Time-dependent Basis Function Approach to Nuclear Scattering

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<u>Outline</u>

- Background and motivation
- Methodology
 - Test case: deuteron dissociation due to Coulomb field
- Conclusion and outlook

Basis Functions in Ab initio Shell Model

 Traditionally basis function approach has been widely used in *ab initio* shell model

 $H|\psi\rangle = E|\psi\rangle$

- By choosing a basis, one casts the quantum manybody problem into the eigenvalue problem of the Hamiltonian matrix
- Eigenvalues mass spectrum
- Eigenvectors → wavefunctions
- See Many Fermion Dynamics nuclear physics (MFDn) for a well-established implementation

P. Maris, M. Sosonkina, J.P. Vary, E.G. Ng and C. Yang, ICCS 2010, Procedia Computer Science 1, 97(2010).

Motivation for Time-dependent Extension

- Technological advances in supercomputing make solving time-dependent Schrödinger equation within reach
 - Moore's law
 - It's time to development approach for the future
- Higher precision results from more differential measurements available due to progress in experimental nuclear physics
- More in-detail and more precise nonperturbative study of the dynamics in nuclear scattering is needed, esp. for strong/time-dependent fields

Example: d+124Sn

• In the lab-frame:

[Ou Li et al, PRL 115, 212501 (2015)]



- Physical motivation: study EoS of nuclear matter, esp. symmetry energy term
- Relative momentum between n and p in the final state is affected by the symmetry energy term in the target nuclear potential
- Quantum Molecular Dynamics (QMD) simulation results available
- Experimentally measurable (at RIKEN)

In Deuteron Center-of-Mass Frame



- The target approaches the projectile and the classical background field is time-dependent
- Trajectory is estimated by QMD calculation
- Background potential is obtained by Skyrme energy density functional approach

Time-dependent Basis Function



- Natural extension of *ab initio* method to time-dependent regime
- Handle background fields explicitly depending on time
- Amplitude level -> quantum interference effects
- Non-perturbative -> strong field physics
- "Snapshots" of the system under investigation
- Take the advantage of high-performance supercomputing

tBF vs tBLFQ

[Zhao, Ilderton, Maris, Vary, PRD 88, 035205 (2013)]

- tBF: time-dependent Basis Function
 - For low-energy quantum mechanics
- tBLFQ: time-dependent Basis Light-front Quantization
 - For relativistic quantum field theory



- tBLFQ uses the Hamiltonian of quantum field theory

 Relativity is naturally built-in
- tBLFQ basis consists of multiple Fock sectors such as

 $|e\downarrow p\rangle = a|e\rangle + b|e\gamma\rangle + c|e\gamma\gamma\rangle + d|eee\rangle + \dots$

<u>Application to Strong QED:</u> Nonlinear Compton Scattering

- $e + n\gamma(laser) \rightarrow e' + \gamma'$
- 10²⁰ photons in a laser: model as background field
- Perturbation theory:
- $\sigma \propto \text{Klein-Nishina} \times \tilde{A}^2$
- At high intensity: non-perturbative treatment needed



Setup for Nonlinear Compton Scattering

• Space-time structure



[Zhao, Ilderton, Maris, Vary, PRD 88, 035205 (2013)] • Two effects: acceleration and radiation

<u>Advantages</u>

- "Snapshots" of the nucleon systems, revealing nuclear dynamics in real time
- Quantum interference is kept during time-evolution
- Study nucleon systems in strong/time-dependent background field
- Nonperturbative effects
- Close connection to light-front quantum field theory -> systematically expandable to quantum field theory treatment

Time-dependent Basis Function Approach

- BLFQ: for quantum field eigenspectrum
- tBLFQ: for quantum field evolution



- Real-time framework: BLFQ ⇒ tBLFQ
- tBLFQ is designed for:
 - time-dependence in dynamical processes
 - in strong/time-dependent background field

General Procedure for tBF

- 1. Write down the Hamiltonian
- 2. Adopt the interaction picture
- 3. Prepare the initial ('in') state
- 4. Evolve the initial state until the background field subsides
- Project the scattering final state onto 'out' states (constructed out of QED eigenstates) and obtain Smatrix element

$$S = \downarrow I (out | Texp(-i \int -\infty \uparrow \infty \blacksquare V \downarrow I) | in) \downarrow I$$

Test Case: Deuteron Dissociation in Coulomb Field



The Coulomb field is due to a passing-by heavy-ion with constant velocity vApproximation: we neglect the center-of-mass motion of the deuteron R; we are interested in the relative motion between p and n only r.

Coordinate System



$$\vec{R} = \frac{\vec{r_p} + \vec{r_n}}{2}$$
 $\vec{r} = \vec{r_p} - \vec{r_n}$

15

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<u>Hamiltonian</u>

 $H_{Full} = H_0 + V_{int}$ $H_0 = KE + V_{QCD}$ $V_{int}(t) = \int A_{\mu} J^{\mu} d\vec{r}$

H_{Full}: total Hamiltonian

H₀: (time-independent) Hamiltonian for deuteron

V_{int}: (time-dependent) interaction between the heavy-ion and deuteron

KE: we keep the kinetic energy of relative motion only V_{QCD}: nucleon-nucleon interaction

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Neutron-Proton Stationary States

- In interaction picture, time evolution is computed in the basis formed by the eigenstates of H₀
- The background field V_{int} induces transitions among the "tower" of eigenstates of H_0
- We need to solve the eigenvalue problem of H₀ and get a "tower" of eigenstates

 $H\downarrow 0 |\psi\rangle = E |\psi\rangle$

• We take V_{QCD} to be JISP16 NN interaction

[A. M. Shirokov et al, PLB 644, 33 (2007)]

19

Deuteron and Its Excitation Spectrum

- As test problem, we retain 3 channels: $({}^{3}S_{1}, {}^{3}D_{1}) {}^{3}P_{0} {}^{3}P_{1}$
- Deuteron has one bound state ground state, all the excited states are scattering states in continuum; we regulate the scattering states by putting the deuteron system in a HO trap with ω=5MeV



Background Field

• We neglect magnetic interaction and keep only electric interaction

$$\begin{aligned} V_{int}(t) &= \int A_{\mu} J^{\mu} d\vec{r} \\ &= \int \rho(\vec{r},t) \varphi(\vec{r},t) d\vec{r} - \int \vec{j}(\vec{r},t) \cdot \vec{A}(\vec{r},t) d\vec{r} \end{aligned}$$

• We perform multipole expansion on Coulomb field

$$\varphi(\vec{x},t) = \frac{Ze}{|\vec{x} - \vec{R}_Z(t)|}$$
$$= Ze \sum_{\lambda\mu} \frac{4\pi}{2\lambda + 1} Y^*_{\lambda\mu} \left(\hat{R}_Z(t)\right) Y_{\lambda\mu}(\hat{x}) \frac{x^{\lambda}}{R_Z^{\lambda+1}(t)}$$

 $R \downarrow Z(t) = b + v t$ is the location of the source

Same time-dependence for same λ

E1 Transitions

• Since $R \downarrow Z \gg x$, we consider E1 transitions onl $V_{int}(1\mu; t) = \frac{4\pi}{3} Ze^2 \sum_{\mu=-1}^{+1} \frac{Y_{1\mu}^*(\hat{R}_Z(t))}{R_Z^2(t)} r_p Y_{1\mu}(\hat{r}_p)$

- E1 transitions shi^{f_1} ^{j_1} D_1 ^{j_1} D_1 A_2 P_0 A_2
- Since we include $ch_{^{3}P_{0}} \rightarrow \uparrow (\overset{^{1}}{}_{S_{1}}, \overset{^{3}}{}_{D_{1}}) \rightarrow \downarrow \overset{^{1}}{\underset{P_{1}}{\overset{\bullet}}} r_{^{3}P_{1}} attern:$

• In interaction/pietur@exp(-iH40 t)



E1 Transition Matrix Elements

$$V_{I;jk}(E1; t) = \frac{4\pi}{3} Ze^2 e^{i\left(\frac{E_j - E_k}{2}\right)t} \sum_{\mu} \frac{Y_{1\mu}^*(\hat{R}(t))}{|R(t)|^2} \int d\vec{r} \ \psi_j^*(\vec{r}) \ \frac{r}{2} \ Y_{1\mu}(\vec{r})\psi_k(\vec{r})$$

$$|\vec{l}| = \begin{bmatrix} 1st; (^3S_1, ^3D_1); M_j = -1 \\ 1st; (^3S_1, ^3D_1); M_j = 0 \\ 1st; (^3S_1, ^3D_1); M_j = +1 \end{bmatrix} E^{=0.65289 \text{ MeV}} Z = 50$$

$$|\vec{l}| = \begin{bmatrix} 1st; (^3S_1, ^3D_1); M_j = -1 \\ 1st; (^3P_0; M_j = 0 \\ 1st; (^3P_1; M_j = -1 \\ 1st; (^3P_1; M_j = +1 \end{bmatrix} E^{=12.0733 \text{ MeV}} b = 7.5 fm$$

$$|t| = 12.7585 \text{ MeV} \qquad \alpha = 1/137.044$$

$$jV \downarrow I(t=0)i =$$

	(0	0	0	-0.000738817	0.00135126	-0.00135126	ο.
		0	0	0	-0.000738817	0.00135126	0.	-0.00135126
		0	0	0	-0.000738817	ο.	0.00135126	-0.00135126
		0.000738817	-0.000738817	0.000738817	0	0	0	0
		0.00135126	-0.00135126	0.	0	0	0	0
		0.00135126	0.	-0.00135126	0	0	0	0
	l	0.	0.00135126	-0.00135126	0	0	0	0

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 $S = \downarrow I \langle out | Texp(-i \int -\infty \uparrow \infty \blacksquare V \downarrow I) | in \rangle \downarrow I$

Choosing Initial State

- Initial state can be chosen according to experimental setup
- Our choice:

• At RIKEN, polarized deuteron beams are available

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Solve Time-dependent Schrödinger Equation

• Time-dependent Schrödinger equation in interaction picture

 $id/dt |\psi(t)\rangle \downarrow I = V \downarrow I(t) |\psi(t)\rangle \downarrow I$

• Formal solution:

 $|\psi(t)\rangle \downarrow I = Texp(-i\int -\infty \uparrow \infty \blacksquare V \downarrow I) |\psi(-\infty)\rangle \\ \downarrow I$

Euler vs MSD Method

Euler:

$$T \quad exp\left[-i\frac{1}{\hbar}\int_0^t V_I(t) \ dt\right] \quad \xrightarrow{\sum \delta t} \quad \left[1 - \frac{i}{\hbar}V_I(t_n)\delta t\right] \left[1 - \frac{i}{\hbar}V_I(t_{n-1})\delta t\right] \ \cdots \ \left[1 - \frac{i}{\hbar}V_I(t_1)\delta t\right]$$

Multi-step differencing (MSD):

$$|\psi, t + \delta t >_I \approx |\psi, t - \delta t >_I - \frac{2i}{\hbar} V_I(t) \, \delta t \, |\psi, t >_I$$

We employ MSD2 for better numerical stability compared to Euler method, since MSD is accurate up to $(V \downarrow I \, \delta t) \, f_2$ while Euler is up to $(V \downarrow I \, \delta t) \, f_1$

Higher order MSDs such as MSD4 or MSD6 are available

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First-Order Perturbation Theory

First-order perturbation theory:

$$\begin{aligned} |\psi; \ t >_{I} &= T_{+} \ exp\left[-i\frac{1}{\hbar} \int_{0}^{t} \ V_{I}(t) \ dt \right] \ |\psi; \ 0 >_{I} \\ &\rightarrow \left[1 - \frac{i}{\hbar} V_{I}(t_{n}) \delta t \right] \left[1 - \frac{i}{\hbar} V_{I}(t_{n-1}) \delta t \right] \ \cdots \ \left[1 - \frac{i}{\hbar} V_{I}(t_{1}) \delta t \right] \ |\psi; \ 0 >_{I} \\ &\rightarrow \left[1 - \frac{i}{\hbar} \delta t \Big(V_{I}(t_{n}) + V_{I}(t_{n-1}) + \cdots + V_{I}(t_{1}) \Big) \Big] |\psi; \ 0 >_{I} \end{aligned}$$

Parameters Used in Numerical Calculation

Z	=	50 (Sn)
b	=	7.5 fm
lpha	=	1/137.04
δT	=	$0.001 \ [MeV]^{-1}$
\mathcal{V} =	=0.1 <i>c</i>	



- Fluctuations are signatures of quantum virtual processes
- Long-term fully quantal treatment vs. classical treatment reveals net quantum effects (work in progress)
- Feeding to states forbidden by first-order perturbation theory



Transition rates diminish when the heavy ion is far way



0.00

T [MeV





$$2T = 10 \text{ MeV}^{-1}$$

$$M_{j} = +1 \text{ Initial State;}$$

$$7 \text{ states Evolution}$$

$$\binom{(^{3}S_{1},^{3}D_{1}); M_{j} = -1}{(^{3}S_{1},^{3}D_{1}); M_{j} = +1}$$

$$^{3}P_{0}; M_{j} = 0$$

$$^{3}P_{1}; M_{j} = -1$$

$$^{3}P_{1}; M_{j} = +1$$

$$= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$^{|\text{Amplitude}|^{2}}$$

$$^{0.0006}$$

$$^{0.0005}$$

$$^{-\text{ MSD2}}$$

0.000

0.000

0.000

-4

 $^{3}P_{0};M_{j}=0$

T [MeV







Dependence on Coupling Constant



As Z increases, transitions deviate from first-order perturbation theory

51 Level-System Evolution (In the 5MeV HO trap)



Initial State Preparation

$$\begin{pmatrix} 1st; ({}^{3}S_{1}, {}^{3}D_{1}); M_{j} = -1 \\ 1st; ({}^{3}S_{1}, {}^{3}D_{1}); M_{j} = 0 \\ 1st; ({}^{3}S_{1}, {}^{3}D_{1}); M_{j} = +1 \\ 2nd; ({}^{3}S_{1}, {}^{3}D_{1}); M_{j} = -1 \\ \vdots \\ 3rd; ({}^{3}S_{1}, {}^{3}D_{1}); M_{j} = +1 \\ 1st; {}^{3}P_{0}; M_{j} = 0 \\ \vdots \\ 3rd; {}^{3}P_{0}; M_{j} = 0 \\ 1st; {}^{3}P_{1}; M_{j} = -1 \\ \vdots \\ 3rd; {}^{3}P_{1}; M_{j} = +1 \\ 1st; ({}^{3}P_{2}, {}^{3}F_{2}); M_{j} = -2 \\ \vdots \\ 3rd; ({}^{3}P_{2}, {}^{3}F_{2}); M_{j} = +2 \\ 1st; {}^{3}D_{2}; M_{j} = -2 \\ \vdots \\ 3rd; {}^{3}D_{2}; M_{j} = +2 \end{pmatrix}$$



Tracking the SAME 7 states













51 states evolution;

Evolution of lowest levels in Extra

1. $({}^{3}P_{2}, {}^{3}F_{2})$ channel,

2. $^{3}D_{2}$ channel

Comment:

As the expansion of level system, deviation between MSD2 scheme and perturbation manifest.



<u>Conclusion</u>

- Time-dependent Basis Function (tBF) is motivated by progresses both in experimental nuclear physics and in supercomputing techniques
- tBF is an nonperturbative *ab initio* method for timedependent problems
- tBF is particularly suitable for strong-field problems
- tBF operates on the level of amplitude
- tBF will hopefully provide further insights into fundamental questions in a more detailed and more differential manner

<u>Outlook</u>

- Observables: phase-space distributions, differential cross sections
- Perform calculation in larger basis space and study convergence with respect to states in continuum
- Compare with classical treatments
- Study the effects of E0, M1, E2, M2... transitions
- Study the sensitivity with respect to different NN interactions, such as Daejeon16
- interactions, such as Daejeon16

 [A. M. Shirokov et al, PLB 761, 81 (2016)]
 Include strong force in the background field
- More realistic center-of-mass motion
 - Trajectory from QMD
 - Direct computation of cm motion (in future)

Thank you!

Ab initio Shell Model vs BLFQ

- Hamiltonian formalism
- Low-energy Nuclear Physics
- Quantum mechanics
- Nucleon degrees of freedom
- Nonrelativistic system
- Particle number is conserved
- Renormalization is tractable
- Galilean boost invariant
- Effective Hamiltonian: complicated

- Hamiltonian formalism
- Hadron Physics
- Quantum field theory
- Parton degrees of freedom
- Relativistic system
- Particle number is not conserved: multi-Fock sectors
- Renormalization is difficult: divergences beset
- Lorentz boost invariant
- Gauge theory: gauge symmetry
- Fundamental Hamiltonian

Light-front vs Equal-time Quantization



Kinematic Generators: P, J

<u>Common Variables in Light-front</u> <u>Dynamics</u>

- Light-front time
- Light-front Hamiltonian
- Longitudinal coordinate
- Longitudinal momentum
- Transverse coordinate
- Transverse momentum
- Equal-time dispersion relation
- Light-front dispersion relation

 $x^{+} = x^{0} + x^{3}$ $P^{-} = P^{0} - P^{3}$ $x^{-} = x^{0} - x^{3}$ $P^+ = P^0 + P^3$ $x^{\perp} = x^{1,2}$ $\boldsymbol{P}^{\perp} = \boldsymbol{P}^{1,2}$ $P^0 = \sqrt{m^2 + \vec{P}^2}$ $P^- = \frac{m^2 + P_\perp^2}{P^+}$

Basis Light-front Quantization

- Solve quantum field theory through eigenvalue problem of light-front Hamiltonian $P^-|\beta\rangle = P_{\beta}^-|\beta\rangle$
 - *P1* : light-front Hamiltonian
 - $|\beta\rangle$: light-front amplitude for mass eigenstates
 - $P\downarrow\beta\uparrow$: eigenvalue (light-front energy) for eigenstate
- Evaluate observables for eigenstate $|\beta\rangle$

 $O \equiv \left< \beta \right| \hat{O} \right| \beta \right>$

Example: Obtain LF QED Hamiltonian

- **QED Lagrangian** $\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\Psi}(i\gamma^{\mu}D_{\mu} m_{e})\Psi$
- Derived Light-front Hamiltonian

QED Hamiltonian in BLFQ Basis

• QED LF-Hamiltonian in a small basis: $|e\rangle + |e\gamma\rangle$, N_{max}=2, K=1.5



• Eigenstates: $|e\rangle_{phys} = 0.9998|e\rangle + 0.0210|e\gamma\rangle$ $|e\gamma\rangle_{scat} = -0.0210|e\rangle + 0.9998|e\gamma\rangle$