Collaboration Workshop “The future of MR-DFT”
Thursday, 25 June, 2015

MR-TDDFT for low-energy heavy ion reactions: Ideas

Kazuyuki Sekizawa

(Warsaw Univ. of Technology, Poland)

2015. 4: I started working at WUT in collaboration with P. Magierski

2015. 3: I have finished my PhD at Univ. of Tsukuba (Supervisor: K. Yabana)

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- multi-nucleon transfer (MNT) reaction
- sub-barrier fusion
- superheavy element (SHE) synthesis

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„ Let's imagine the future of MR-DFT!! ”

Any comments/questions/criticisms are welcome!!

Outline

1. Introduction: Drawbacks in “SR-TDEDF”
2. Method: “MR-TDEDF” with a multi-Slater-determinant
3. “Ideas” for MNT / subbarrier fusion / SHE synthesis
4. Summary

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Action to be minimized:

$$S = \int_{t_1}^{t_2} dt \ \big\langle \Phi(t) \big| i\hbar\partial_t - \hat{H} \big| \Phi(t) \big\rangle \qquad \left(S = \int_{t_1}^{t_2} dt \ \left[i\hbar \sum_{i=1}^{N} \langle \phi_i(t) | \partial_t | \phi_i(t) \rangle - E[\rho(t)] \right] \right)$$

Trial w.f.: a *single* Slater determinant

$$\Phi(x_1, \cdots, x_N, t) = \frac{1}{\sqrt{N!}} \det\{\phi_i(x_j, t)\}$$

Single-particle wavefunctions

$$\phi_i(x, t) \qquad (\, i = 1, \cdots, N; \ x \equiv (\mathbf{r}, \sigma)\,)$$

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Variation $\frac{\delta S}{\delta \phi_i^*(t)} = 0$ leads to:

$$i\hbar \, \partial_t \phi_i(x, t) = \hat{h}[\rho(t)] \phi_i(x, t)$$

: TDEDF (or TDHF, TDKS) equations

One-body density

$$\rho(\mathbf{r}, t) = \sum_{i,\sigma} \big| \phi_i(x, t) \big|^2$$

Single-particle Hamiltonian

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✓ No empilical parameters: Input is an EDF only

✓ Sucessfully applied:

- Giant resonances (linear response, RPA)
- Heavy ion reactions (fusion, transfer, quasi-fission, fission, ...)

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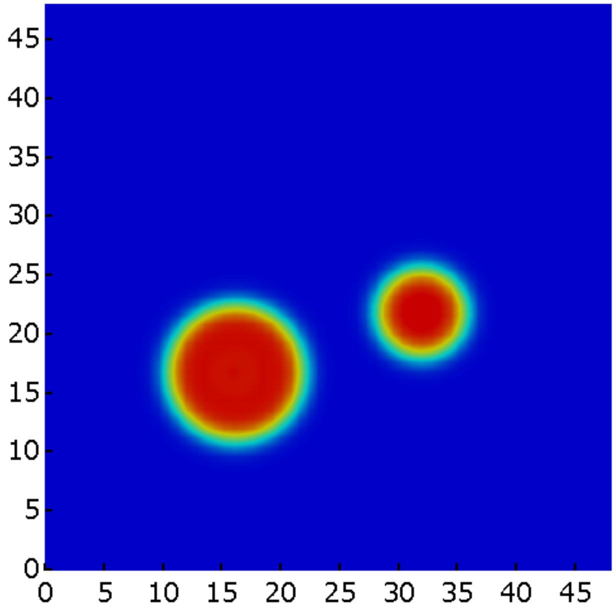
Ex. 1: Multi-nucleon transfer (MNT) reaction

^{40}Ca+^{124}Sn at E_{lab}=170 MeV, b=3.96 fm



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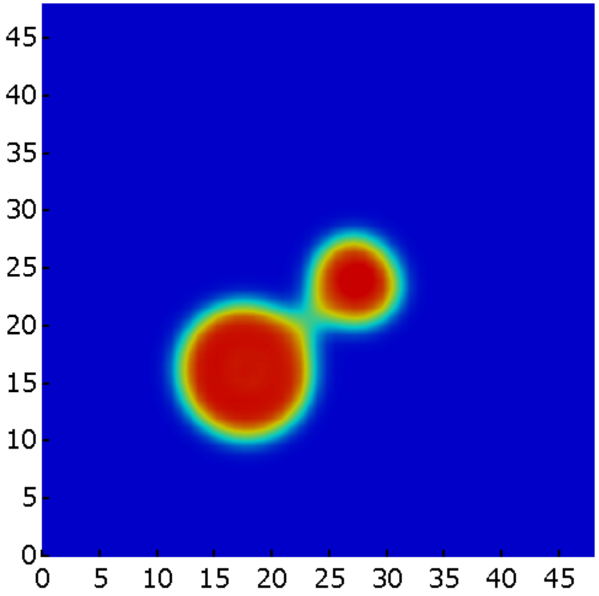

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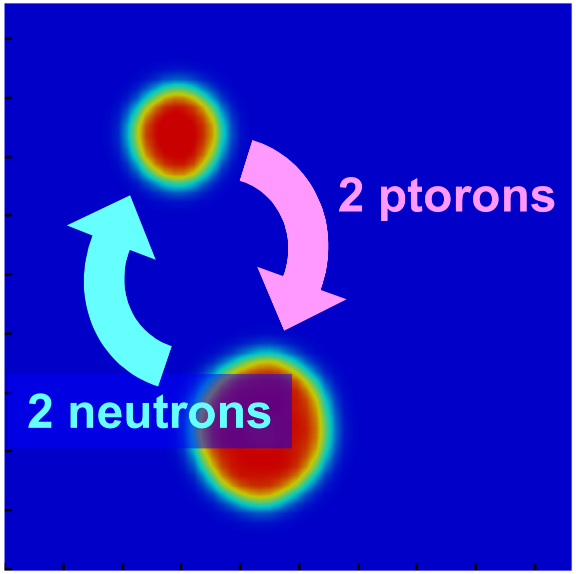

✓ At most 2 neutrons/protons were transferred on average

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PNP: C. Simenel, PRL**105**(2010)192701

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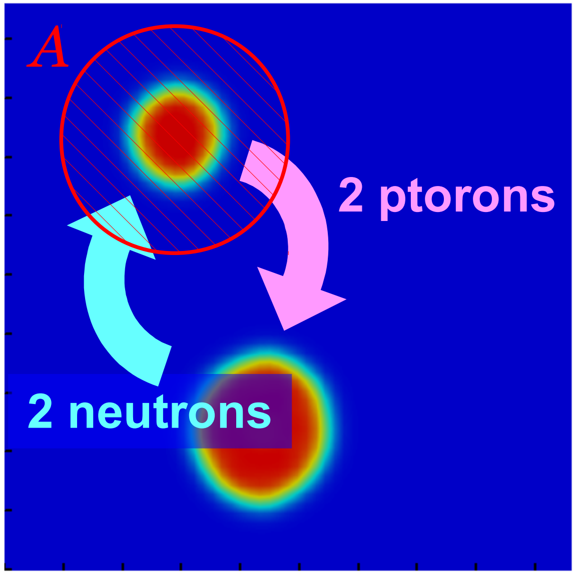

✓ At most 2 neutrons/protons were transferred on average

✓ Particle-number projection technique can be applied:

- Probability: *n* nucleons are inside the volume *A*

$$P_n = \langle\Phi|\hat{P}_n|\Phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{in\theta}\det\{\langle\phi_i|\phi_j\rangle_B + e^{-i\theta}\langle\phi_i|\phi_j\rangle_A\}$$

$$\hat{P}_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta\;\; e^{i(n-\hat{N}_A)\theta}$$: Particle-number projection op.

- Cross section for a nucleus containing *N*, *Z* nucleons

$$\sigma_{N,Z} = 2\pi\int db\; b\, P_N(b)P_Z(b)$$

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K.S., K.Yabana, PRC**88**(2013)064614

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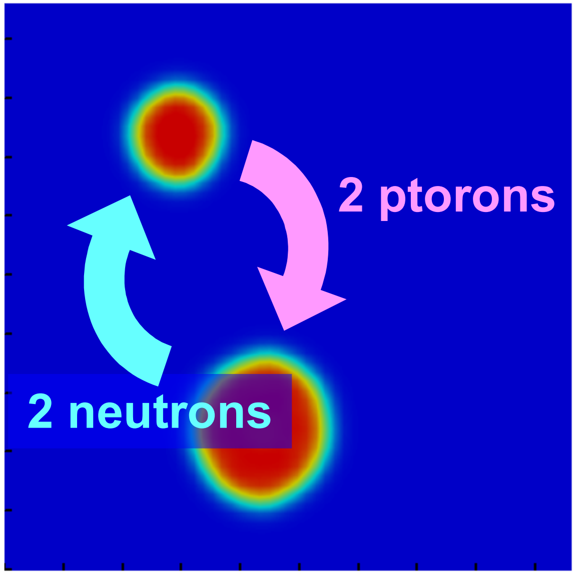

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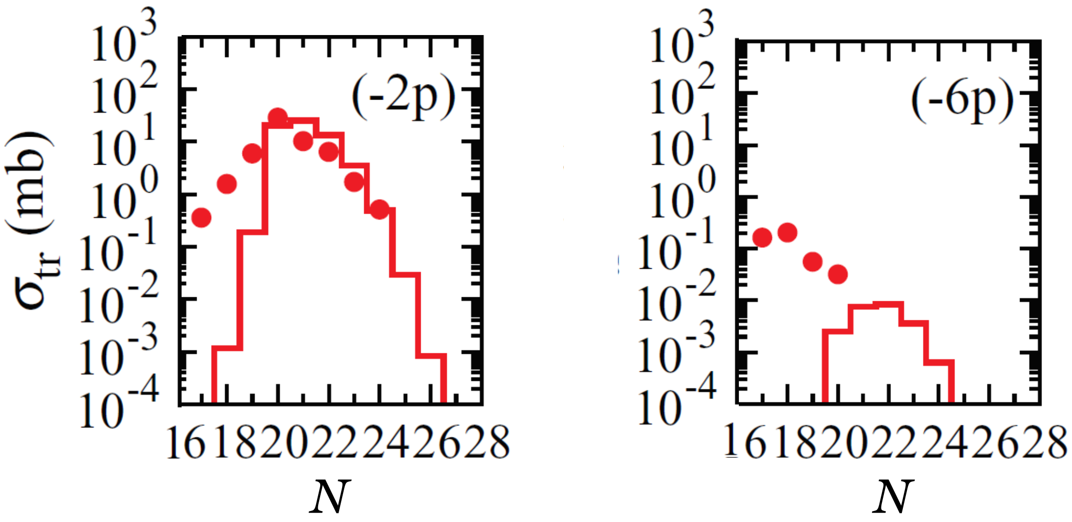
✓ Result:
- Reasonable description alound the average
- Underestimate many-nucleon transfer channels



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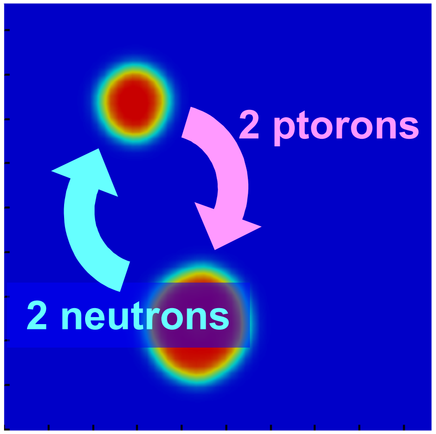

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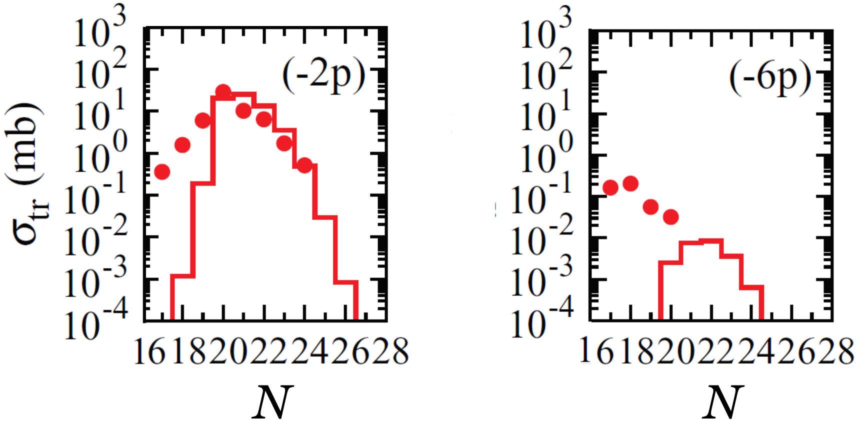

✓ Possible reason: We don't have a mean-field for 6-proton transfer channel

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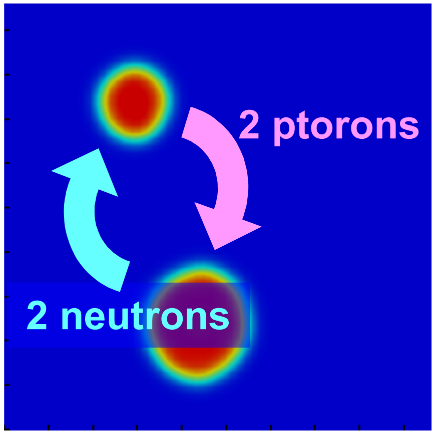

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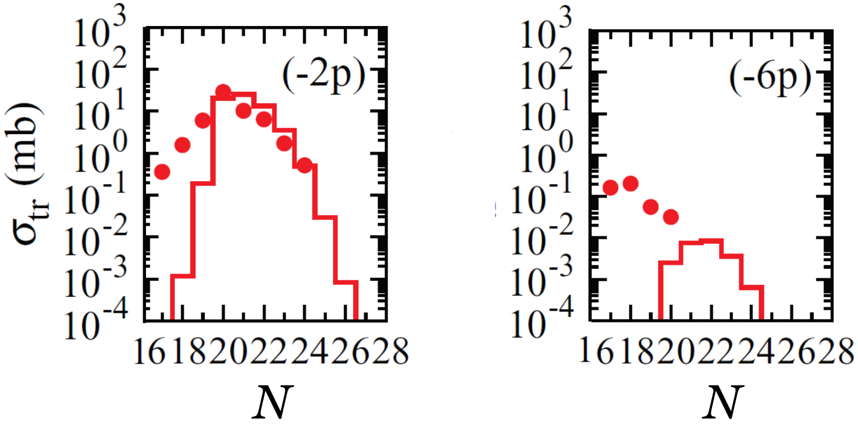

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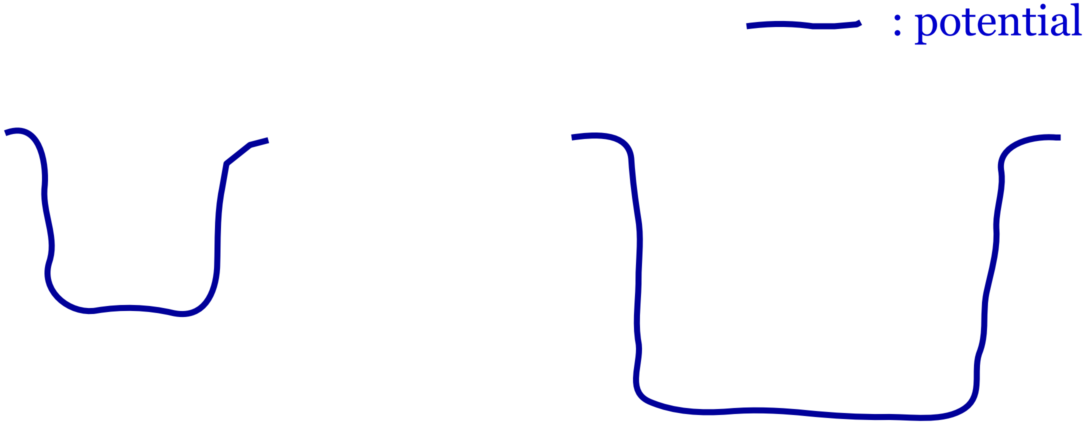
Naive picture



: potential for neutrons

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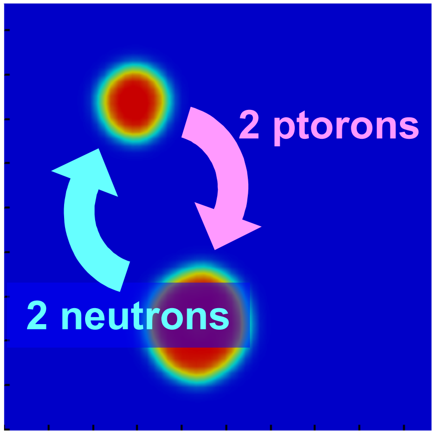

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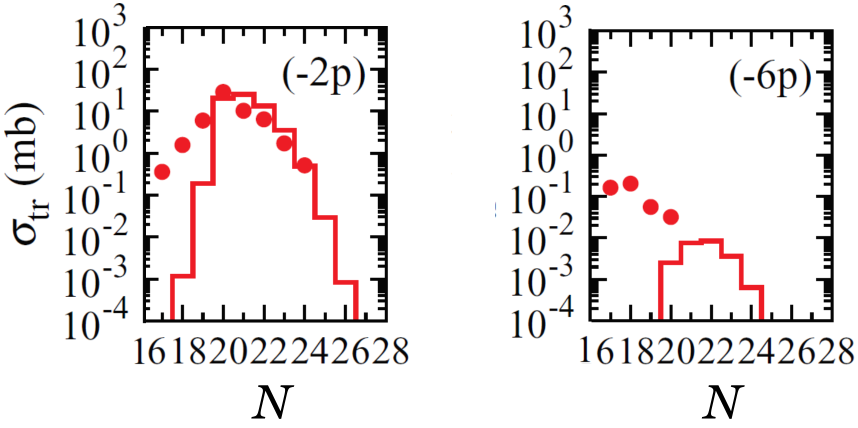

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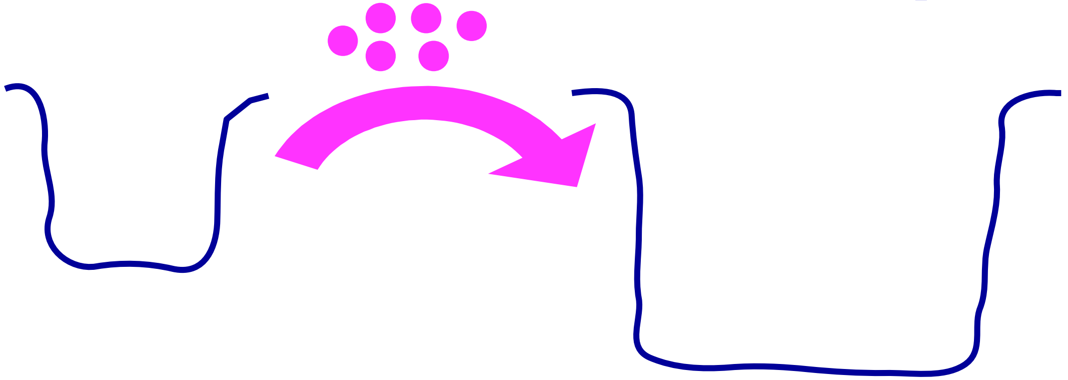

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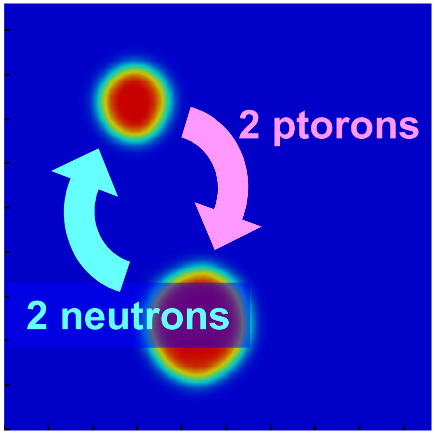

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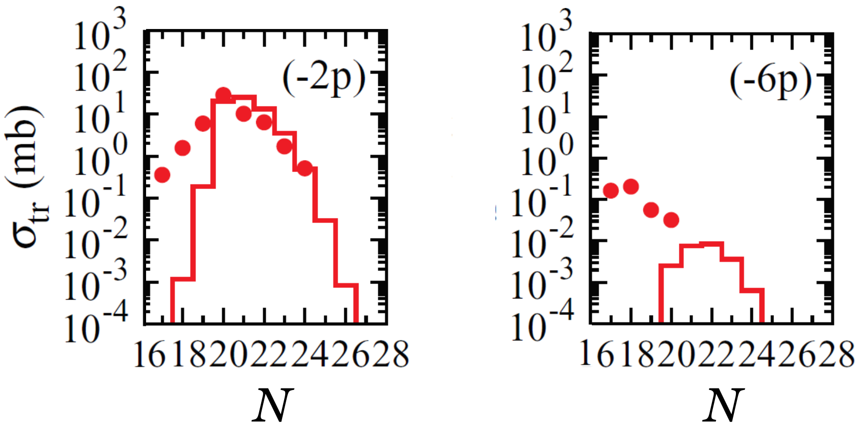

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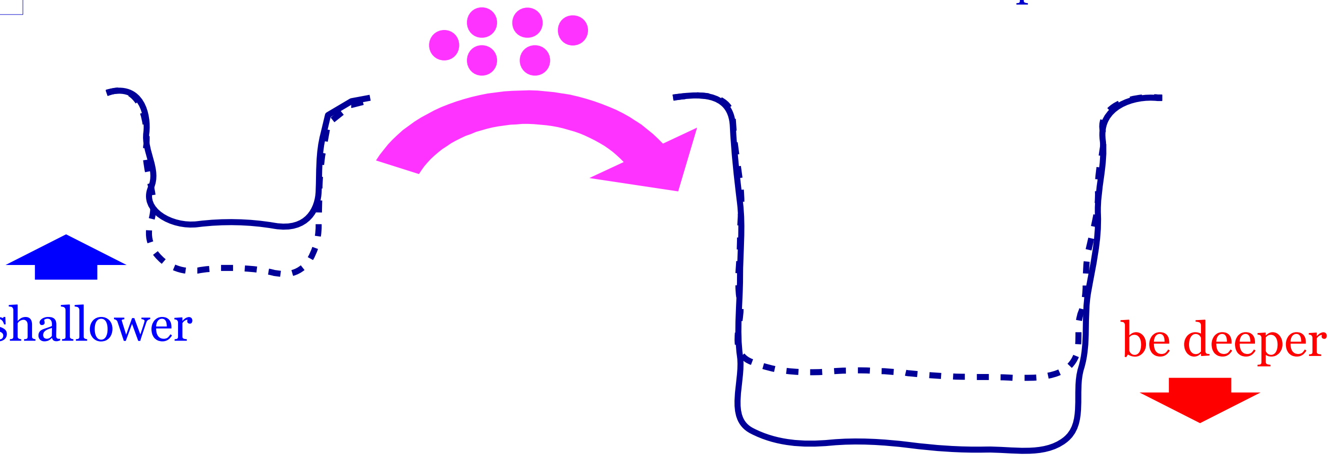

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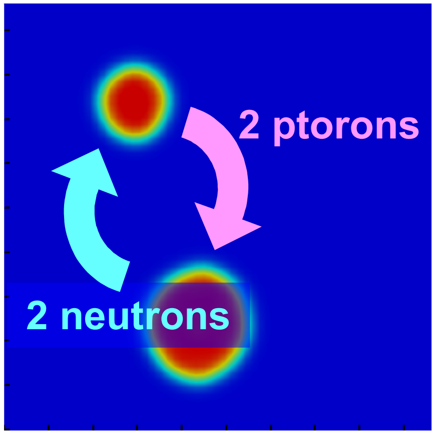

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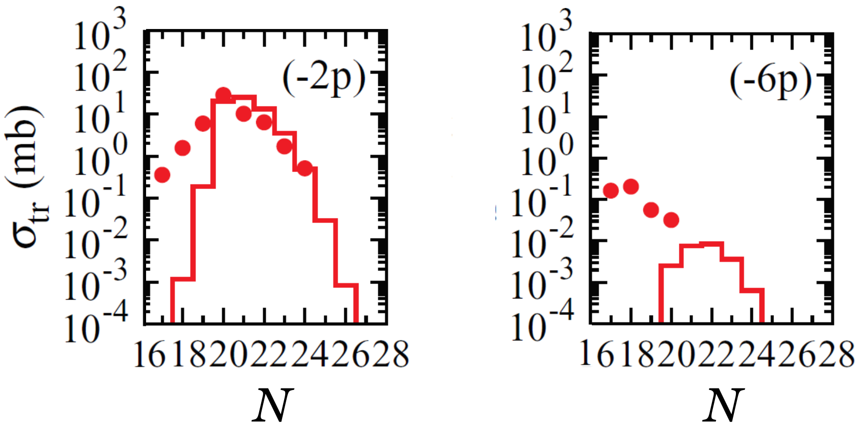

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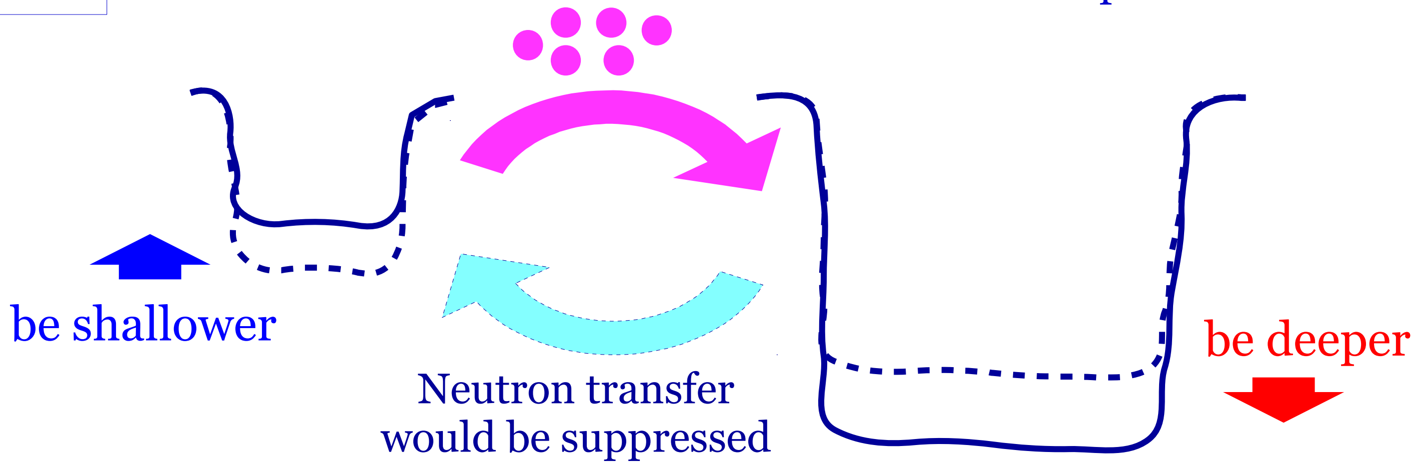

be shallower

Neutron transfer would be suppressed

be deeper

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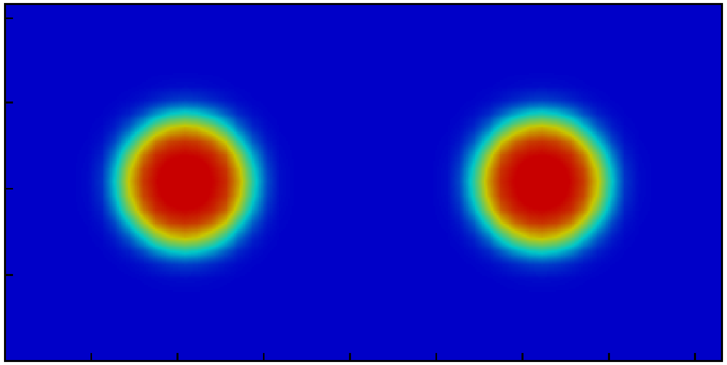
- Subbarrier fusion: Absence of quantum tunneling of the many-body wavefunction
- SHE synthesis:

Ex. 2: Subbarrier fusion

^{40}Ca+^{40}Ca at $E_{\mathrm{c.m.}}$=64 MeV <V_{B}



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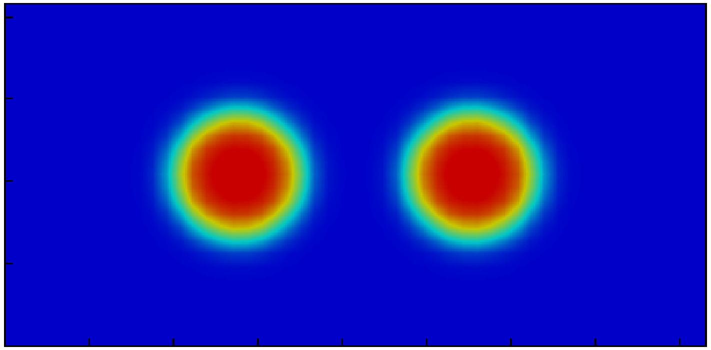

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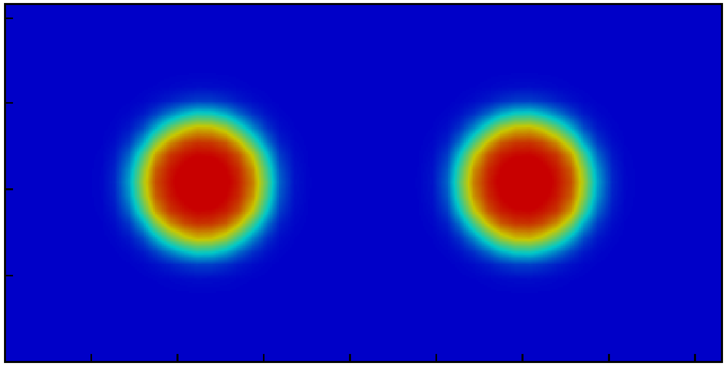

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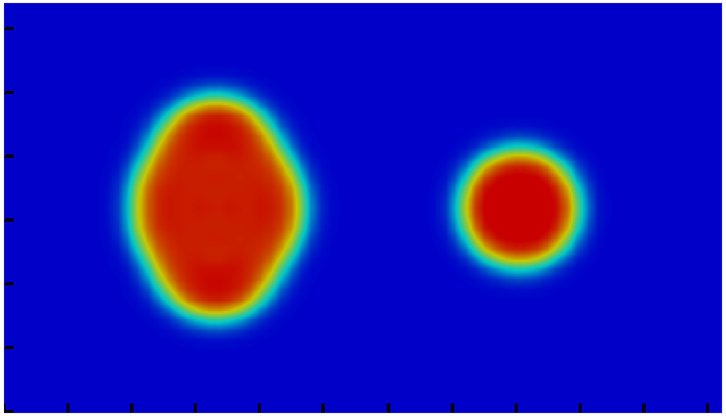
^{64}Ni+^{238}U ⟶ ^{302}120 ? (E_{lab}=428 MeV, b=0 fm)



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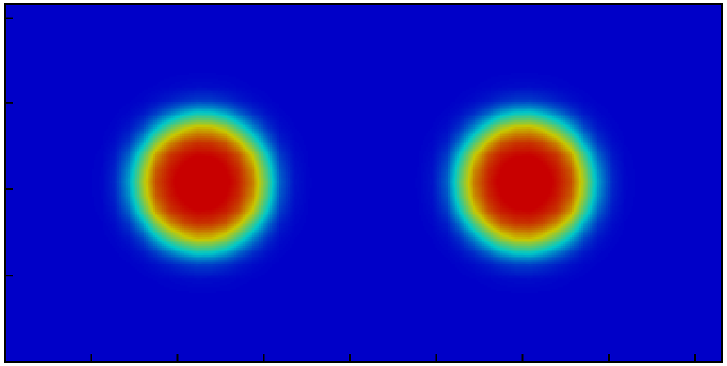

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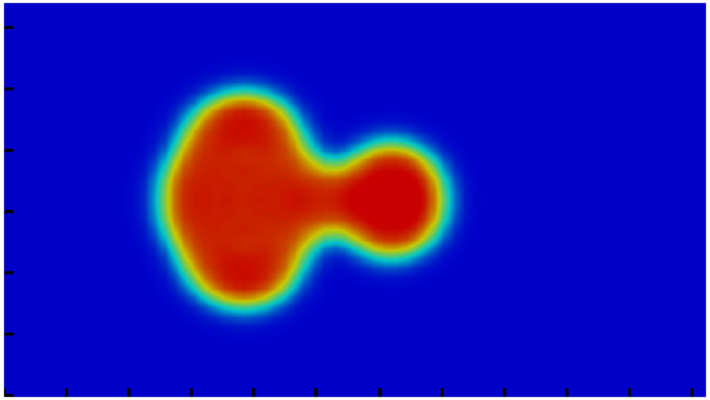

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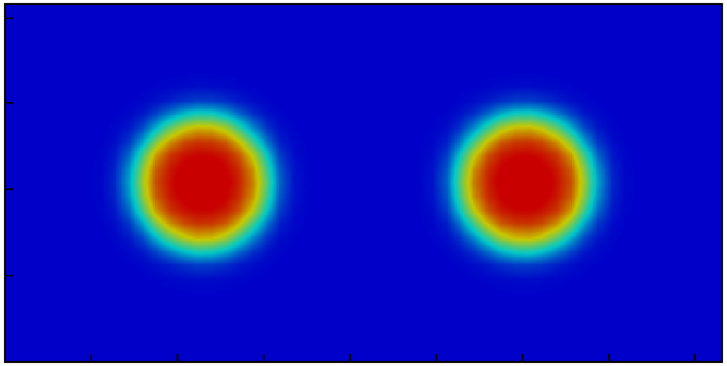

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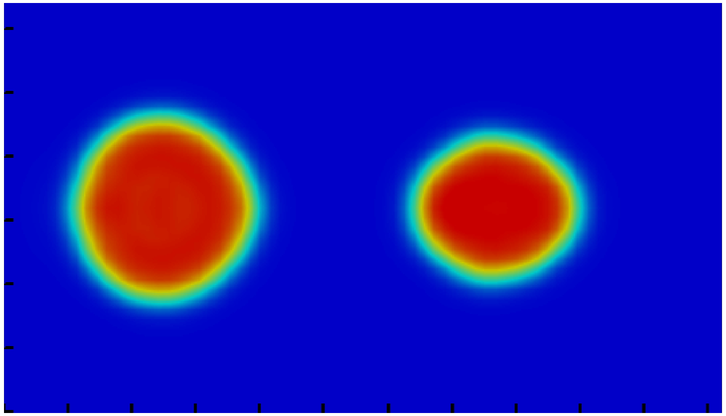

✓ In this case P_{fusion}=0, but we would also like to have a tiny, finite fusion probability

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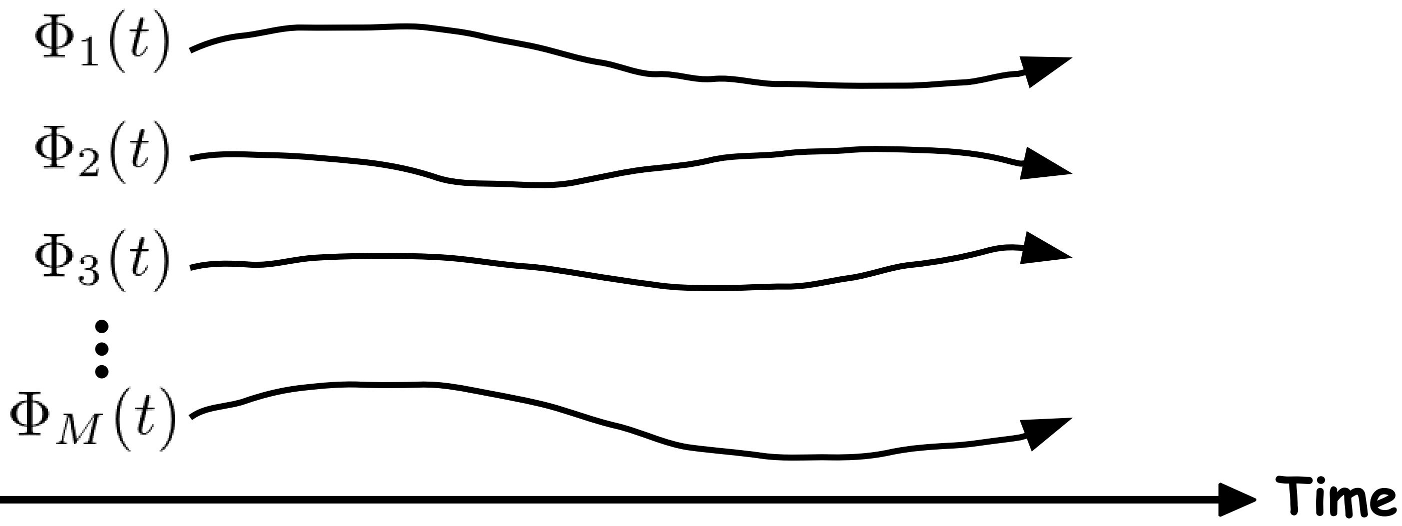

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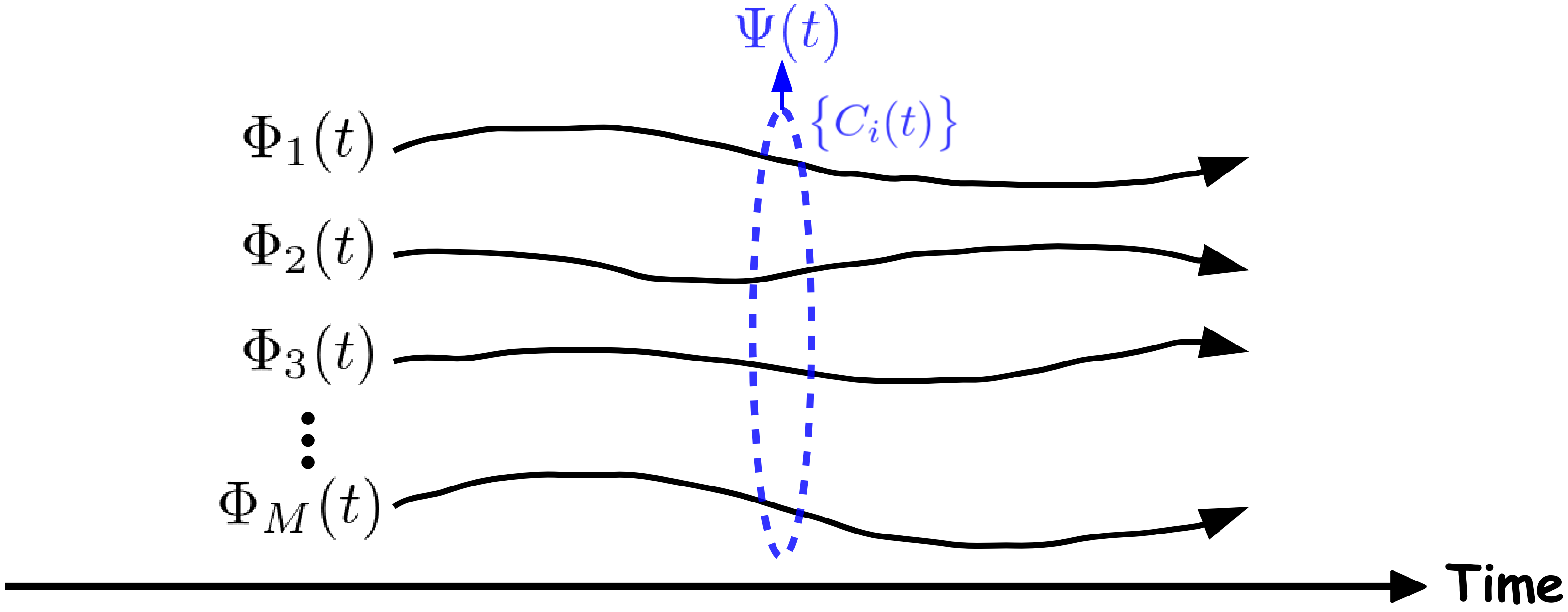

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$\Psi(t) = \sum_i C_i(t)\, \Phi_i(t)$: Multi-Slater-determinant

"MR-TDEDF": Equation for the coefficients $C_i(t)$

Action to be minimized:

$$\Psi(t) = \sum_i C_i(t)\,\Phi_i(t)$$: **Multi-Slater-determinant**

$$S = \int_{t_1}^{t_2} dt\ \big\langle \Psi(t) \big| i\hbar\partial_t - \hat{H} \big| \Psi(t) \big\rangle$$

$$= \int_{t_1}^{t_2} dt \sum_{ij} C_i^*(t) \big\langle \Phi_i(t) \big| \Big(i\hbar\, \dot{C}_j(t) \big| \Phi_j(t) \big\rangle + i\hbar\, C_j(t) \partial_t \big| \Phi_j(t) \big\rangle - C_j(t) \hat{H} \big| \Phi_j(t) \big\rangle \Big)$$

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$$= \int_{t_1}^{t_2} dt \sum_{ij} C_i^*(t) \Big(i\hbar\,\dot{C}_j(t) \underline{\mathcal{N}_{ij}(t)} + C_j(t) \underline{\mathcal{A}_{ij}(t)} - C_j(t) \underline{\mathcal{H}_{ij}(t)} \Big)$$

Norm kernel

$$\mathcal{N}_{ij}(t) = \big\langle \Phi_i(t) \big| \Phi_j(t) \big\rangle$$

A transition matrix

$$\mathcal{A}_{ij}(t) = \big\langle \Phi_i(t) \big| i\hbar\partial_t \big| \Phi_j(t) \big\rangle$$
$$= \det\Big\{ \langle \phi_k^{(i)}(t) \big| \hat{h}^{(j)}(t) \big| \phi_l^{(j)}(t) \rangle \Big\}$$

Interaction kernel

$$\mathcal{H}_{ij}(t) = \big\langle \Phi_i(t) \big| \hat{H} \big| \Phi_j(t) \big\rangle$$

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Interaction kernel

$$\mathcal{H}_{ij}(t) = \big\langle \Phi_i(t) \big| \hat{H} \big| \Phi_j(t) \big\rangle$$

Variation $\dfrac{\delta S}{\delta C_i^*(t)} = 0$ leads to:

Equation for the coefficients $\{C_i(t)\}$

$$i\hbar\, \mathcal{N}(t)\, \dot{\mathcal{C}}(t) = \Big(\mathcal{H}(t) - \mathcal{A}(t) \Big) \mathcal{C}(t)$$

where

$$\mathcal{C}(t) \equiv \begin{pmatrix} C_1(t) \\ C_2(t) \\ \vdots \\ C_M(t) \end{pmatrix}$$

Outline

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Ideas: MR-TDEDF for MNT reaction

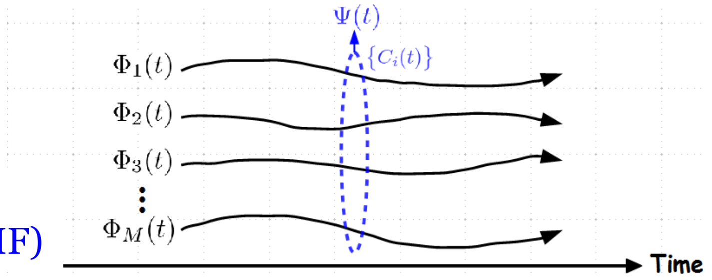
Ex. 1: MNT

Choise of $\Phi_i(t)$?

$$\Psi(t) = \sum_i \boxed{C_i(t)}\,\boxed{\Phi_i(t)}$$

Determined by variation

Calculated by SR-TDEDF (TDHF)



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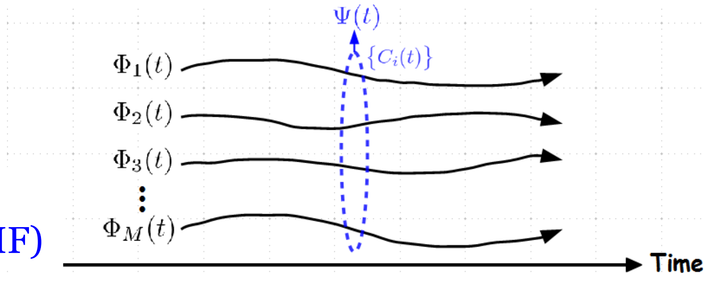
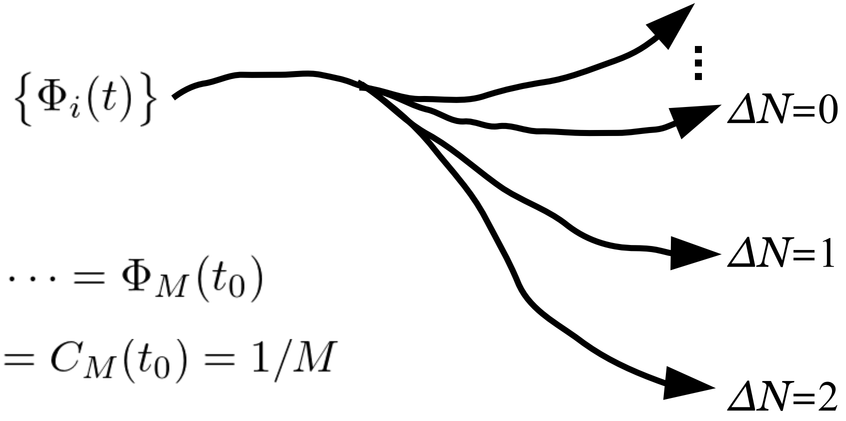


① Transfer-constrained SR-TDEDF (TDHF)

C. Simenel, J. Phys. G **41**(2014)094007

$$S' = \int_{t_1}^{t_2} dt\ \langle \Phi(t) | i\hbar\partial_t - \hat{H} - \lambda \hat{N}_A | \Phi(t) \rangle$$



$$\Phi_1(t_0) = \Phi_2(t_0) = \cdots = \Phi_M(t_0)$$

$$C_1(t_0) = C_2(t_0) = \cdots = C_M(t_0) = 1/M$$

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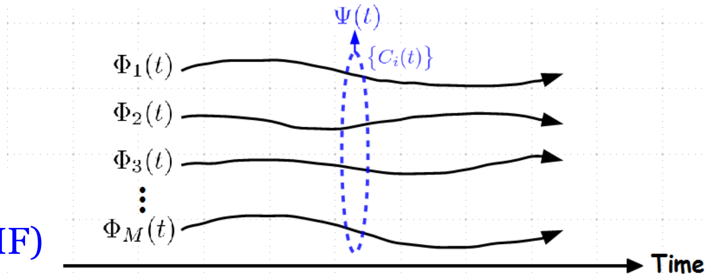

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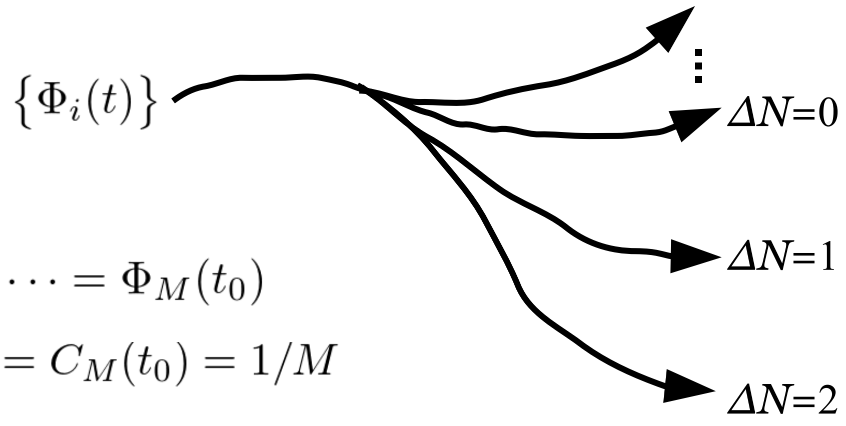

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---

② Use different projectile / target combinations

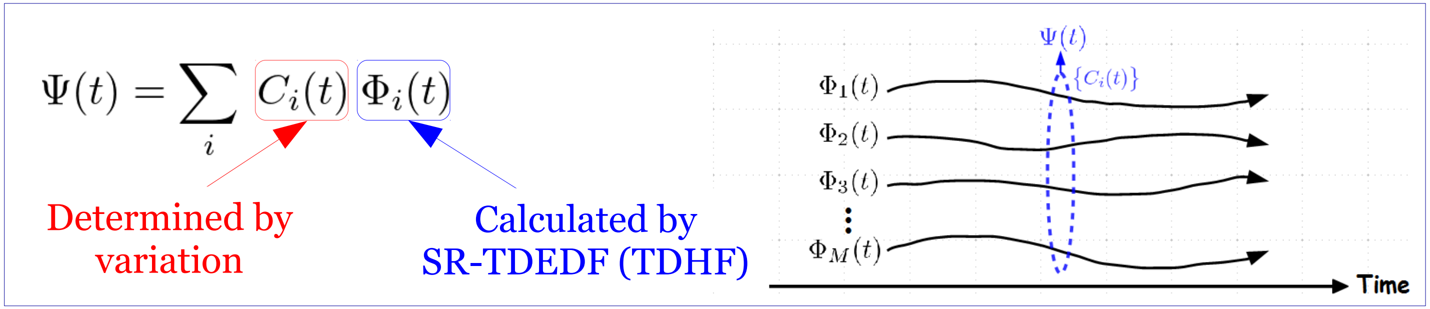
$\Phi_1(t)$ = ^{40}Ca+^{124}Sn , $\Phi_2(t)$ = ^{42}Ca+^{122}Sn , $\Phi_3(t)$ = ^{18}Ar+^{126}Te , ···

$$C_1(t_0) = 1 \qquad C_{i\neq 1}(t_0) = 0$$

Ideas: MR-TDEDF for subbarrier fusion / SHE synthesis

Ex. 2: Subbarrier fusion

Choise of $\Phi_i(t)$?

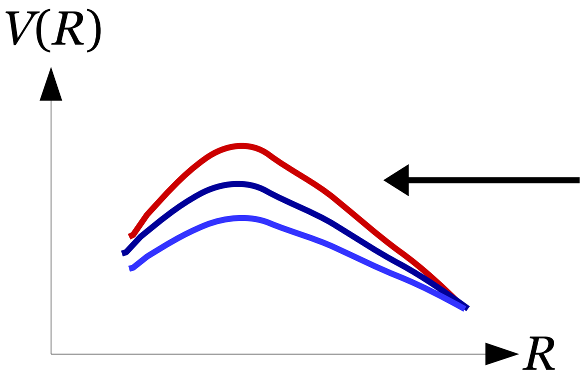


$$\Psi(t) = \sum_i \boxed{C_i(t)}\,\boxed{\Phi_i(t)}$$

Determined by variation

Calculated by SR-TDEDF (TDHF)

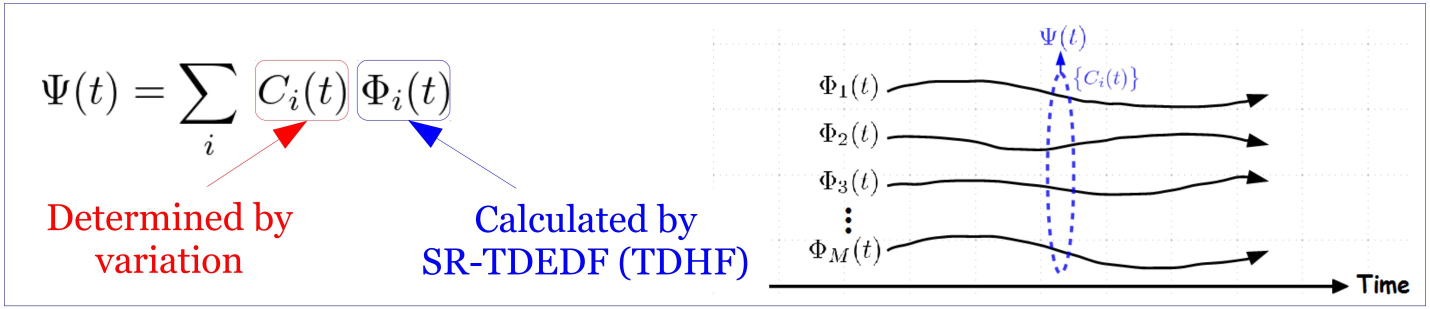
① Modify the nucleus-nucleus potential



Ideas: MR-TDEDF for subbarrier fusion / SHE synthesis

Ex. 2: Subbarrier fusion

Choise of $\Phi_i(t)$?



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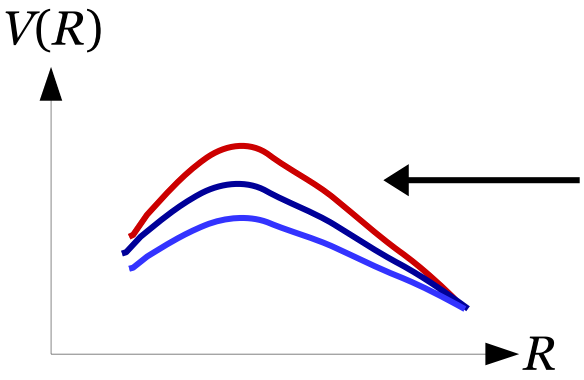
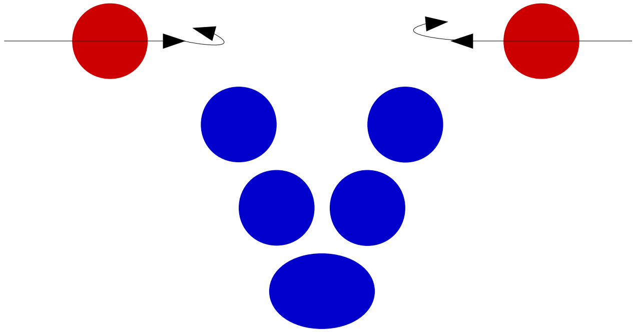


② Put static solutions in addition to SR-TDEDF



$\Phi_1(t)$: SR-TDEDF

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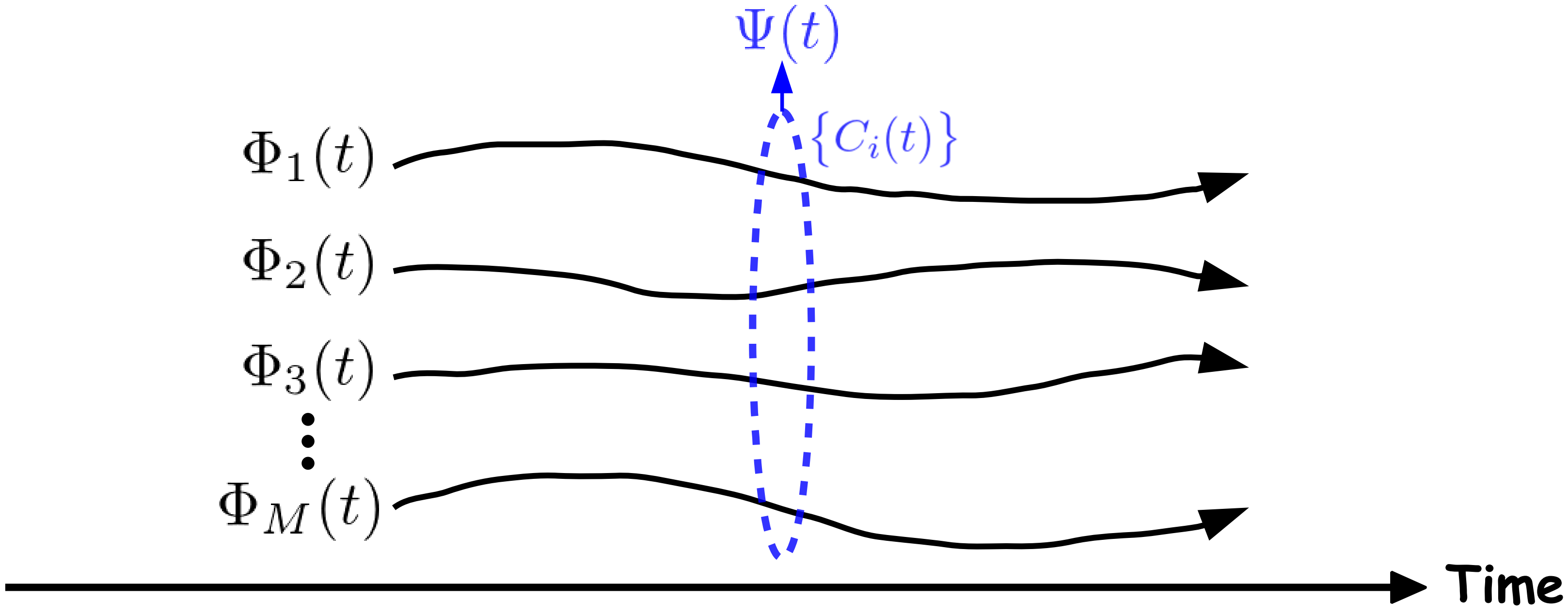

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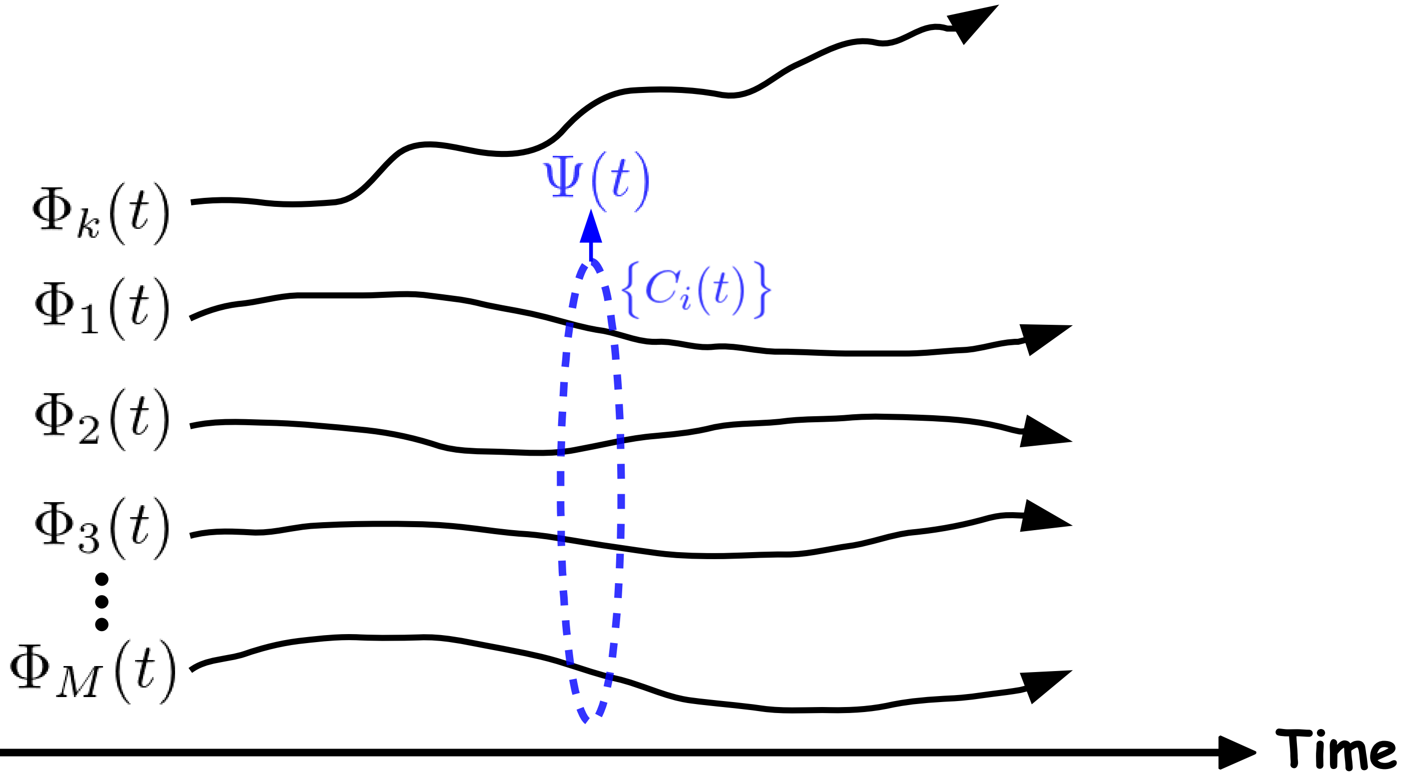

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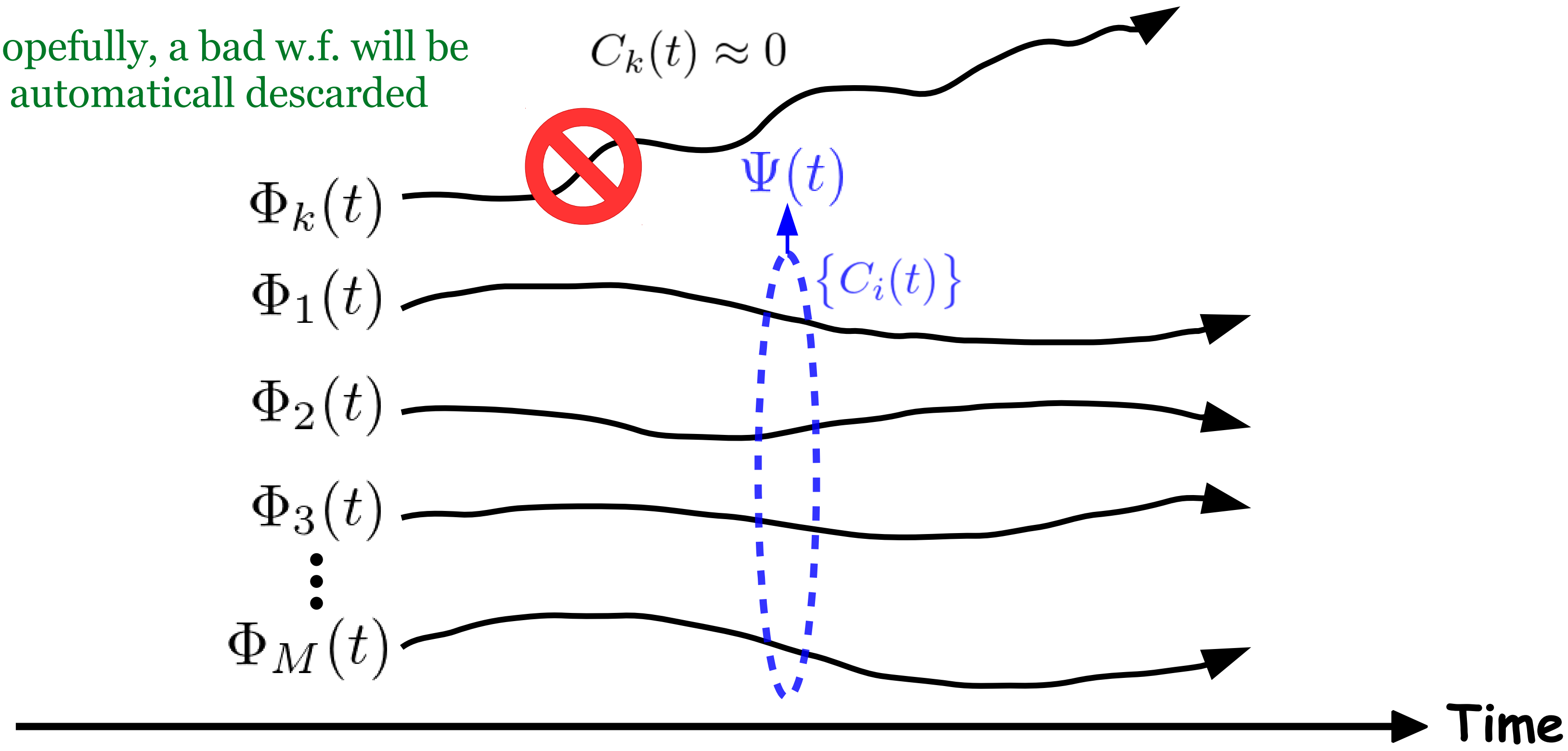

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Calculated by
SR-TDEDF (TDHF)

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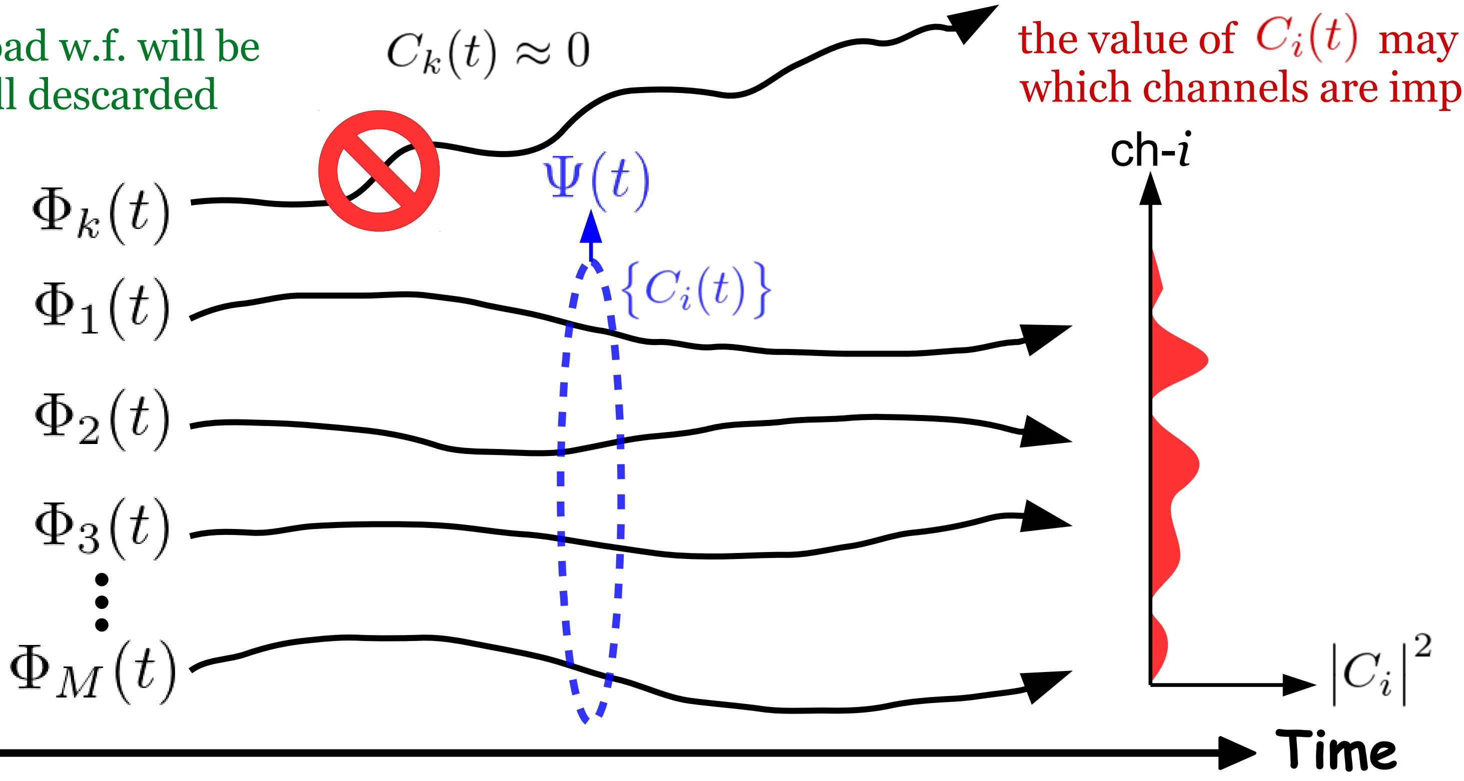
the value of $C_i(t)$ may tell us
which channels are important



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We have considered a possible use of the multi-Slater-determinant:

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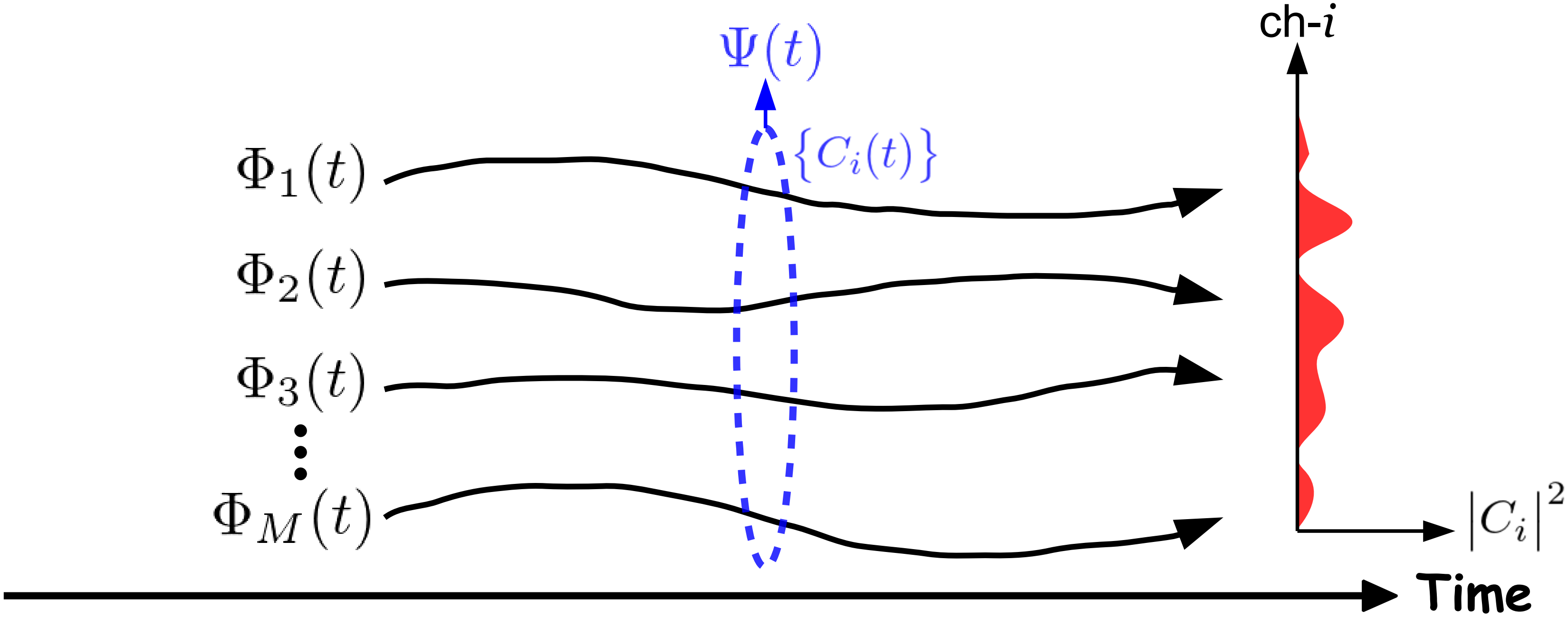
Although there are many practical problems, we can try it in the near future!



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Thank you for your attention.