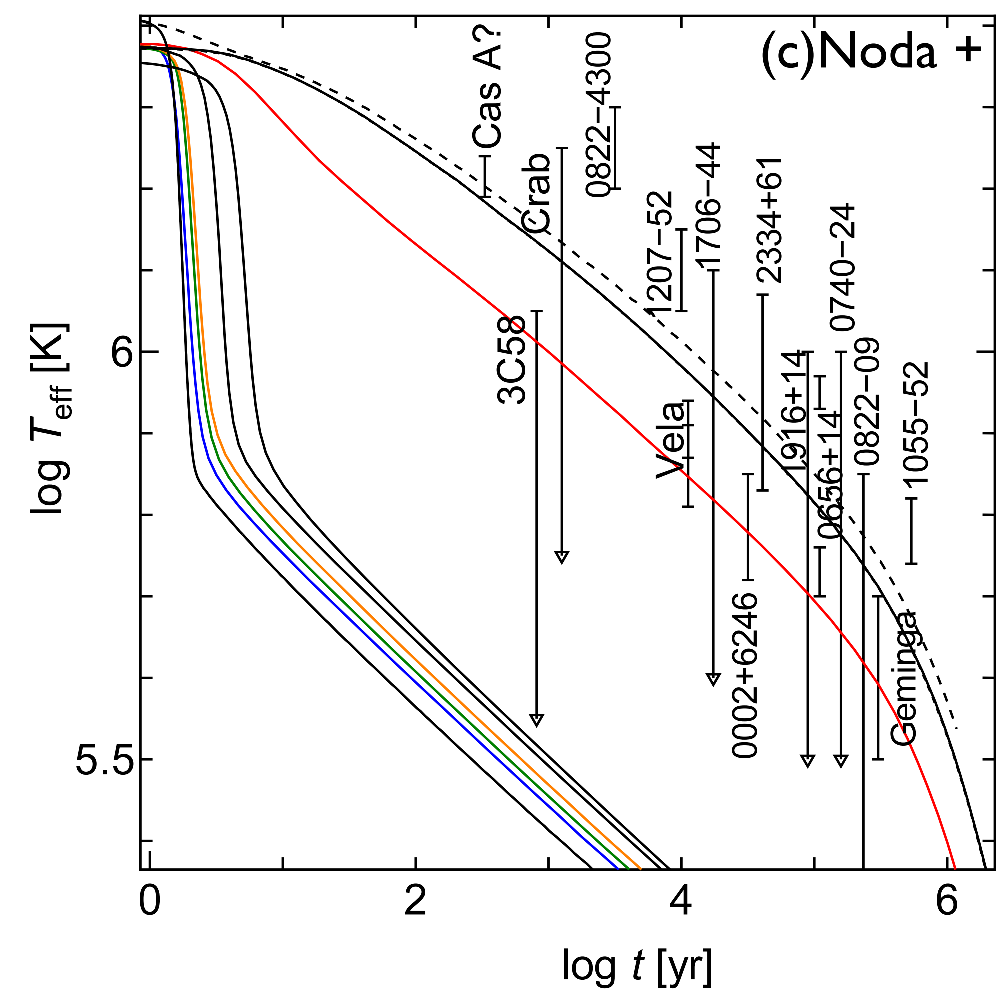
$$c_v e^{\Phi} \frac{\partial T}{\partial t} + \nabla \cdot (e^{2\Phi} \boldsymbol{F}) = e^{2\Phi} Q$$

thermal diffusion eq.

heat capacity

flux (thermal conductivity)

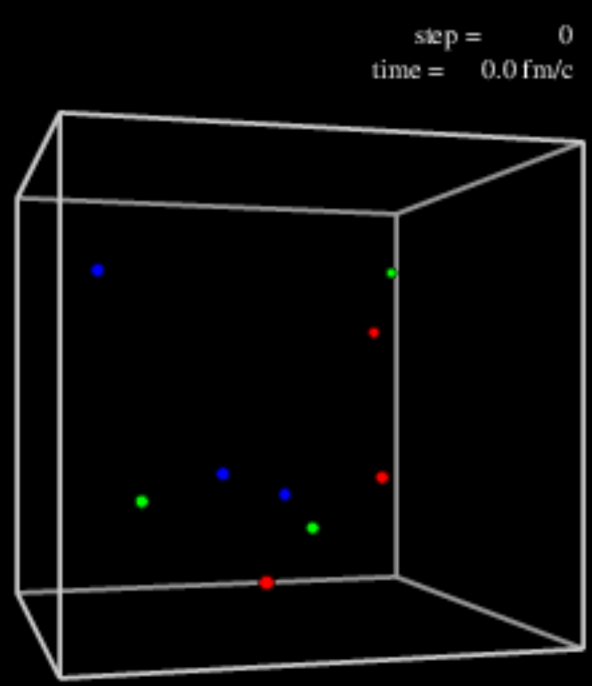
cooling rate (neutrino) + heating rate (magnetic field)



FROM QCD TO NS MATTER

Lattice QCD

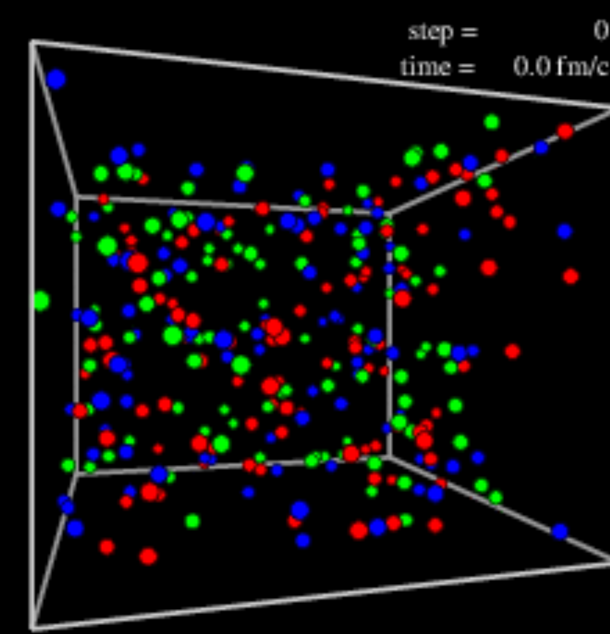
size	～ 10 fm
number	6 (, 9)



There are the limits by the sign problem.

Neutron Star matter

1～10 n_0



↑

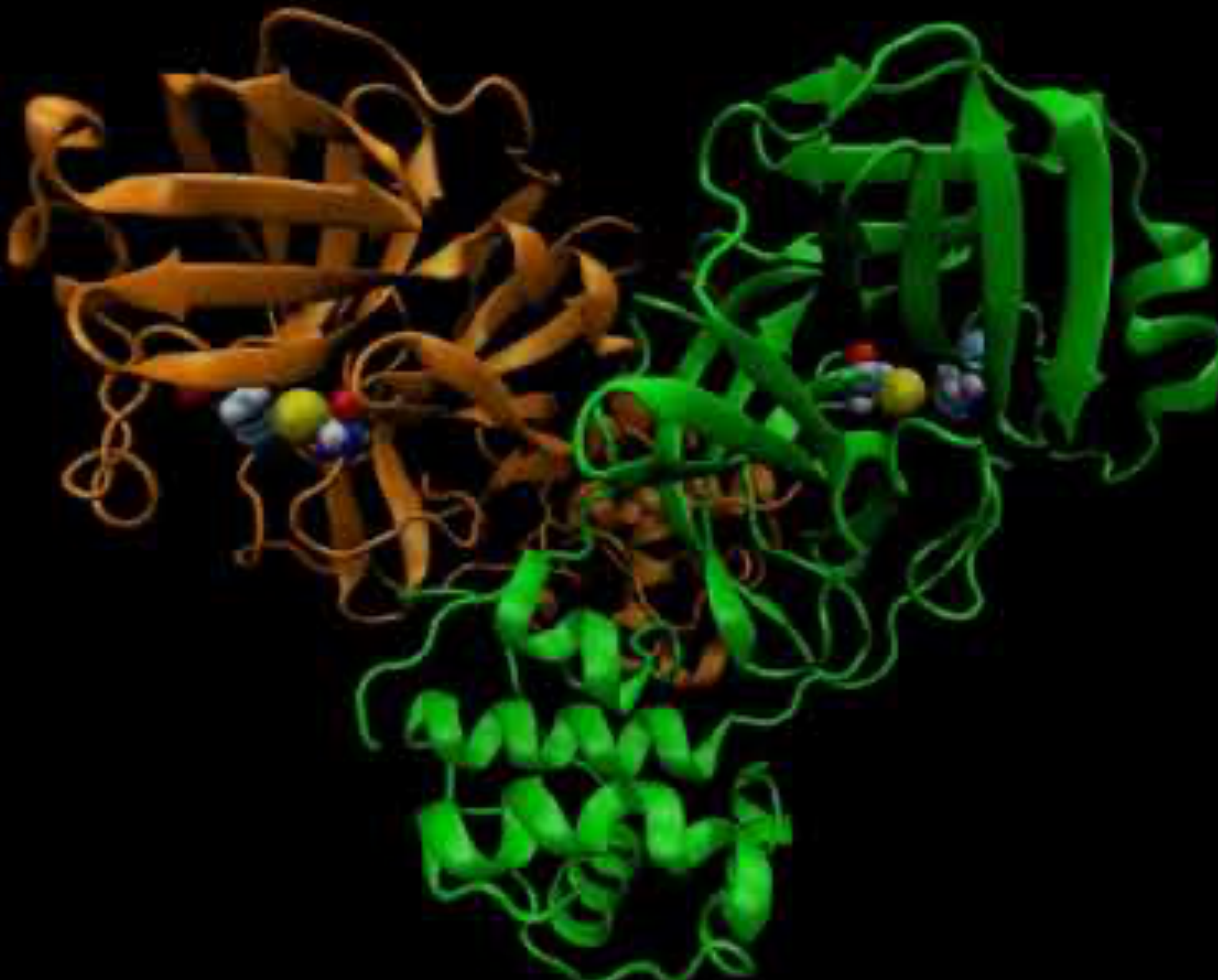
Using the results (interactions) from LQCD, we conduct the Color molecular dynamics(CMD) simulations.

MD simulations can not be the 1st principle.

They work well to study the medicines and/or DNA, etc..

Resent works with Molecular Dynamics

SARS-CoV-2 Main Proteases (c) Taiji et al. at RIKEN



COLOR QMD

See also
Maruyama, Hatsuda (2000) PRD

number of variables

$$\{x, y, z, Px, Py, Pz, \alpha, \beta, \theta, \varphi\}_i$$

10 variables on each particle

time evolution

$$\frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} \qquad \mathcal{L} = \left\langle \Psi \middle| i\hbar\frac{d}{dt} - \hat{H} \middle| \Psi \right\rangle$$

wave functions

$$\Psi = \prod_{i=1}^{3A} \phi_i(\mathbf{r})\chi_i \qquad \chi_i = f_i s_i c_i$$

f_i ... flavors (fixed)

s_i ... spins (fixed now) ↑ ↓

$$c_i \equiv \begin{pmatrix} \cos\alpha_i e^{-i\beta_i}\cos\theta_i \\ \sin\alpha_i e^{+i\beta_i}\cos\theta_i \\ \sin\theta_i e^{i\varphi_i} \end{pmatrix} \begin{matrix} \text{R} \\ \text{G} \\ \text{B} \end{matrix}$$

$$\phi_i(\mathbf{r}) \equiv (\pi L^2)^{-\frac{3}{4}} \exp[-(\mathbf{r}-\mathbf{R}_i)^2/2L^2 - i\mathbf{P}_i\mathbf{r}]$$

cooling of the system

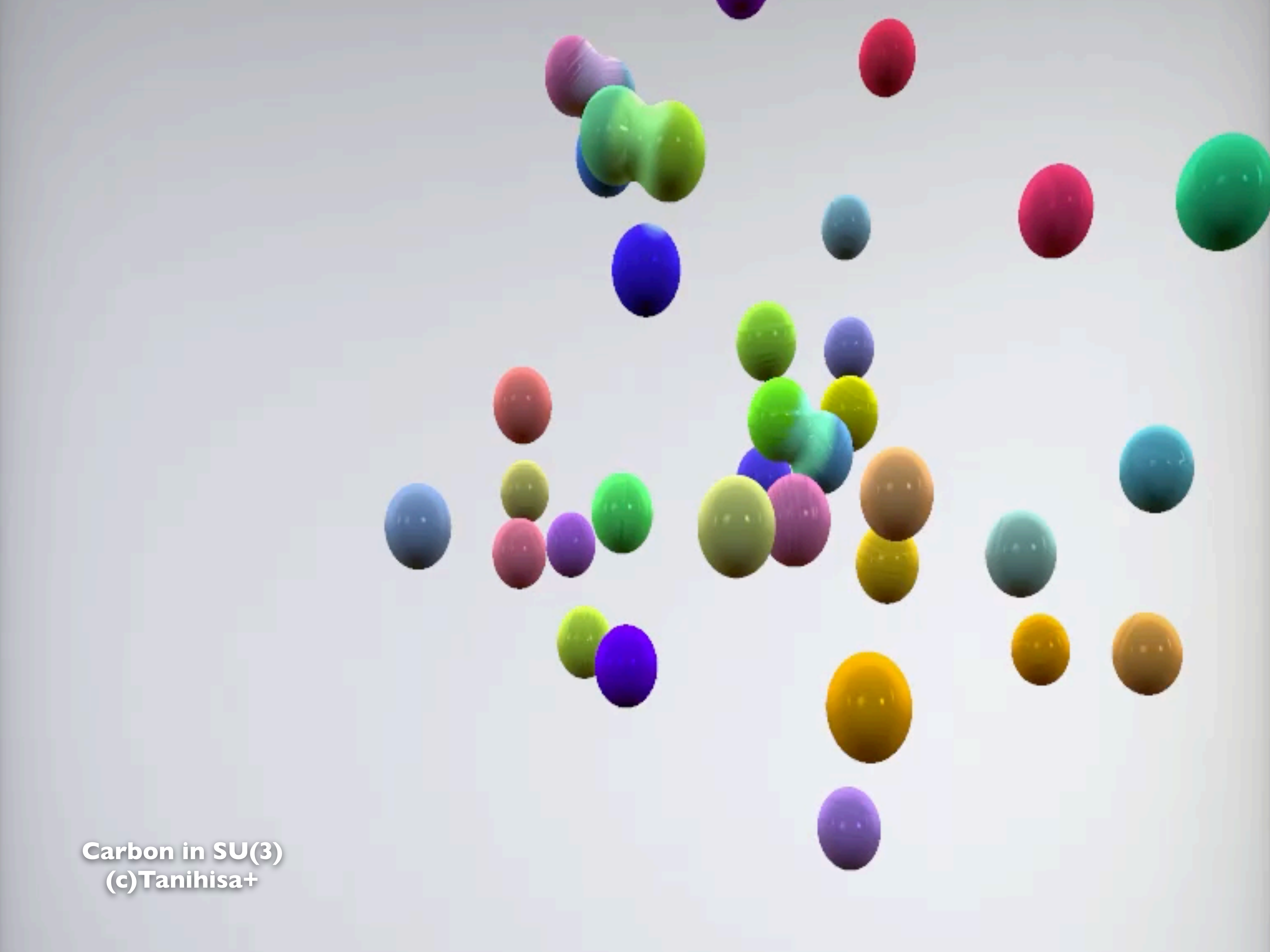
$$\dot{\mathbf{R}}_i = \frac{1}{3}\sum_{j\in\{i\}}\left[\frac{\partial H}{\partial \mathbf{P}_j} + \mu_P\frac{\partial H}{\partial \mathbf{R}_j}\right]$$

$$\dot{\mathbf{P}}_i = \frac{1}{3}\sum_{j\in\{i\}}\left[-\frac{\partial H}{\partial \mathbf{R}_j} + \mu_P\frac{\partial H}{\partial \mathbf{P}_j}\right]$$

confinement conditions

$$\begin{cases} |\mathbf{R}_i - \mathbf{R}_j| < d_{cluster} \quad (i, j = 1, 2, 3) \\ \sum_{a=1}^{8}\left[\sum_{i=1}^{3}\langle\chi_i|\lambda^a|\chi_i\rangle\right]^2 < \varepsilon \end{cases}$$

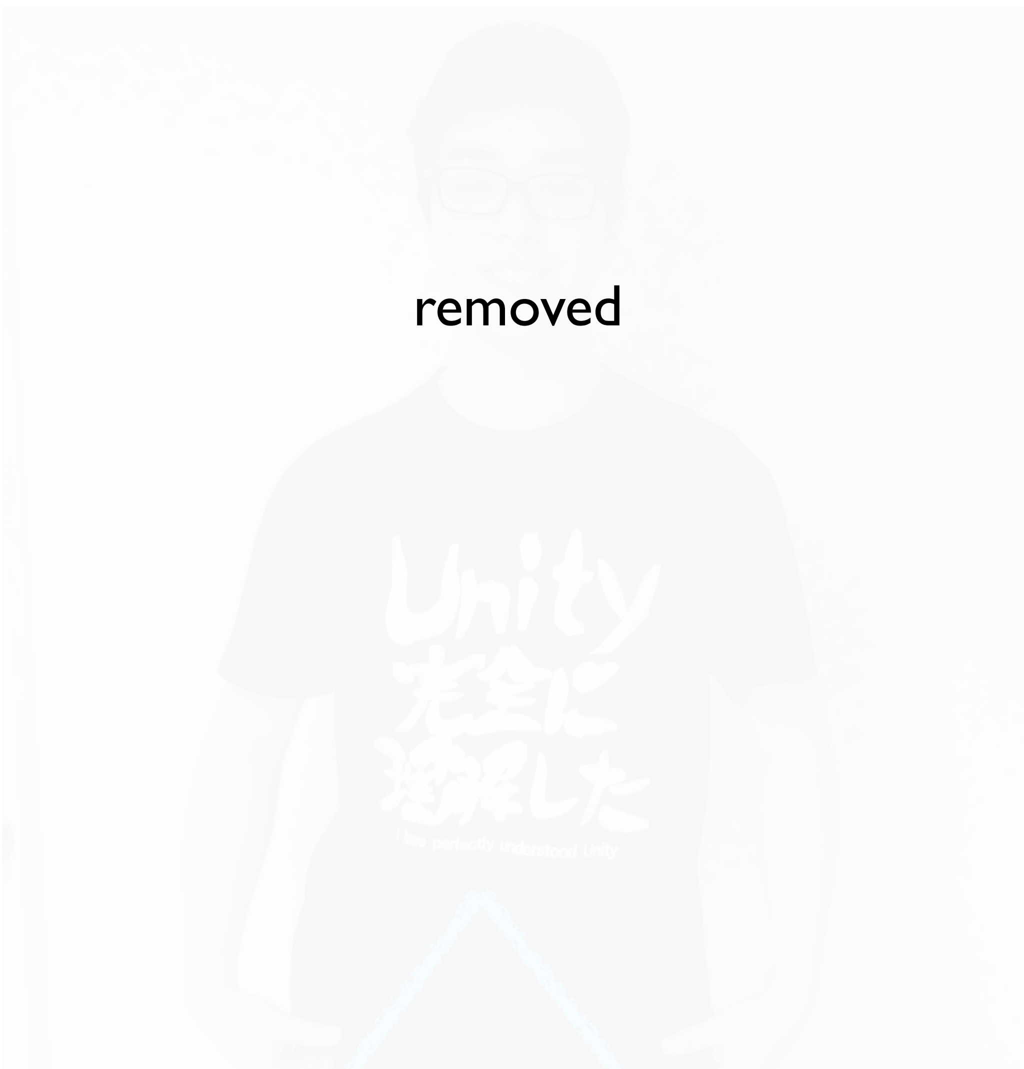
λ^a being the Gell-Mann matrices


Carbon in SU(3)
(c)Tanihisa+

Visualization of CMD

Thanks to the students.

Hakozaki

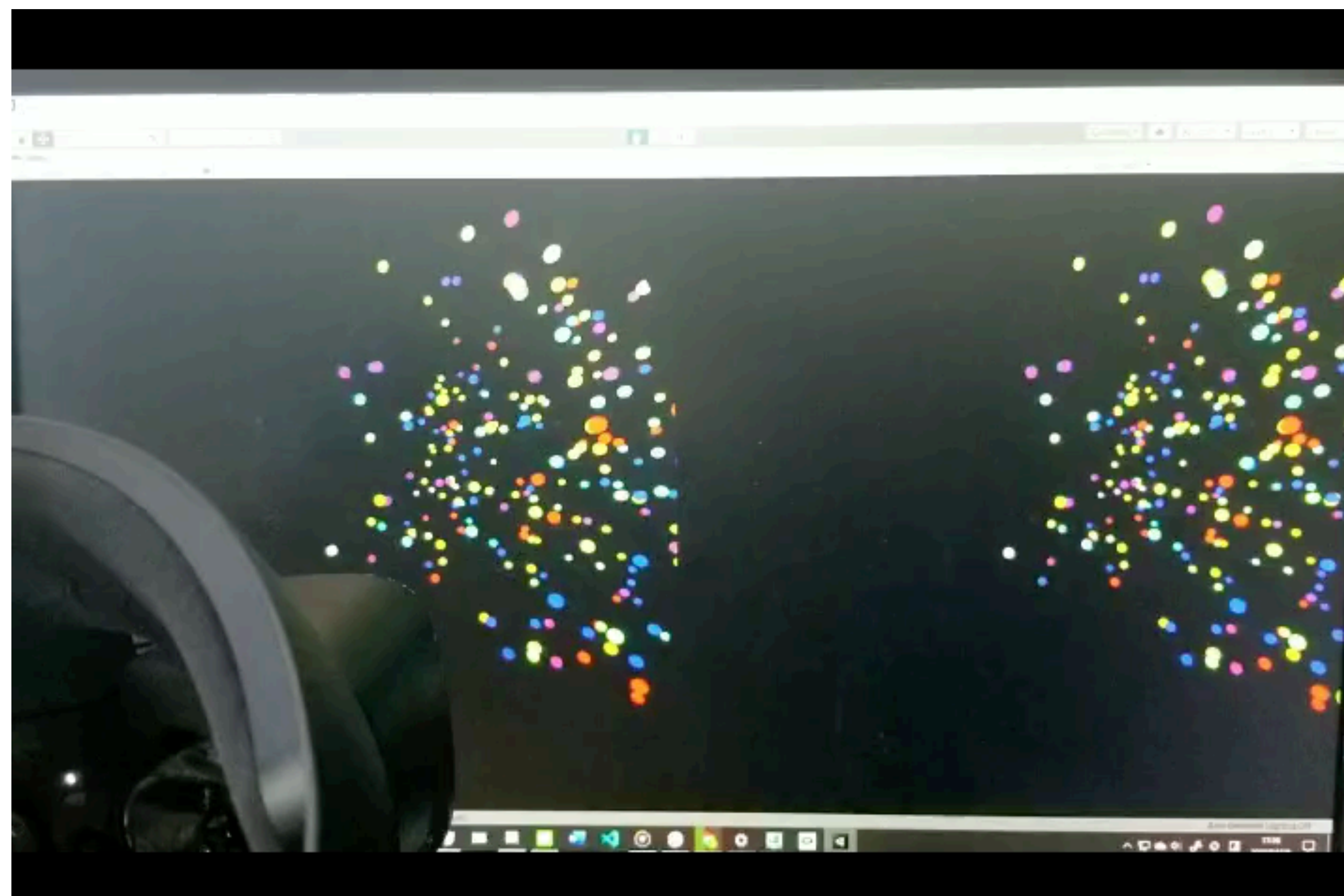


"I have perfectly understood **unity**(visualization)".

Youtube Link(VR)

https://www.youtube.com/watch?v=nolC0UmR3Is&feature=youtu.be

oculus(VR)



INTERACTIONS IN CMD

$$\hat{H} = \sum_i \sqrt{m^2 + \hat{\mathbf{p}}_i^2} + \frac{1}{2}\sum_{i,j\neq i} \hat{V}_{ij}$$

$$\hat{V}_{ij} = -\sum_{a=1}^{8} t_i^a t_j^a V_C(\hat{r}_{ij}) + V_M(\hat{r}_{ij}) + V_{Pauli}(r) + V_{coul}(r)$$

$$V_C(r) \equiv Kr - \alpha_s \frac{e^{-\mu r}}{r} + V_{spin}(r)$$

$$V_{spin}(r) = \frac{\kappa'}{m_i m_j r_{0ij}^2} \frac{1}{r_{ij}} e^{-(r_{ij}/r_{0ij})^2} \quad s_i s_j$$

$$V_M(r) \equiv -\frac{g_{\sigma q}^2}{4\pi}\frac{e^{-\mu_\sigma r}}{r} + \frac{g_{\omega q}^2}{4\pi}\frac{e^{-\mu_\omega r}}{r} + \frac{\sigma_i^3 \sigma_j^3}{4}\frac{g_{\rho q}^2}{4\pi}\frac{e^{-\mu_\rho \hat{r}_{ij}}}{\hat{r}_{ij}}$$

$$V_{Pauli} = \frac{C_p}{(q_0 p_0)^3} \exp\left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2}\right] \delta_{\chi_i \chi_j}$$

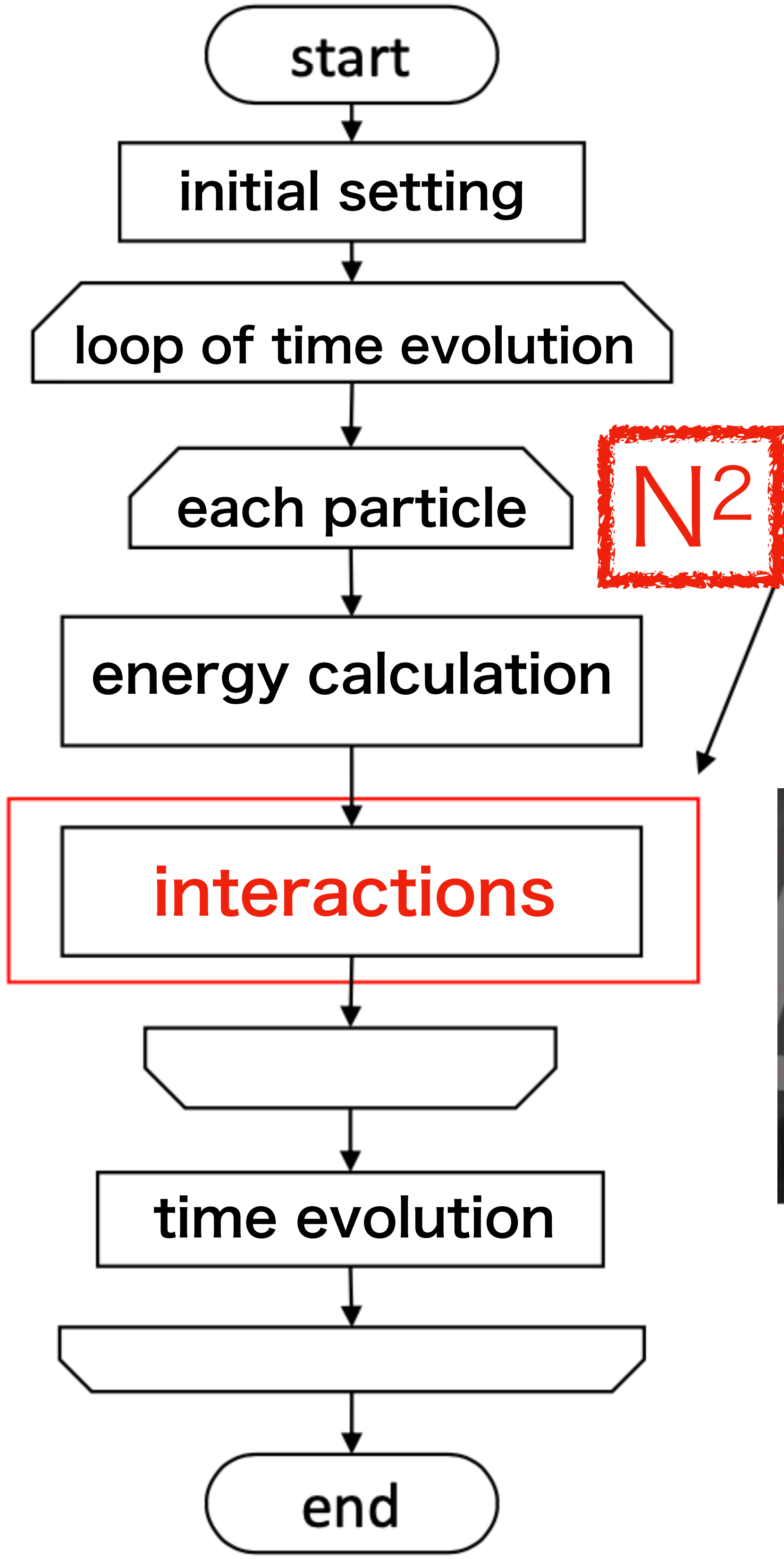
$t^a = \lambda^a/2$ with λ^a being the Gell-Mann matrices

- V_C ..quark-quark interactions
- V_{spin} ..spin-spin interactions
- V_M quark-meson interactions
- V_{Pauli} ..Pauli interactions

*We only take into account the correlation between only 2 particles.

⇒order of calculations～O(N^2)

Procedure



- The main part of calculations (∼90%).

→ The main target to be improved.

- Super computer in JAEA
- parallel computings(OpenACC)

Device : HPE SGI 8600 in JAEA
CPU : Intel Xeon Gold 6428R
(3.0GHz, 35.75MB cache)X 2CPU
Core number per node : 48
GPU : NVIDIA Tesla V100 SX2 32GB memory
(FP64/GPU : 2560)x4GPU
Memory per node : 384 GB

How to reduce numerical costs ?

Tree method from N-body simulations in astrophysics

$$0 = \sum_{j \neq i}^{N} G m_j \frac{\boldsymbol{x}_j - \boldsymbol{x}_i}{(|\boldsymbol{x}_j - \boldsymbol{x}_i|^{+}\varepsilon^2)^{3/2}} + \text{repulsion (by pressure \& rotation)}$$

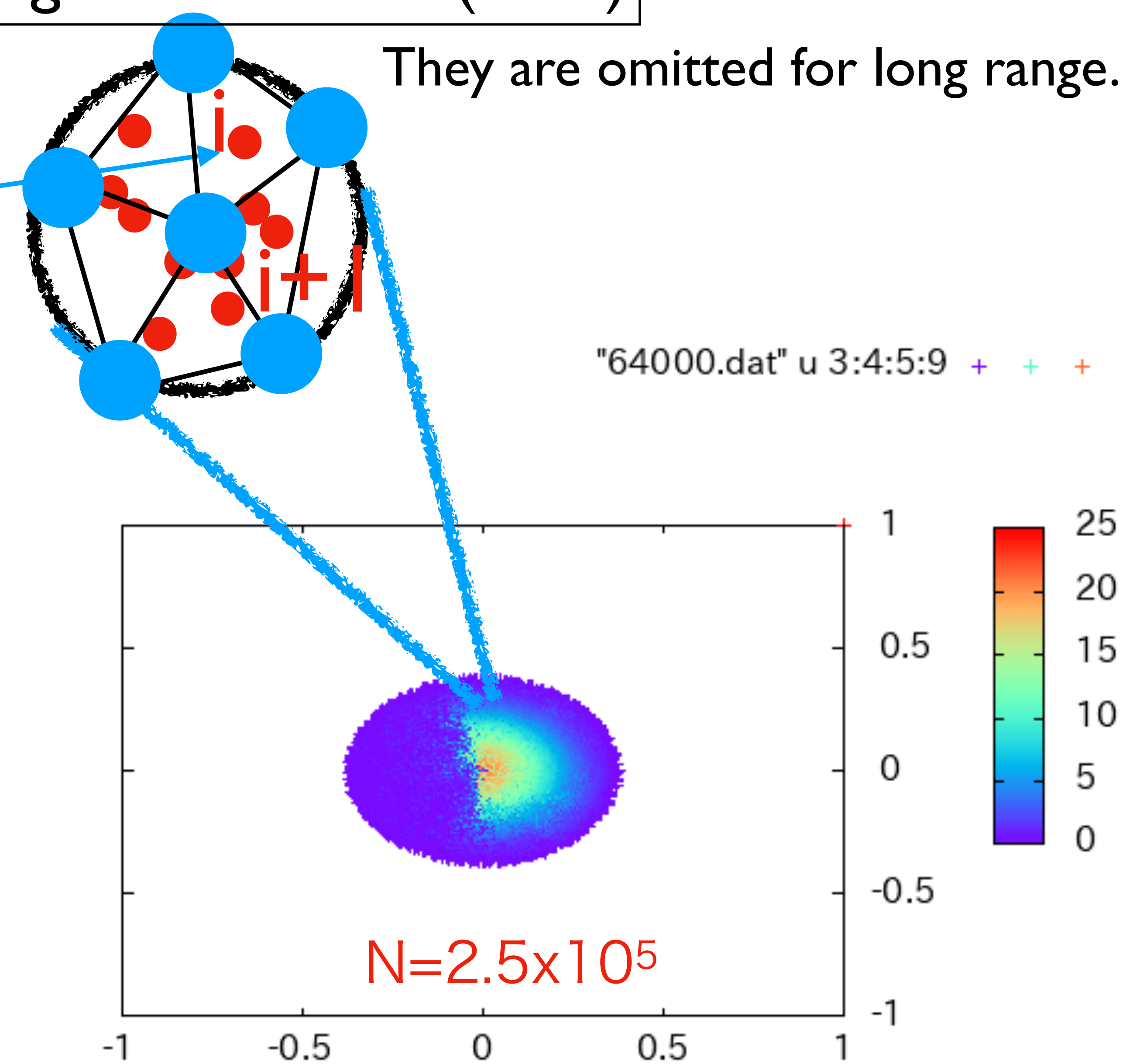
Gravitation — long range correlations(global)

pressure — short range correlations(local)

rotation — single correlations

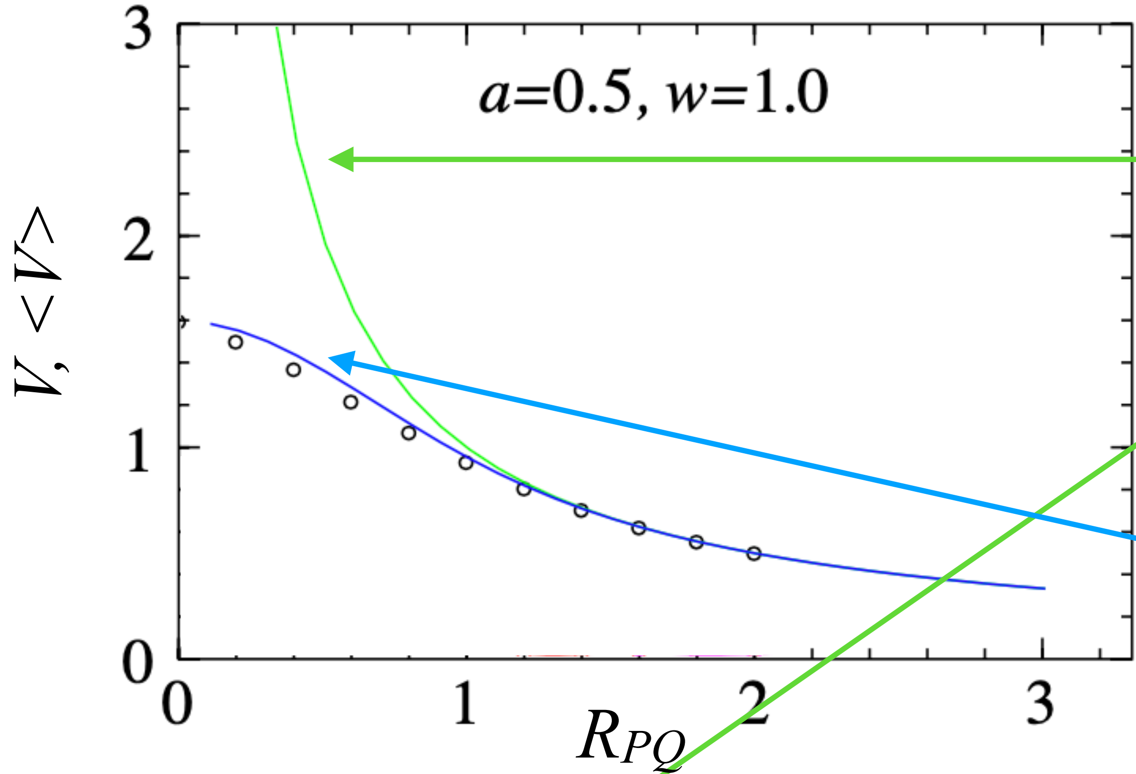
They are omitted for long range.

j



Gravitations from **i** and **i+1** are same for **j** sometimes.
→They should be summarized.

Double folding model

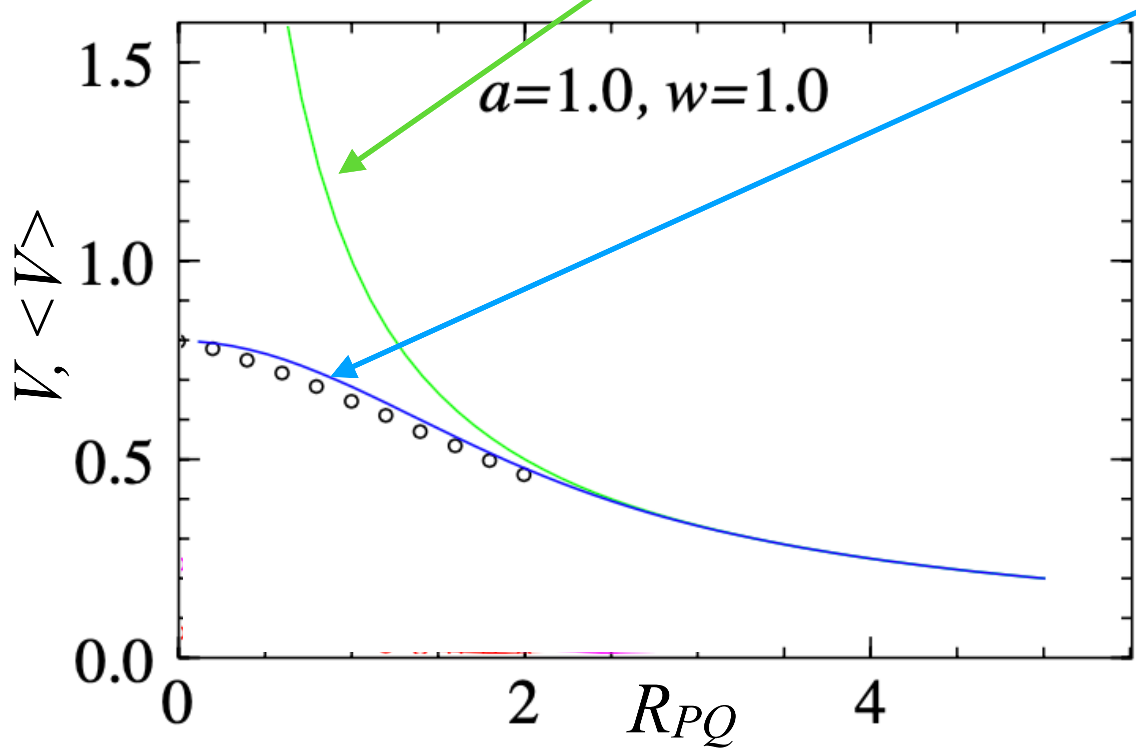


Yukawa-type interactions

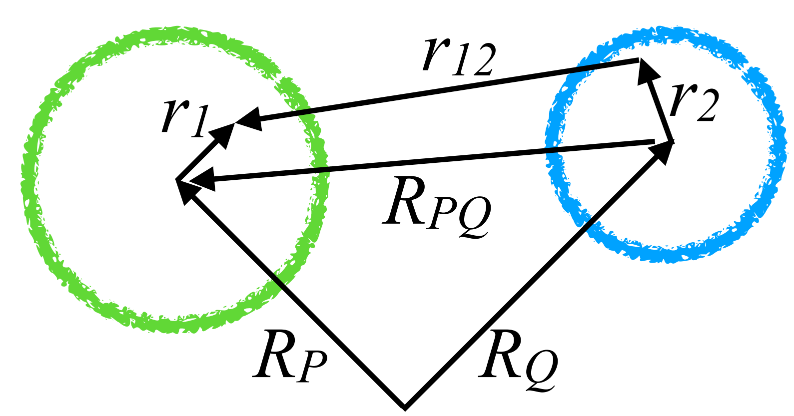
$$V = c\frac{e^{-\mu R_{PQ}}}{R_{PQ}}$$

Double foldings of Yukawa-type interactions (Expected values)

No divergence



$$< V > = c\int \exp(-pr_{1P}^2)\frac{e^{-\mu r_{12}}}{r_{12}}\exp(-qr_{2Q}^2)dr_1 dr_2$$



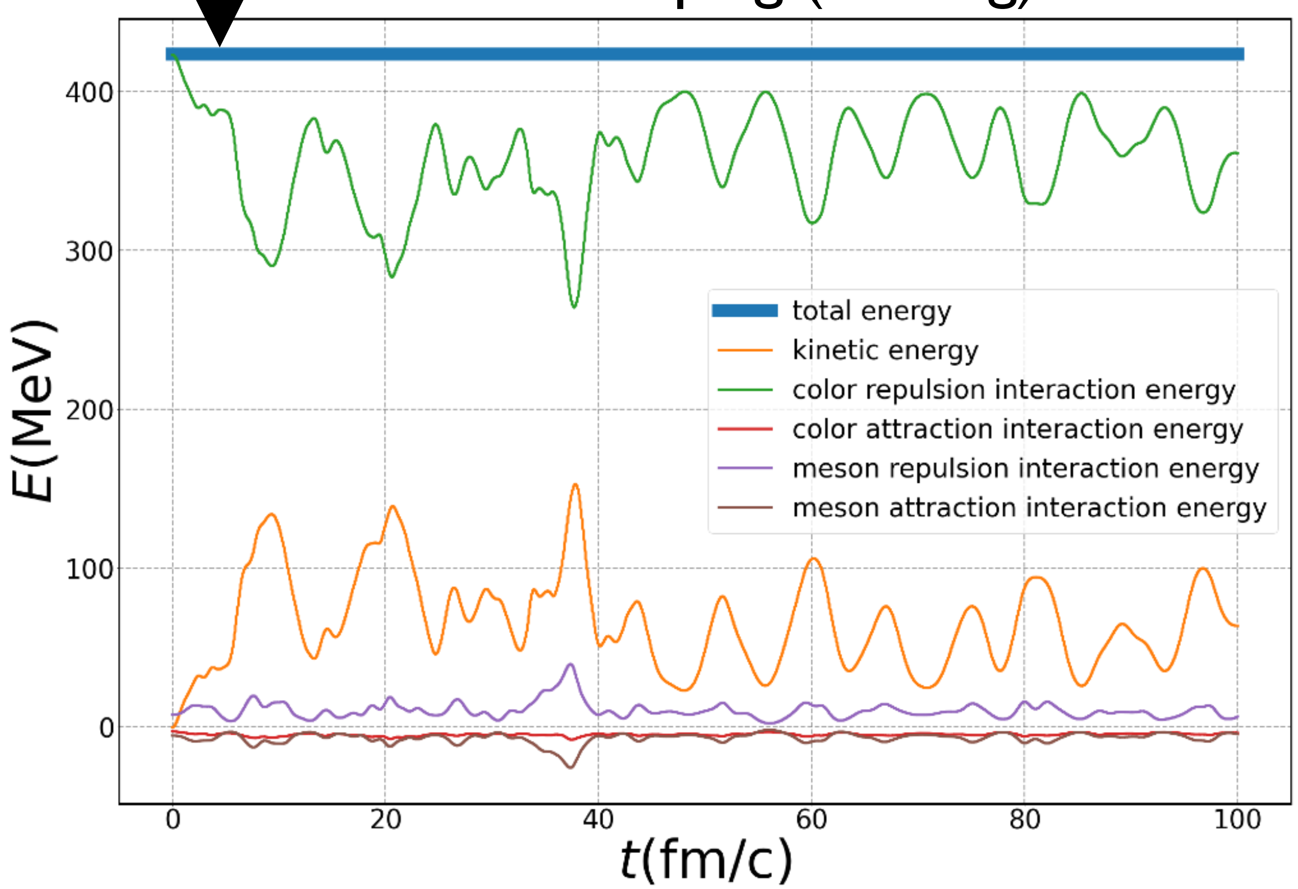
Positions are expected values in MD.

Energy conservation

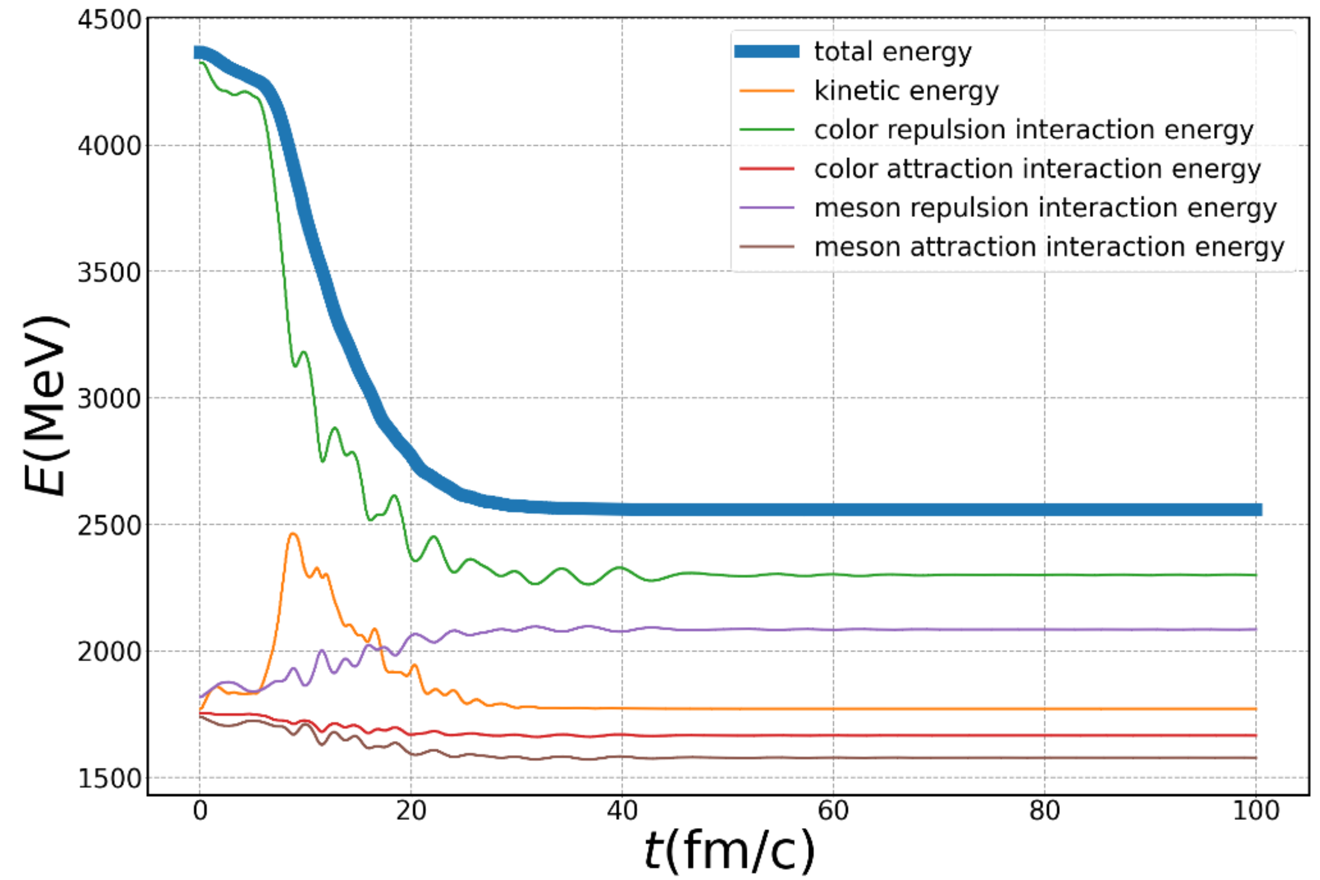
one of the accuracy checks

total energy

without dumping (cooling) terms



including dumping (cooling) terms



$$\dot{\mathbf{R}}_i = \frac{1}{3} \sum_{j \in \{i\}} \left[\frac{\partial H}{\partial \mathbf{P}_j} + \mu_R \frac{\partial H}{\partial \mathbf{R}_j} \right]$$

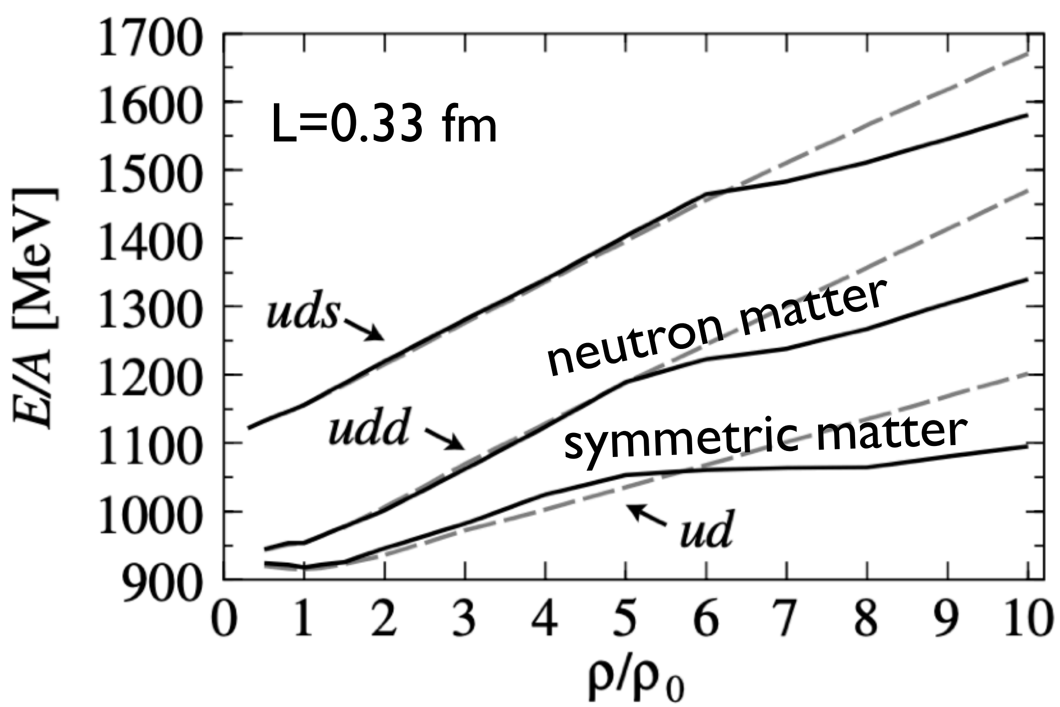
$$\dot{\mathbf{P}}_i = -\frac{1}{3} \sum_{j \in \{i\}} \left[\frac{\partial H}{\partial \mathbf{R}_j} + \mu_P \frac{\partial H}{\partial \mathbf{P}_j} \right]$$

(c) Mukobara+

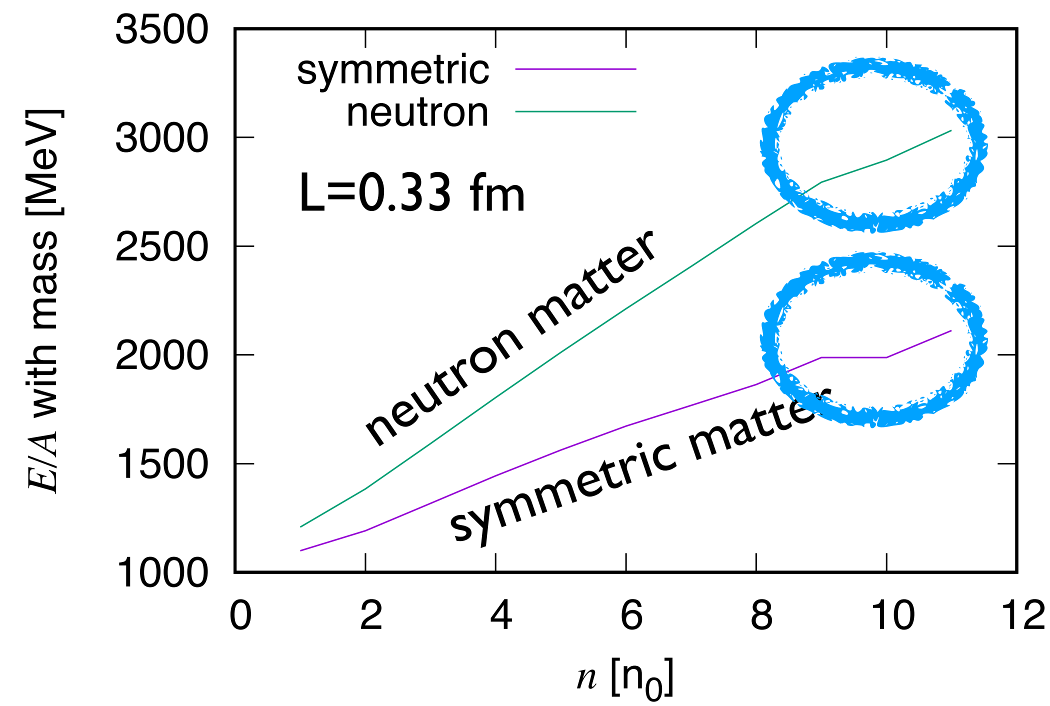
EOS from color molecular dynamics

without spin cases

Akimura et al. EPJA 25,405(2005)



Our preliminary result



- non-linear σ meson coupling

$$\frac{1}{2-\varepsilon}\left(-\frac{g_{\sigma q}^2}{4\pi}\right)\left(\sum_{j\neq i, j\in l}^{n}\frac{e^{-\mu_\sigma \hat{r}_{ij}}}{\hat{r}_{ij}}\right)^{1-\varepsilon}$$

- non-relativistic kinetic energy

$$\frac{\mathbf{P}_i^2}{2m_i}$$

- color fixed calculations

- σ meson coupling

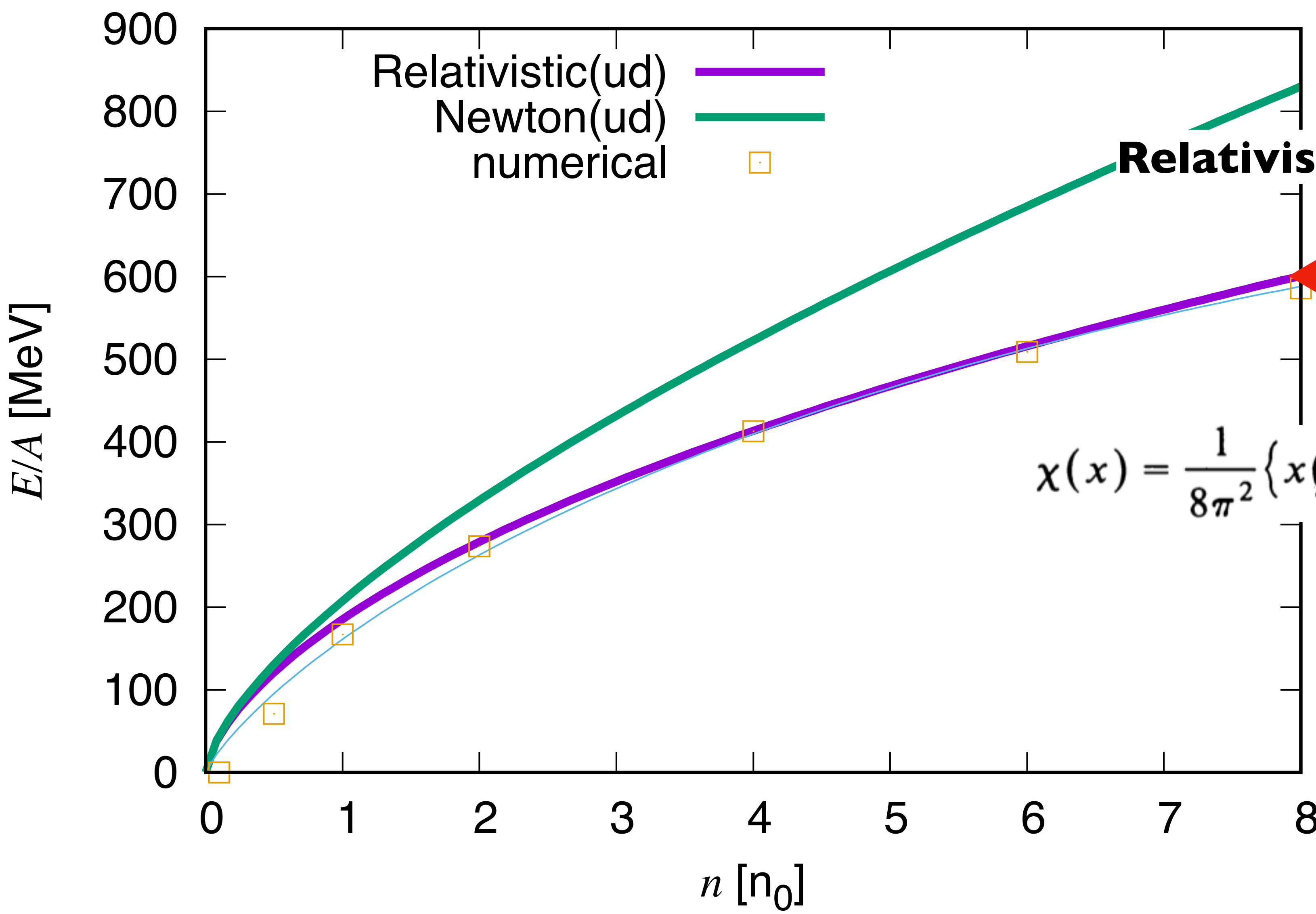
$$\frac{1}{2}\sum_{i,j\neq i} -\frac{g_{\sigma q}^2}{4\pi}\frac{e^{-\mu_\sigma r}}{r}$$

- relativistic kinetic energy

$$\sum_i\left(\sqrt{m^2+\hat{\mathbf{p}}_i^2} - m\right)$$

- color evolutions

Free kinetic energy for fermions and Pauli interaction



Relativistic Free kinetic energy for fermions

$$\epsilon = \frac{gmc^2}{\lambda^3}\chi(x)$$

$$\chi(x) = \frac{1}{8\pi^2}\left\{x(1+x^2)^{1/2}(1+2x^2) - \ln\left[x + (1+x^2)^{1/2}\right]\right\}$$

$$n = \frac{4\pi^2 g}{3h^3}{p_F}^3 \qquad x = \frac{p_F}{mc}$$

$$g = \text{spin} \times \text{color} \times \text{flavor}$$

Effective Pauli interaction

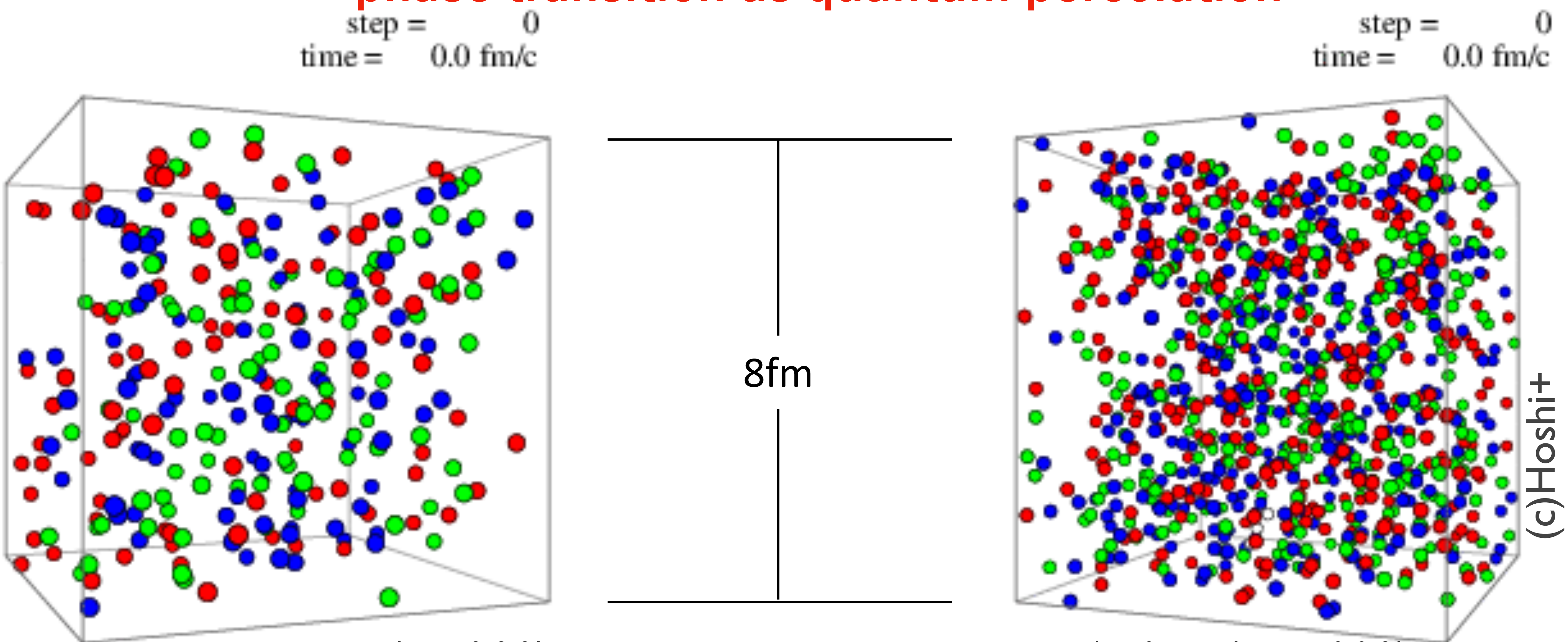
$$V_{\text{Pauli}} = \frac{C_p}{(q_0 p_0)^3}\exp\left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2}\right]\delta_{\chi_i\chi_j}$$

Introduced to show the antisymmetric effects.

These parameters, Cp, q0, p0 are optimized to reproduce the kinetic energy for fermions

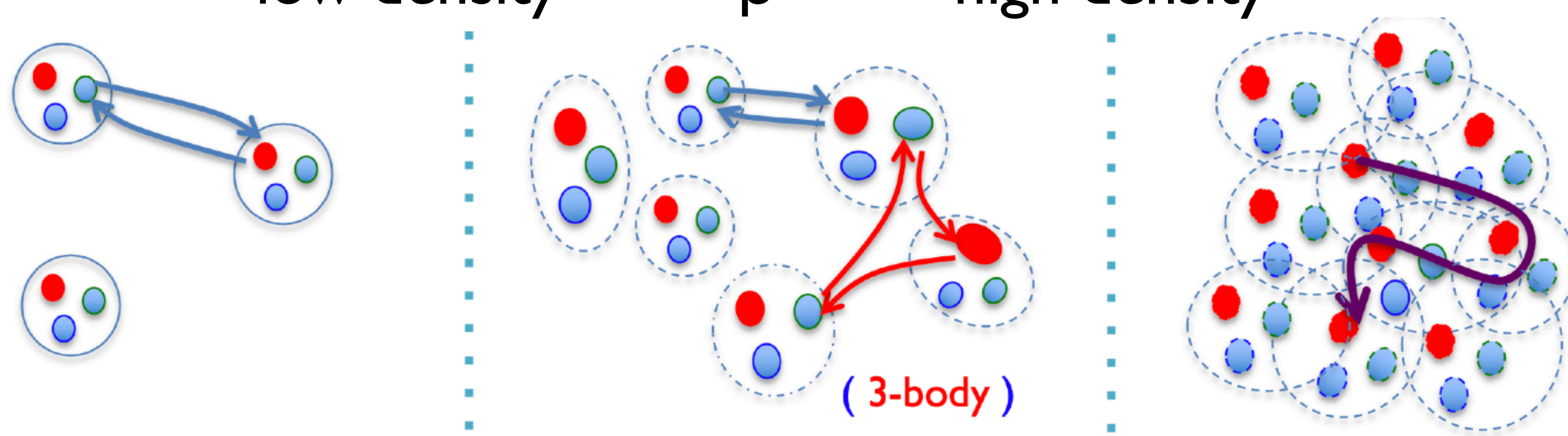
Many body cases

phase transition as quantum percolation



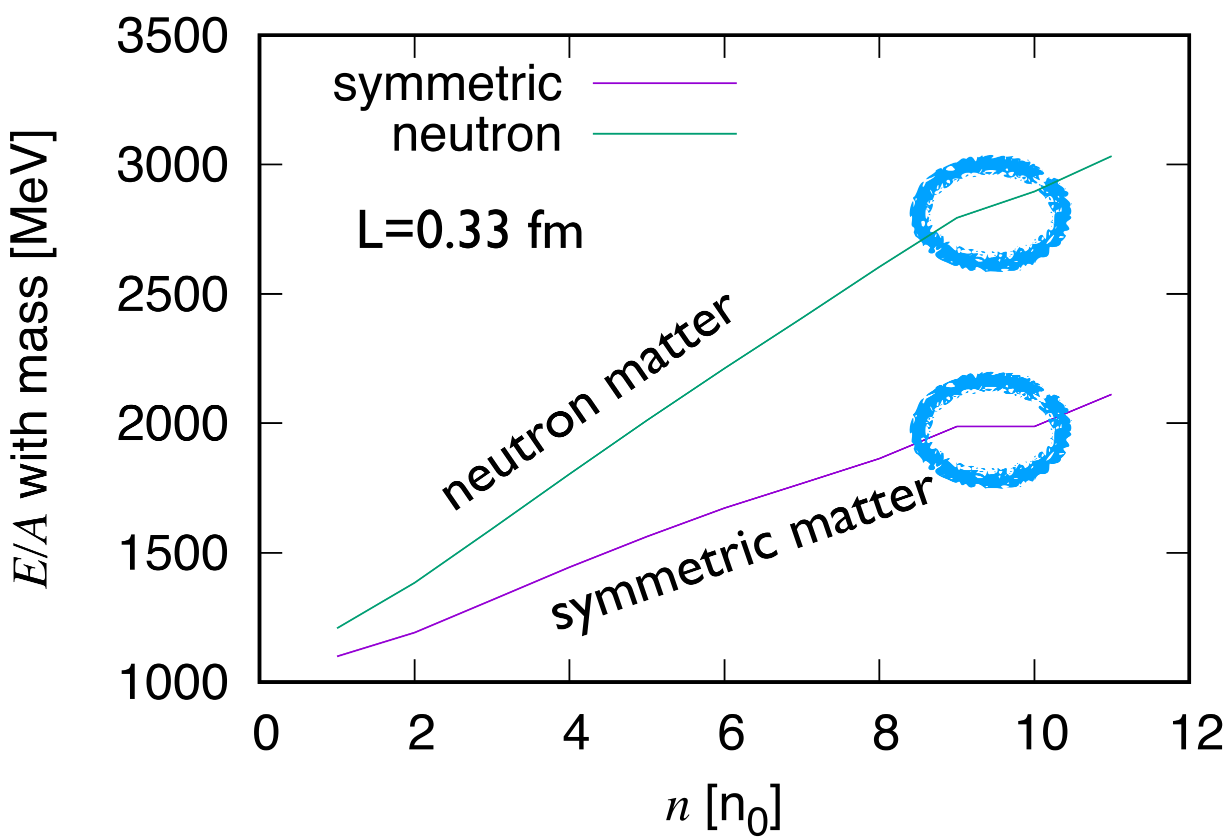
$\rho=1.17\rho_0$(N=288) $\rho=4.10\rho_0$ (N=1008)

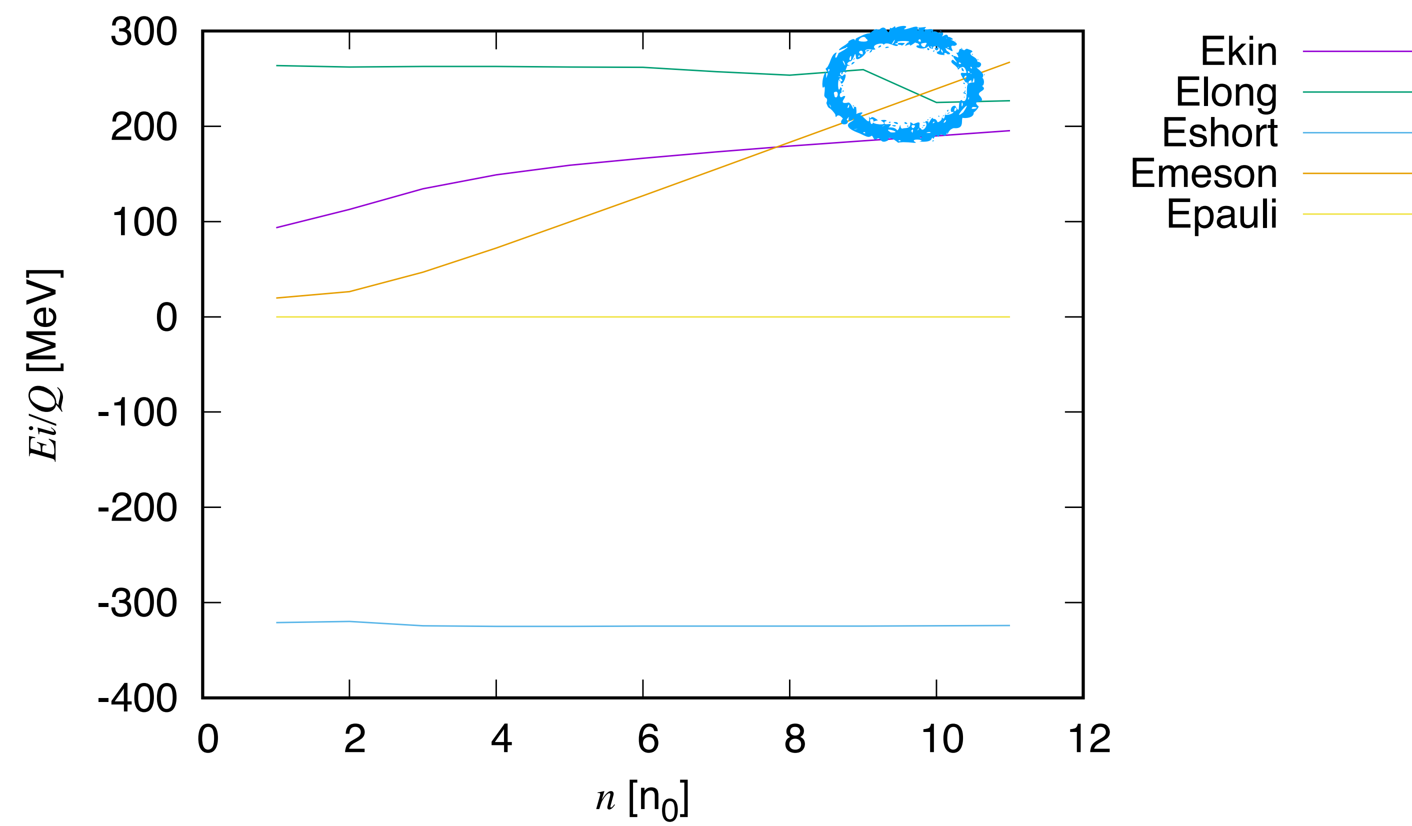
low density <— ρ —> high density



Kojo-Powell-Song-Baym 2014

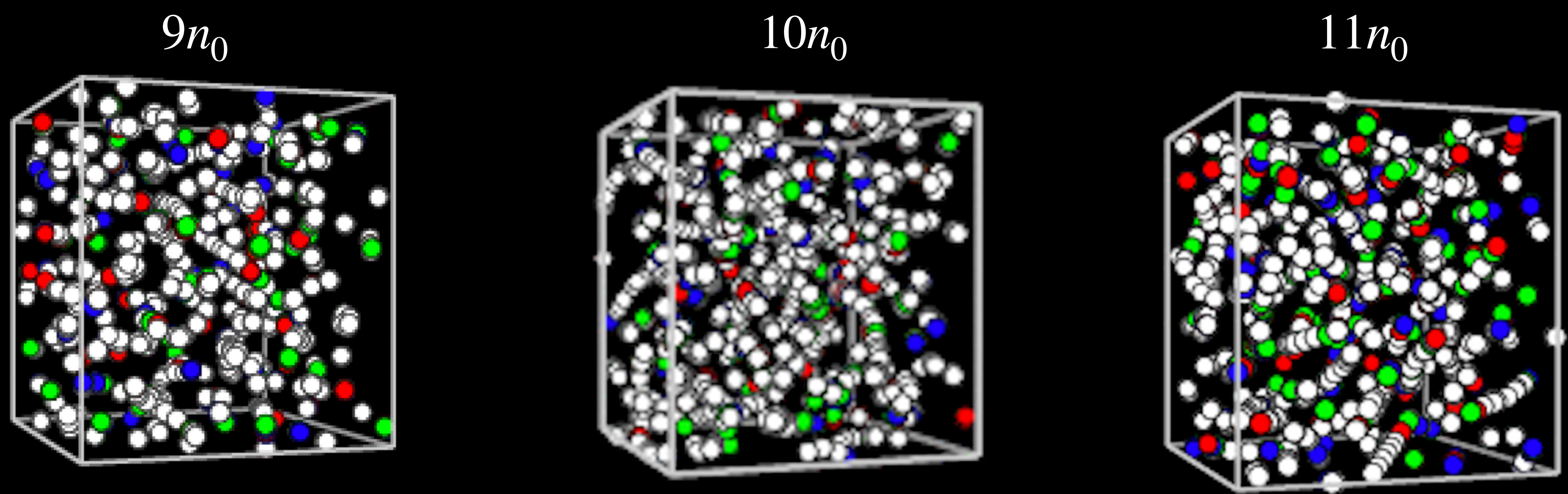
Energy component for cross over EOS

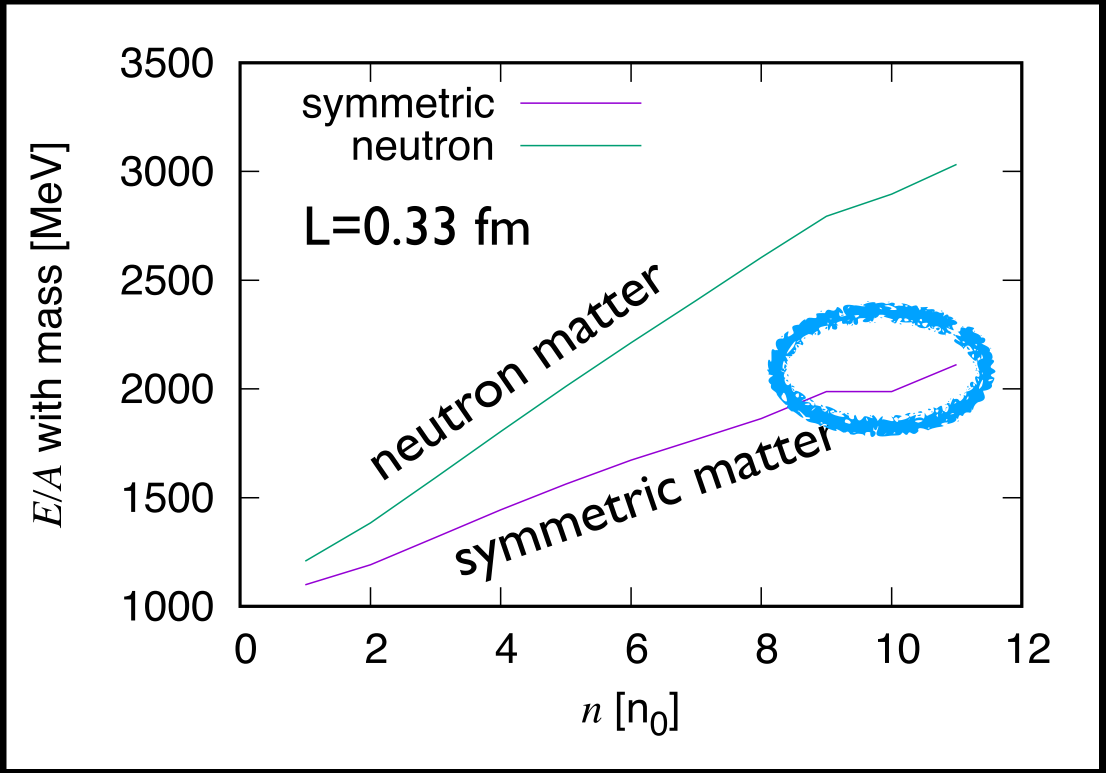




- Elong (confinement potential) → Phase transition (order)
- Emeson (quark-meson couplings) + Ekin(kinetic term) → Hardness of EOS

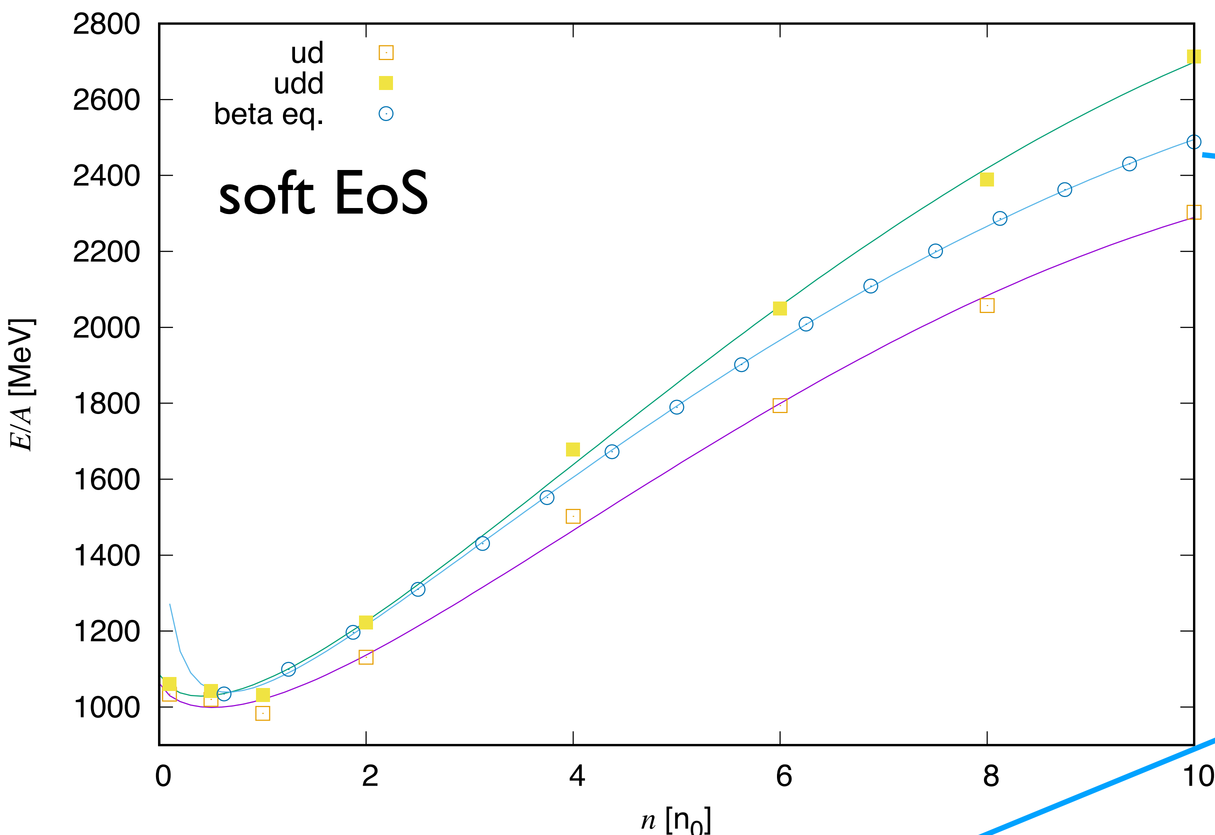
Many body system around phase transition

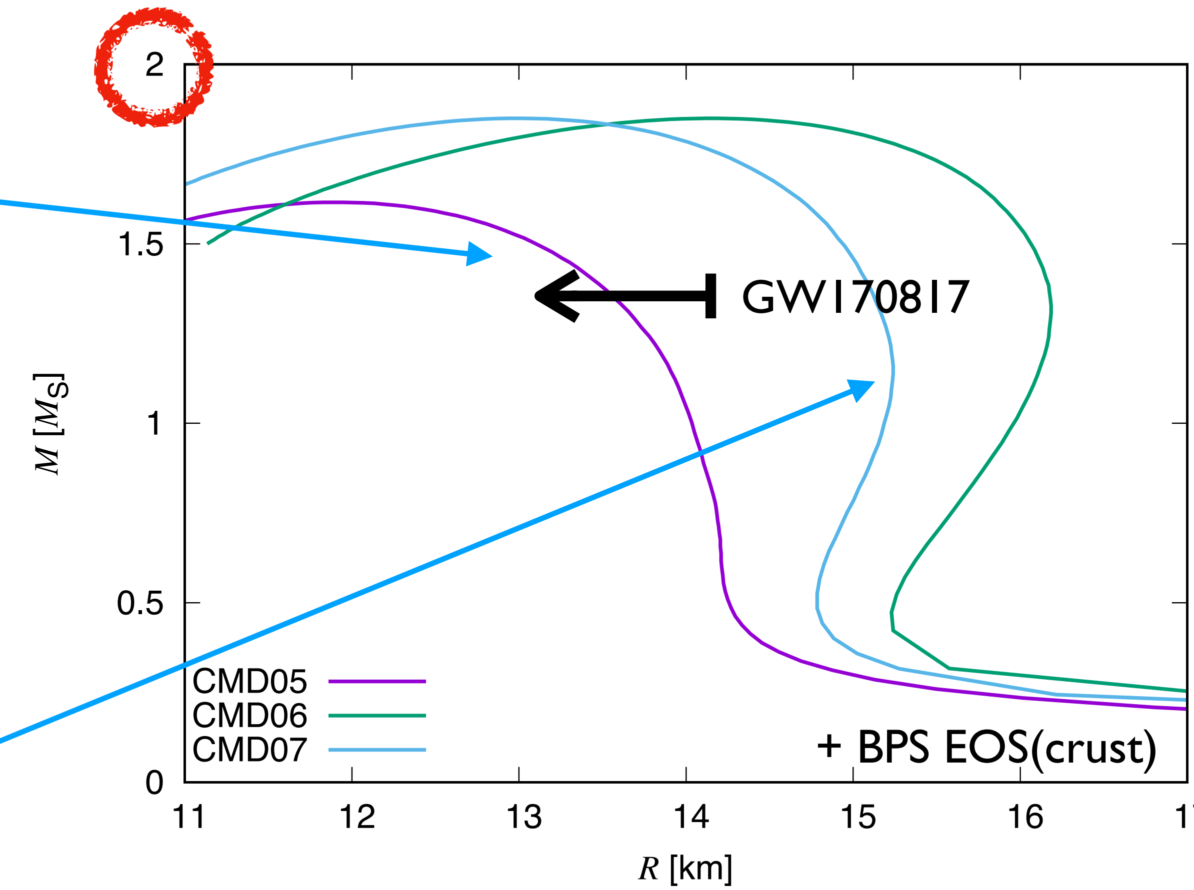


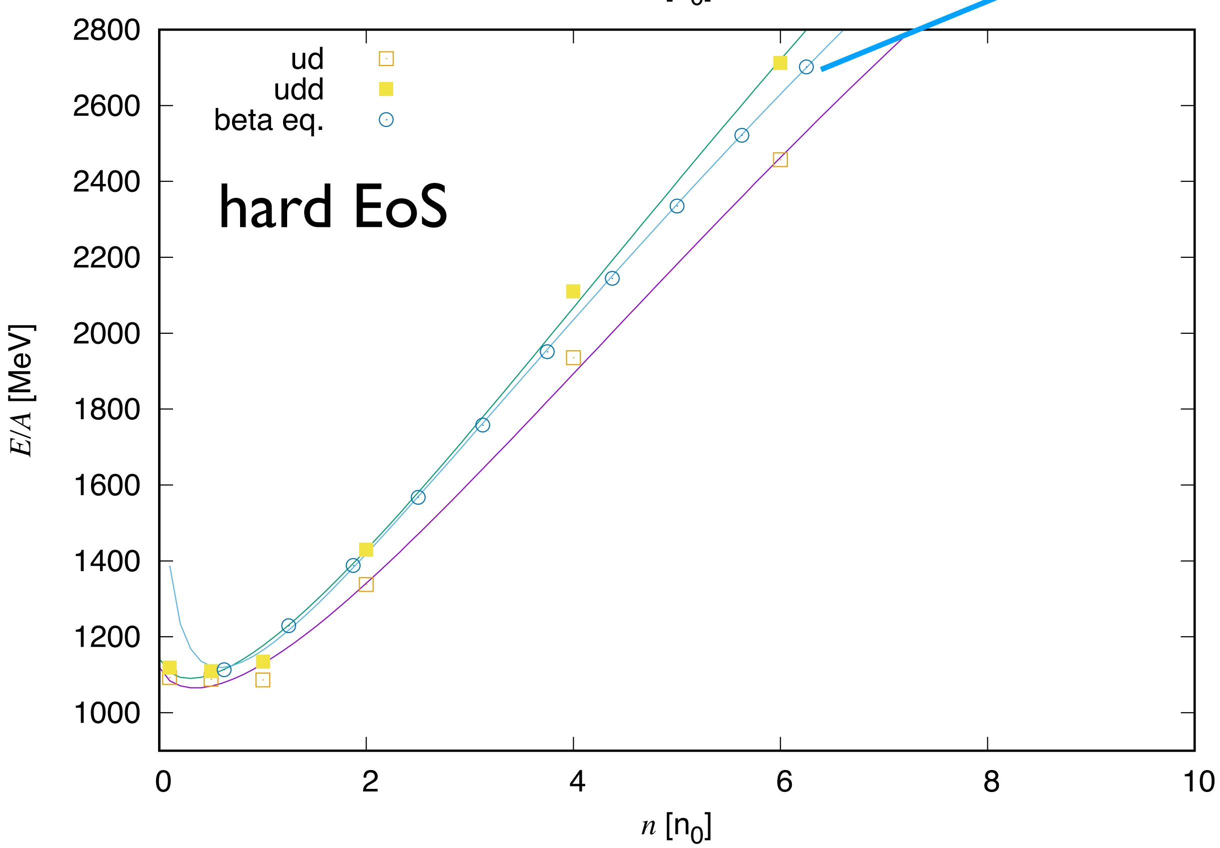


Deconfinement occurs gradually dependent on density.

First trial calculations for MR relations





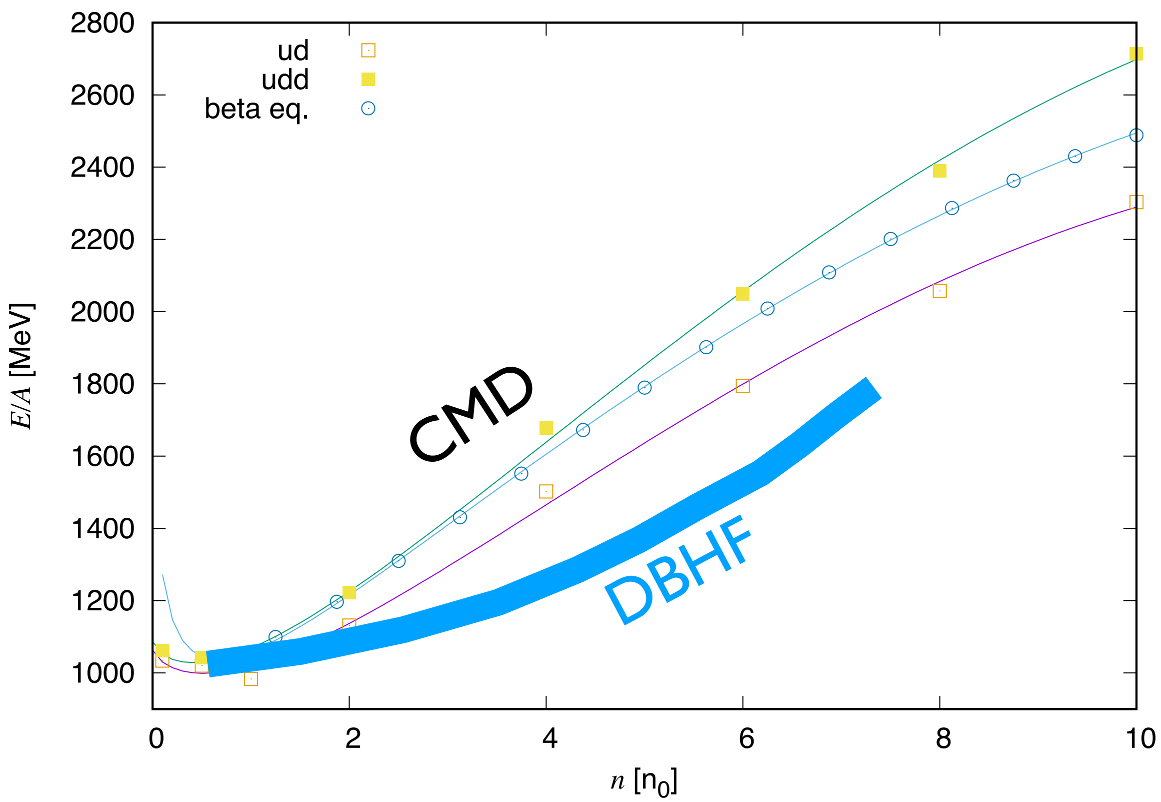


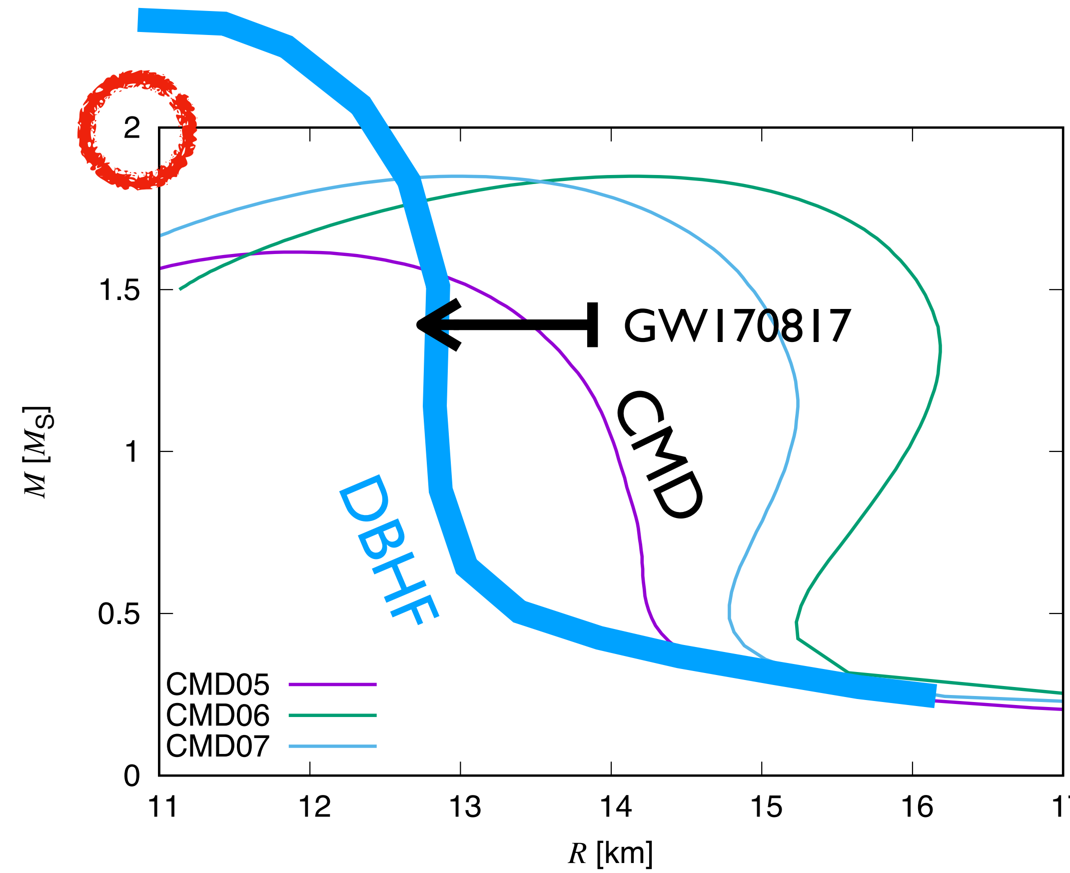
- Large *R* for Large *M* !
- Maximum masses are Less than 2Ms !

⟹ Something is lack.

What type of E/A(interaction) is favored?

Comparison with Dirac Bruckner Hartree Fock (Bonn-B potential)





DBHF: Parabolic shape, namely "soft" at low density and "hard" at high density.

CMD: Almost linear shape, compared with DBHF.

Origins of the non-linear effects:
color magnetic interactions? relativistic interactions? many body interactions?
Or the other interactions?

Color magnetic interaction for N quarks

Jaffe, PRD 15, 281 (1978), Oka & Yazaki, PTP 66, 556 15, 281 (1981)

$$-\sum_{i\neq j}^{N}\{\underset{\sim}{\lambda}\vec{\sigma}\}_i\cdot\{\underset{\sim}{\lambda}\vec{\sigma}\}_j = 8N-\tfrac{1}{2}C_6^N+\tfrac{4}{3}S_N(S_N+1)+C_3^N$$

where we use quadratic Casimir operators

$$C_6^N=\sum_{r=1}^{35}\Big(\sum_{i=1}^{N}\mu_i^r\Big)^2,\quad C_2^N=4S_N(S_N+1)=\sum_{k=1}^{3}\Big(\sum_{i=1}^{N}\sigma_i^k\Big)^2,\quad C_3^N=\sum_{a=1}^{8}\Big(\sum_{i=1}^{N}\lambda_i^a\Big)^2.$$

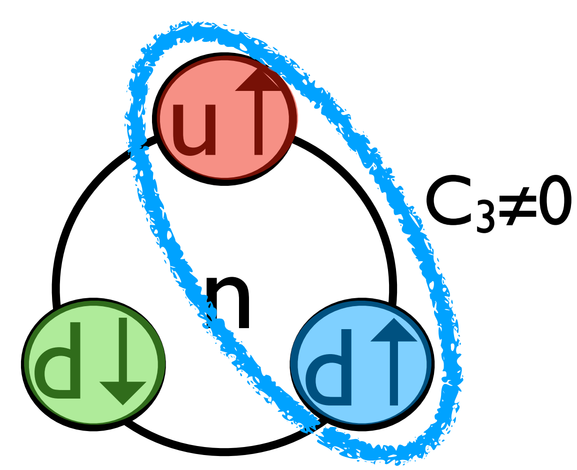
e.g.

$n\cdots$ N=3, C_6=33*2, S=1/2, C_3=0 $\Longrightarrow$ -8

$\Delta\cdots$ N=3, C_6=21*2, S=3/2, C_3=0 $\Longrightarrow$ +8

But what about N>>3 ?

In our molecular dynamics,
we need 2-body effective interaction
corresponding N-body systems.



$n\cdots$ Σ sij=-1/2-1/2+1/4=-3/4=-S(S+1)

OPTIMIZATION OF INTERACTIONS IN CMD

interactions with colors

$$\hat{V}_{\text{color}} = \frac{1}{2}\sum_{i=1,j\neq i}^{n}\left(-\sum_{a=1}^{8}\frac{\lambda_i^a\lambda_j^a}{4}\left(K\hat{r}_{ij} - \frac{\alpha_s}{\hat{r}_{ij}}\right)\right)$$

↑or↓

$$V_{ij}^{CS} = \frac{\kappa'}{m_i m_j r_{0ij}^2}\frac{1}{r_{ij}}e^{-(r_{ij}/r_{0ij})^2}\lambda_i^c\lambda_j^c\,\sigma_i\cdot\sigma_j$$

$$r_{0ij} = (\alpha + \beta\mu_{ij})^{-1}.\quad \mu_{ij} = m_i m_j/(m_i + m_j)$$

Aaron et al. EPJA 56,93(2020)

～1/(2m)

αs	κ'	K	α	β	$m_{u,d}$	m_s	L
1.25	0.5	750 MeVfm^{-1}	2.1 fm^{-1}	0.552	0.362 GeV	0.538 GeV	0.346 fm

Akimura et al. EPJA 25,405(2005) etc. **Optimized in this study.**

2-body spin correlations

$$<\frac{\sigma_i}{2}\cdot\frac{\sigma_j}{2}> = \frac{1}{4}(\uparrow\uparrow),\quad -\frac{3}{4}(\uparrow\downarrow)$$

(I,S)	$(\frac{1}{2},\frac{1}{2})$ N,P	$(\frac{1}{2},\frac{3}{2})$ Δ	$(0,\frac{1}{2})$ Λ	$(1,\frac{1}{2})$ Σ	$(1,\frac{3}{2})$ Σ^*	$(\frac{1}{2},\frac{1}{2})$ Ξ	$(\frac{1}{2},\frac{3}{2})$ Ξ^*
M_B	0.90	1.24	1.075	1.07	1.41	1.21	1.58
Expt.	0.938	1.232	1.115	1.189	1.382	1.315	1.532

2-body spin correlations consistent with 3-body spin correlations

$$<\frac{\sigma_i}{2}\cdot\frac{\sigma_j}{2}> = \frac{1}{4}(\uparrow\uparrow),\quad -\frac{1}{2}(\uparrow\downarrow)$$

(I,S)	$(\frac{1}{2},\frac{1}{2})$ N, P	$(\frac{1}{2},\frac{3}{2})$ Δ	$(0,\frac{1}{2})$ Λ	$(1,\frac{1}{2})$ Σ	$(1,\frac{3}{2})$ Σ^*	$(\frac{1}{2},\frac{1}{2})$ Ξ	$(\frac{1}{2},\frac{3}{2})$ Ξ^*
M_B	0.938	1.233	1.115	1.177	1.379	1.328	1.531
Expt.	0.938	1.232	1.115	1.189	1.382	1.315	1.532

others

Akimura et al. EPJA 25,405(2005)

quark-meson coupling

$$V_{\text{meson}}(r) \equiv -\frac{g_{\sigma q}^2}{4\pi}\frac{e^{-\mu_\sigma r_{ij}}}{r_{ij}} + \frac{g_{\omega q}^2}{4\pi}\frac{e^{-\mu_\omega r_{ij}}}{r_{ij}} + \frac{\sigma_i^3\sigma_j^3}{4}\frac{g_{\rho q}^2}{4\pi}\frac{e^{-\mu_\rho \hat{r}_{ij}}}{\hat{r}_{ij}}$$

pauli interaction

$$\langle V_{\text{pauli}}(r)\rangle \equiv \frac{C_p}{(q_0 p_0)^3}\exp\left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2}\right]\delta_{\chi_i\chi_j}$$

Summary and Discussion

Summary

- We have studied EoS from CMD with dynamical color evolutions.
- We have found cross over EOS, which is consistent with Akimura et al. 2005.
- Note that we have also found 1st order phase transition for the other parameter sets.
- We need more realistic E/A. ← Color-magnetic int.? Relativistic? Others?

Discussion

- What should be effective two-body color magnetic interactions corresponding N-body system?
- How to take into account the vacuum effects (chiral condensations).