# Basis Generator Method Calculations for Ion-Atom Collisions of Relevance to Neutral Beams in Fusion Plasma


Tom Kirchner

YORK UNIVERSITÉ UNIVERSITY

redefine THE POSSIBLE.

# Prelude I: the past

Basis Generator Method (BGM) =
basis-expansion approach to time-dependent quantum problems

- General idea
  Lüdde et al, JPB **29**, 4423 (1996)
- Implemented and applied mostly to atomic collision problems
  - One-centre based description first
    Kroneisen et al, JPA **32**, 2141 (1999)
  - Followed by two-centre based description (TC-BGM)
    Zapukhlyak et al, JPB **38**, 2353 (2005)
  - Extended to molecules
    Lüdde et al, PRA **80**, 060702(R) (2009)
- Most calculations on few-electron systems

# Prelude II: the future

This CRP mostly deals with hydrogen beams

- Expand on previous work for *p*-H
  Keim et al, JPB **38**, 4045 (2005)
- Consider partially-stripped ions
  Schenk & TK, PRA **91**, 052712 (2015)
- Study atomic processes of neutral beams of He and Li
  Baxter & TK, PRA **93** (2016); TK et al, PRA **89** (2014), **...**

# Outline

1. Intro ✓
2. Theory I: (TC)-BGM
3. Examples of previous work I: the $p$-H system (and a bit more)
4. Theory II: the few-electron problem
5. Examples of previous work II: He (and a bit more)
6. Summary

## 2. Theory I: (TC)-BGM

# Basis expansion methods

Time-dependent Schrödinger equation (TDSE)

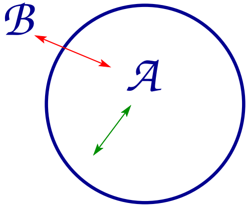
$$i\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

attacked via

$$|\psi(t)\rangle = \sum_{k=0}^{K} c_k(t)|\xi_k\rangle$$

basis expansion $=$ projection onto finite $\mathcal{A} \subset \mathcal{H}$

each state is coupled to complementary space via optical potential

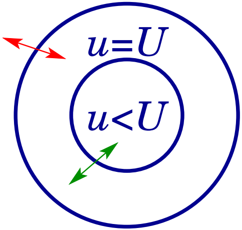


# Basis Generator Method

Expansion in adapted model space $\mathcal{A}^{UV}$

$$|\psi(t)\rangle = \sum_{u=0}^{U} \sum_{v=1}^{V} c_{uv}(t) |\phi_v^u\rangle$$

only states of outermost 'shell' of $\mathcal{A}^{UV}$ are coupled to complementary space




If population of outermost shell $\rightarrow 0$

$\Rightarrow$ finite representation exact

# BGM equations

- 'Generating' basis

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$
$$\hat{H}_0|\phi_v^0\rangle = \varepsilon_v|\phi_v^0\rangle \; , \quad v = 1, \ldots, V$$

- Hierarchy of dynamically adapted subspaces

$$|\phi_v^u\rangle = (\hat{H} - i\partial_t)|\phi_v^{u-1}\rangle \; , \quad u = 1, \ldots, U$$
$$= (\hat{H} - i\partial_t)^u|\phi_v^0\rangle \; , \quad v = 1, \ldots, V$$

- Explicit construction of states complicated

$$|\phi_v^1\rangle = \hat{V}|\phi_v^0\rangle$$
$$|\phi_v^2\rangle = \{-\frac{1}{2}\nabla^2\hat{V} + \hat{V}^2 - i\partial_t\hat{V} - \nabla\hat{v}\nabla\}|\phi_v^0\rangle$$

# BGM strategy

- It's not the states, it's the space!
- Try to find alternative basis $\{\chi_\nu^\mu, \nu = 1, \ldots, N, \mu = 1, \ldots, M\} \equiv \mathcal{R}^{MN}$ with following properties:

  1. initial state $|\phi_\nu^0\rangle \in \mathcal{R}^{0N}$
  2. $\hat{H} - i\partial_t$ maps each $|\chi_\nu^\mu\rangle$ onto finite linear combination of $\{|\chi_\nu^\mu\rangle\}$

  if (1) and (2) are met $\Rightarrow \mathcal{A}^{UV} \subset \mathcal{R}^{MN}$
- Propagate TDSE in $\mathcal{R}^{MN}$!

# BGM practice I

Collisions in semiclassical approximation

- For two-center Coulomb problem conditions are met by

$$|\chi_\nu^{\mu_1\mu_2}\rangle = W_p^{\mu_1} W_t^{\mu_2} |\phi_\nu^0\rangle$$

with regularized potentials

$$W_{p,t} = [x_{p,t}^2 + y_{p,t}^2 + z_{p,t}^2 + \epsilon_{p,t}^2]^{-\frac{1}{2}}$$

- Complicated matrix elements

$$\langle \chi_\nu^{\mu_1\mu_2} | \hat{H} - i\partial_t | \chi_{\nu'}^{\mu_1'\mu_2'} \rangle$$

- Practice: $|\chi_\nu^\mu\rangle = W_p^\mu |\phi_\nu^0\rangle$ or $|\chi_\nu^\mu\rangle = W_t^\mu |\phi_\nu^0\rangle$

Kroneisen et al. J. Phys. A 1999

# BGM practice II

- $\langle \chi_\nu^\mu | \hat{H} - i\partial_t | \chi_{\nu'}^{\mu'} \rangle$ can be calculated
- $W_p$ or $W_t$?
- Recall: for

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

"exact" first-order basis states:

$$|\phi_v^1\rangle = (\hat{H} - i\partial_t)|\phi_v^0\rangle = \hat{V}|\phi_v^0\rangle$$

$\rightarrow$ favours $W_p$ (if $\hat{H}_0$ = target Hamiltonian)

- $|\chi_\nu^\mu\rangle = W_p^\mu |\phi_\nu^0\rangle$ have two-centre character and overlap with bound projectile states
$\rightarrow$ calculate capture by projection

# Two-centre (TC)-BGM

- Add projectile states to basis for better description of capture
- Include translation factors

$$\phi_v^0(\mathbf{r}) = \begin{cases} \phi_v(\mathbf{r}_t)\exp(i\mathbf{v}_t\mathbf{r}) & \textit{if } v \le V_t \\ \phi_v(\mathbf{r}_p)\exp(i\mathbf{v}_p\mathbf{r}) & \text{else} \end{cases}$$

$$\chi_v^\mu(\mathbf{r}, t) = [W_p(t)]^\mu \phi_v^0(\mathbf{r}) \qquad v = 1, \ldots, V_t$$

- TC-BGM = TCAO + (special) pseudostates for quasimolecular couplings and transitions into continuum

# *3.* Examples I: collisions with H(1s)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **38** (2005) 4045–4055 doi:10.1088/0953-4075/38/22/009

**Lyman-$\alpha$ line polarization after proton impact on atomic hydrogen**

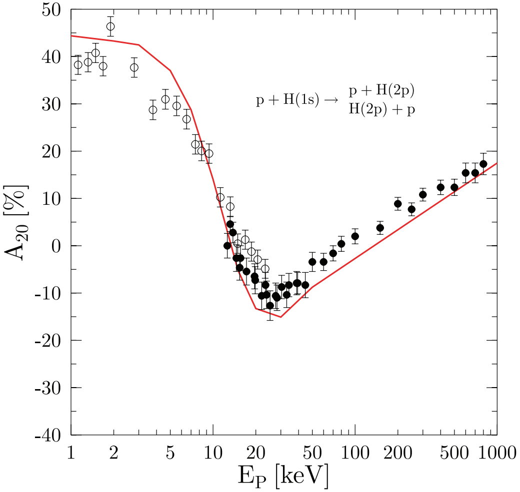
**M Keim[1,2], A Werner[3], D Hasselkamp[4], K-H Schartner[4], H J Lüdde[1], A Achenbach[1] and T Kirchner[2]**

- Integral alignment parameter

$$A_{20} = \frac{6\Pi(Ly_\alpha)}{\Pi(Ly_\alpha) - 3} = \frac{\sigma_{2p_1} - \sigma_{2p_0}}{2\sigma_{2p_1} + \sigma_{2p_0}}$$

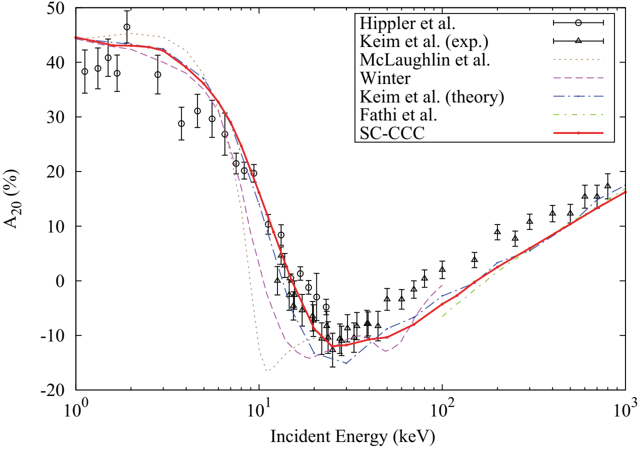
- TC-BGM basis: KLMNO eigenstates of target and projectile, and 100 pseudostates

# $p$-H($1s$): integral alignment



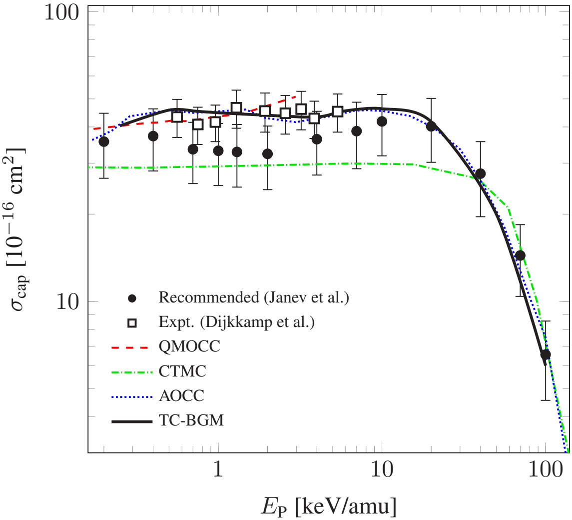

Keim et al., JPB **38** 4045 (2005)

# $p$-H($1s$): integral alignment



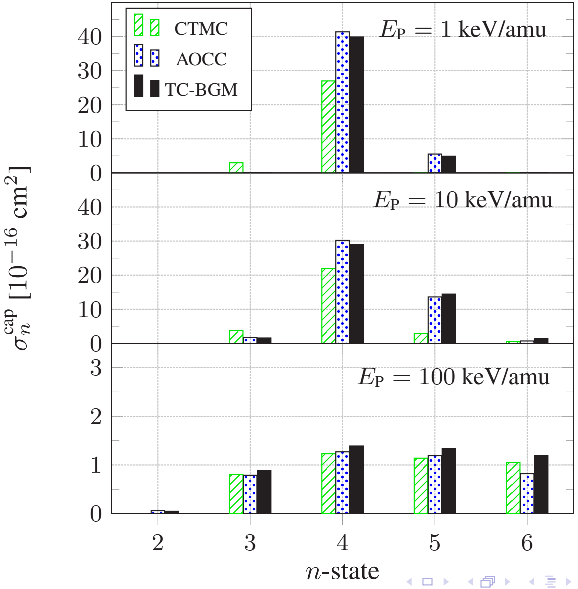

Avazbaev et al., PRA **93**, 022710 (2016)

# $O^{6+}(1s^2)$-H($1s$): electron capture




QMOCC, AOCC, CTMC: Wu et al., JPB **45** 235201 (2012)

# $O^{6+}(1s^2)$-H$(1s)$: electron capture



## *4.* Theory II: the few-electron problem

# Few-electron problem I

- Explicit solution is hard
- Ansatz (independent electrons – IEM):

$$\hat{H}_e(t) \;\to\; \sum_{j=1}^{N} \hat{h}_j(t), \quad i\partial_t \psi_j(\boldsymbol{r}, t) = \hat{h}(t)\psi_j(\boldsymbol{r}, t)$$

$$\hat{h}(t) \;=\; -\frac{1}{2}\Delta - \frac{Z_T}{r} - \frac{Z_p}{|\boldsymbol{r} - \boldsymbol{R}(t)|} + v_{ee}(\boldsymbol{r}, t)$$

- Choice of $v_{ee}$ defines model
- Time-dependent density functional theory (TDDFT) provides foundation

# Few-electron problem II

Choices:

$$
\begin{aligned}
v_{ee}(\boldsymbol{r}, t) &= v_{ee}^{0}(r) && \text{no response} \\
v_{ee}(\boldsymbol{r}, t) &= f(t) v_{ee}^{0}(r) && \text{global target response}^{*} \\
v_{ee}(\boldsymbol{r}, t) &= v_{ee}[\psi_j](\boldsymbol{r}, t) && \text{microscopic response}
\end{aligned}
$$

- TC-BGM can be used within IEM
- Model uncertainties (IEM) $\leftrightarrow$ numerical uncertainties (convergence etc.)

* Kirchner *et al.*, PRA 2000

# Few-electron problem III

Single-particle solutions $\to$ many-electron info

- Option 1: IEM (multinomial) analysis
  e.g. single and double capture for $N = 2$:

$$P_1 = 2p_{\mathrm{cap}}(1 - p_{\mathrm{cap}})$$
$$P_2 = p_{\mathrm{cap}}^2$$

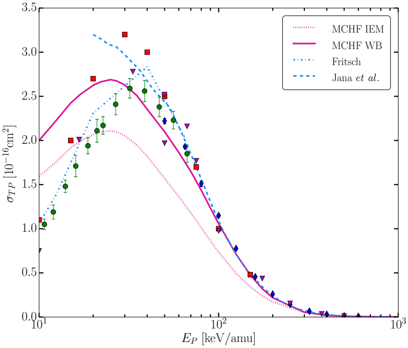
- Option 2: determinants (density matrices)*
- Further options: correlation integrals**, single-active electron (SAE) model, ...
  $P_{\mathrm{SAE}} = 2p_{\mathrm{cap}} = P_{\mathrm{net}} = P_1 + 2P_2$
  analysis = source of model uncertainties

*Lüdde and Dreizler, JPB 1985; **Baxter and TK, PRA 2016

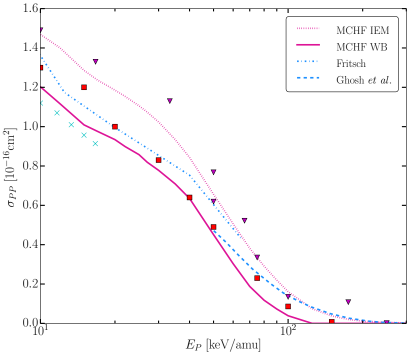
# 5. Examples II: He (and a bit more)

# $He^{2+}$- He: single and double capture

## single capture



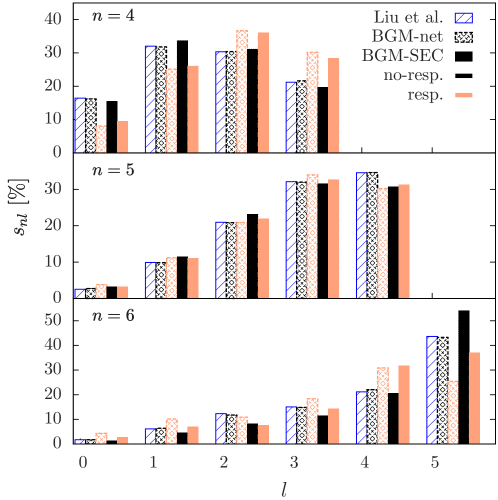

## double capture




——: two-electron ——: DFT-based

Baxter and Kirchner, PRA **93**, 012502 (2016)

# $Ne^{10+}$- He: single capture



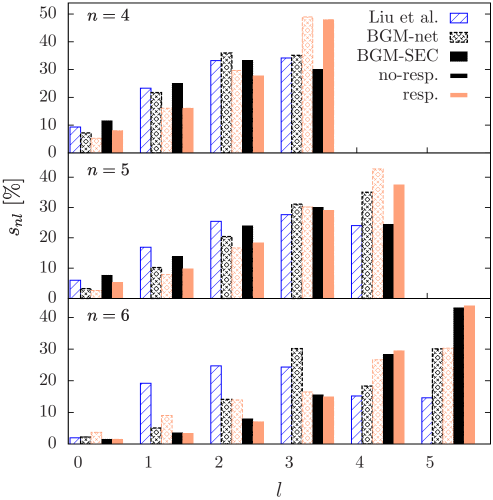

$$s_{nl} = \sigma_{nl} / \sum_{nl} \sigma_{nl}$$

Liu et al., PRA **89**, 012710 (AOCC)

BGM: PRA **92**, 032712

$E_P = 4.54$ keV/amu

# $Ne^{10+}$- Ne: single capture



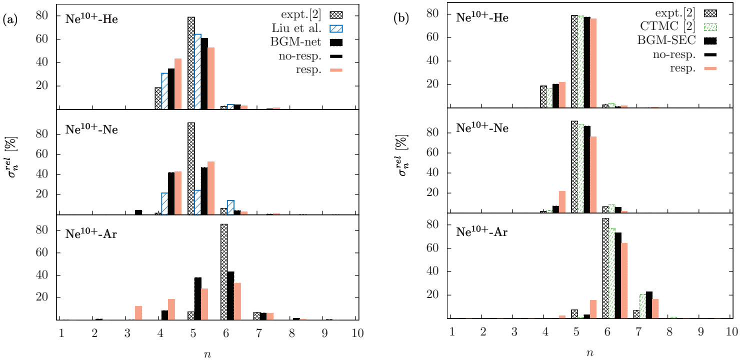

$$s_{nl} = \sigma_{nl} / \sum_{nl} \sigma_{nl}$$

Liu et al., PRA **89**, 012710 (AOCC)

BGM: PRA **92**, 032712

$E_P = 4.54$ keV/amu

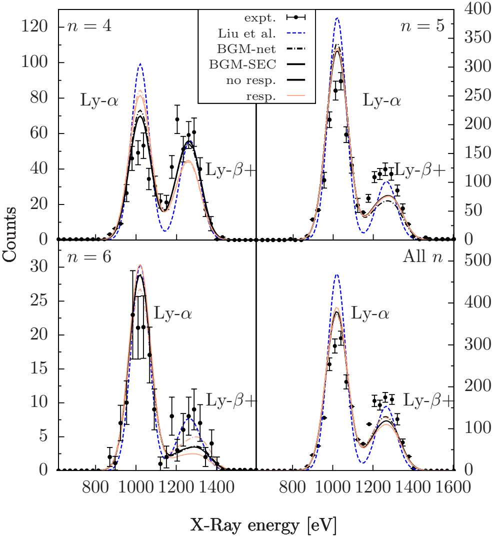
# $Ne^{10+}$- He,Ne,Ar: single *n*-capture




$E_P = 4.54$ keV/amu

Liu et al., PRA **89**, 012710
BGM: PRA **92**, 032712
CTMC and Expt: Ali et al., Astrophys. J. Lett. **716**, L95

# $Ne^{10+}$- He: x-ray spectra



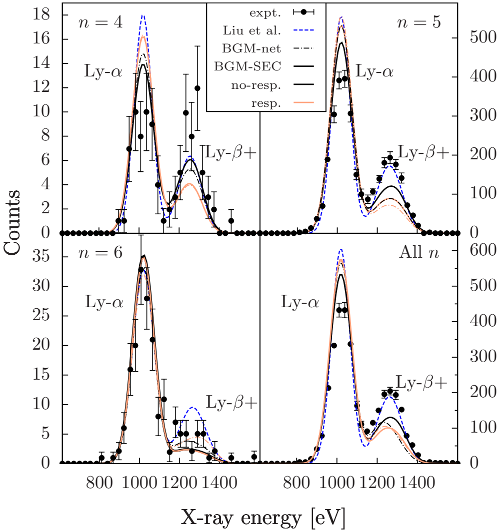

Expt.: Ali et al., Astrophys. J. Lett. **716**, L95

Liu et al., PRA **89**, 012710

BGM: PRA **92**, 032712

$E_P = 4.54$ keV/amu

# $Ne^{10+}$- Ne: x-ray spectra




Expt.: Ali et al., Astrophys. J. Lett. **716**, L95

Liu et al., PRA **89**, 012710

BGM: PRA **92**, 032712

$E_P = 4.54$ keV/amu

# Summary

(TC)-BGM: coupled-channel method within semiclassical approximation

Collisions with hydrogen

- successful alignment parameter calculation for *p*-H
- Shell-specific capture into highly-charged projectiles

Few-electron problems

- IEM variants
- DFT perspective
- Partially stripped projectiles can be handled

## Thanks to ...

| | |
|---|---|
| York University | M. Baxter |
| | A. Leung |
| U Frankfurt | H. J. Lüdde |

**... and to you for your attention!**