Understanding the isovector channel of nuclear interaction through heavy ion charge-exchange reactions

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Authors:

Burrello S. 1,2, Bellone J.I. 2,3, Colonna M. 2, Lay J.A. 1, Lenske H. 4



² INFN - LNS, Catania, Italy

³ Dpt. di Fisica e Astronomia, Università di Catania, Italy

⁴ Institut für Theoretische Physik, JLU Giessen, Germany



Isovector channel of interaction ⇒ Symmetry energy in Equation of State (EOS)

$$\frac{E}{A}(\rho,\beta) \approx \frac{E}{A}(\rho,\beta=0) + S(\rho)\beta^2 \qquad S(\rho) = J + L\left(\frac{\rho - \rho_0}{3\rho_0}\right) + \dots \qquad \beta \equiv \frac{\rho_n - \rho_p}{\rho}$$

- ullet Collective phenomena in many-body systems \Rightarrow properties of interaction
- ullet Probing collective **nuclear response** \Rightarrow Heavy-Ion (HI) collisions
- Dipole excitations in neutron-rich nuclei:
 - Giant Dipole Resonance (GDR)
 - Pygmy Dipole Resonance (PDR)
 - [S. Burrello et al., arXiV:1807.10118, (2018).]

■ Isospin-flip transitions
 ⇒ Charge-exchange reactions

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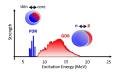
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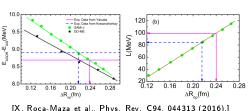
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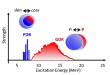
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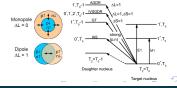
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- Isospin-flip transitions
 - ⇒ Charge-exchange reactions



- Charge-exchange (CEX) reactions: nuclei keep mass constant but change charge
- Contribution of various mechanisms

multi-step transfers via intermediate states (sequential pick-up/stripping processes)
 direct conversion of nucleon (N) (through meson exchange)

$$_{z}^{a}a+_{Z}^{A}A\rightarrow_{z\pm1}^{a}b+_{Z\mp1}^{A}B$$

Fermi (F) and Gamow-Teller (GT) transitions

$$V_{NN} = \sum_{S,T} \left[V_{ST}^{c} \left(\sigma_{1} \cdot \sigma_{2} \right)^{S} + V_{1T}^{t} S_{12} \right] \left(\tau_{1} \cdot \tau_{2} \right)^{T}$$

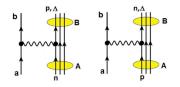
- Light ions $\Rightarrow \left(\frac{d\sigma}{d\Omega}\right)_{\theta=0} \propto B(GT)_{\beta}$ Monopole \Rightarrow analogy to GT of β -decay [Taddeucci T.N. et al., Nucl. Phys. A469, 125 (1987)]
- Heavy ions ⇒ complex many-body nature

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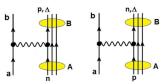
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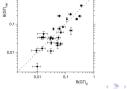
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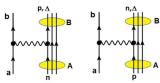
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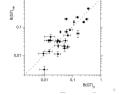
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- Direct reaction ⇒ Distorted Wave Born Approximation (DWBA)
- Single CEX A(a,b)B cross section (c.s.) ($lpha\equiv$ initial, $eta\equiv$ final, $\hat{J}\equiv\sqrt{2J+1}$)

$$\frac{d\sigma}{d\Omega} = \frac{E_{\alpha}E_{\beta}}{(2\pi\hbar^2)^2} \frac{k_{\beta}}{k_{\alpha}} \frac{1}{\hat{J_a}^2 \hat{J_A}^2} \sum_{\substack{m_{\beta}, m_{A} \in \alpha \\ m_{\beta}, m_{\beta} \in \beta}} \left| M_{\alpha\beta} \right|^2, \quad M_{\alpha\beta}(\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}) = \sum_{S,T} \int d^3\mathbf{p} \, \mathcal{K}_{\alpha\beta}^{(ST)}(\mathbf{p}) \, \mathcal{N}_{\alpha\beta}(\mathbf{k}_{\alpha}, \mathbf{k}_{\beta}, \mathbf{p})$$

$$\mathcal{K}_{\alpha\beta}^{(ST)} \Rightarrow$$
 Structure part

$$\mathcal{N}_{\alpha\beta} \Rightarrow \mathsf{Reaction}$$
 part

- Distortion factor $\mathcal{N}_{\alpha\beta} = \delta(\mathbf{p} (\mathbf{k}_{\alpha} \mathbf{k}_{\beta})) = \delta(\mathbf{p} \mathbf{q}_{\alpha\beta}) \Rightarrow$ Plane Wave (PWBA)
- Factorization at low $q_{\alpha\beta} \Rightarrow \beta$ -decay Nuclear Matrix Elements (NME)

[Lenske H. et al., Phys. Rev. C (2018), submitted]

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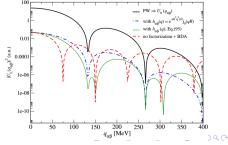
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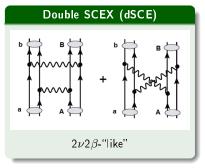
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Second order CEX reactions: double charge-exchange (DCEX) reactions

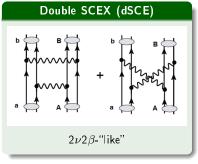


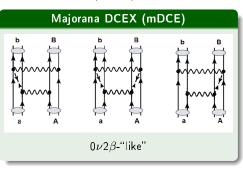
Majorana DCEX (mDCE)

 $0\nu 2\beta$ -"like"

- Missing theory for reaction mechanism ⇒ renewed experimental interest
- double CEX \Leftrightarrow neutrino-less 2β (0 $\nu2\beta$) decay \Rightarrow NUMEN project @LNS [Cappuzzello, F. et al., EPJ A51 (2015)]
- ⁴⁰Ca(¹⁸O, ¹⁸Ne)⁴⁰Ar @ 15 AMeV
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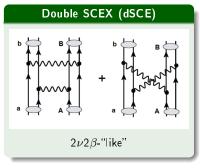


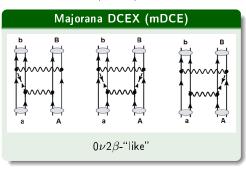


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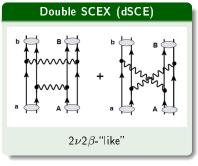


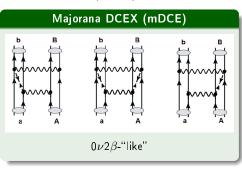


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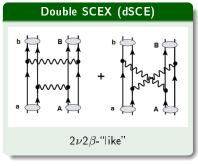
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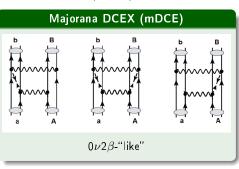




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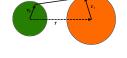




ullet Optical potential \Rightarrow double-folding integrals

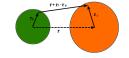
$$U_{pt}(\mathbf{r}) = \int d\mathbf{r}_t \int d\mathbf{r}_p \rho_t(\mathbf{r}_t) \rho_p(\mathbf{r}_p) V_{NN}(\mathbf{r} + \mathbf{r}_t - \mathbf{r}_p)$$

• Analytical Form Factors (FF): $F_L(r) \propto \left(\frac{\partial U}{\partial r}\right)$



• dSCE vs mDCE: - same θ distribution

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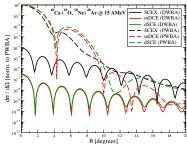
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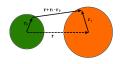
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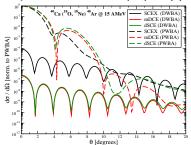
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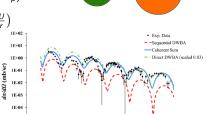
dSCE vs mDCE: diffraction pattern and distortion

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 $heta_{lab}({
m deg})$ [M. Cavallaro et al., EPJ WC 66, (2014)]

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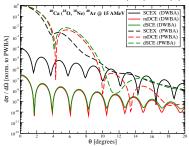
1E-05 1E-06

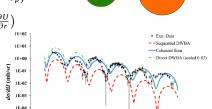
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 - ◆ロ → ◆母 → ◆ き → ◆ き → り へ ○

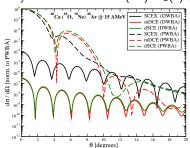
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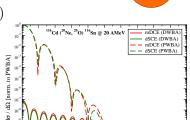
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θ [degrees]

• dSCE vs mDCE: - same θ distribution \Rightarrow analogy with transfer - similar distortion factor $N_D = \left(\frac{d\sigma/d\Omega(DWBA)}{d\sigma/d\Omega(PWBA)}\right)_{\alpha}$

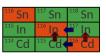
WARNING

Distortion effects act only once also in two-step process!



Isolate CEX from exp. cross section
 ⇒ description of competing processes

¹¹⁶ Sn	¹¹⁷ Sn	¹¹⁸ Sn
¹¹⁵ In	ن ¹¹⁶ In	¹¹⁷ In
¹¹⁴ Cd	115 Cd	116 Cd



- Transfer sensitive to N-nucleus mean-field potential ⇒ no probe for F and GT
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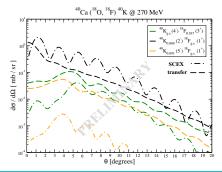
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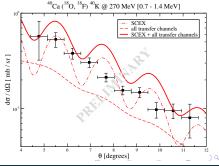
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Final remarks and conclusions

Summary

- Collective modes for isovector channels: dipole and isospin-flip excitations
- Charge-exchange reactions with heavy ions in view of experimental interest
- Interplay with multi-nucleon transfers feeding same outgoing channels

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- Role of distortion effects in direct and two-step double charge exchange
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Further developments and outlooks

- Complete theory of double charge exchange, of interest in 2β -decay studies
- Full determination of higher order combination of multi-transfer
- Behavior of nuclear interaction in isospin channels: support to RIB

Acknowledgements



KIND ATTENTION!



F. Cappuzzello, C. Agodi, M. Cavallaro, D. Carbone, S. Tudisco, D. Lo Presti, J. R. B. Oliveira, P. Finocchiaro, M. Colonna, D. Rifuggiato, L. Calabretta, D. Calvo, L. Pandola, L. Acosta, N. Auerbach, J. Bellone, R. Bijker, D. Bonanno, D. Bongiovanni, T. Borello-Lewin, I. Boztosun, O. Brunasso, S. Burrello, S. Calabrese, A. Calanna, E.R. Chávez Lomelí, G. D'Agostino, P.N. De Faria, G. De Geronimo, F. Delaunay, N. Deshmukh, J.L. Ferreira, M. Fisichella, A. Foti, G. Gallo, H. Garcia, V. Greco, M.A. Guazzelli, A. Hacisalihoglu, F. Iazzi, R. Introzzi, G. Lanzalone, J.A. Lay, F. La Via, H. Lenske, R. Linares, G. Litrico, F. Longhitano, J. Lubian, N. Medina, D.R. Mendes, M. Moralles, A. Muoio, A. Pakou, H. Petrascu, F. Pinna, S. Reito, A. D. Russo, G. Russo, G. Santagati, E. Santopinto, R.B.B. Santos, O. Sgouros, S.O. Solakci, G. Souliotis, V. Soukeras, A. Spatafora, D. Torresi, R.I.M. Vsevolodovna, V.A.B. Zagatto, A. Yildirin

Acknowledgements



THANK YOU FOR YOUR KIND ATTENTION!



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Backup slides

BACKUP SLIDES

First exploratory steps: unit cross section

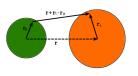
- Optical potential ⇒ double-folding integrals
 - Love & Franey V_{NN} interaction
 - Hartree-Fock-Bogoliubov density profiles

$$U_{pt}(\mathbf{r}) = \int d\mathbf{r}_t \int d\mathbf{r}_p \rho_t(\mathbf{r}_t) \rho_p(\mathbf{r}_p) V_{NN}(\mathbf{r} + \mathbf{r}_t - \mathbf{r}_p)$$

Analytical Form Factors (FF

$$F_L(r) = J_0 \ N_L \left(\frac{\partial U}{\partial r}\right), \quad \frac{1}{N_L} = \int dr \ r^2 \left(\frac{r}{R}\right)^L \left(\frac{\partial U}{\partial r}\right)$$

DCEX c.s. with schematic FF



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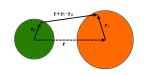
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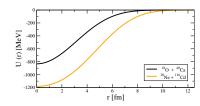
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DCEX c.s. with schematic FF

Single state dominance
 ⇒ dSCE ~ [FF(a)]²
 Closure approximation

 \Rightarrow mDCE $\sim \langle k' | FF^* | k \rangle$





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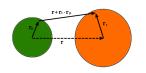
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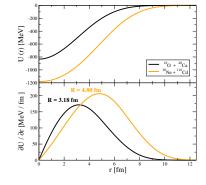
DCEX c.s. with schematic FF

• Single state dominance

Closure approximation

 \Rightarrow mDCE $\sim (k'|FF^2|k)$





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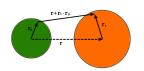
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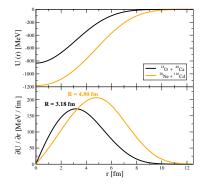
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- DCEX c.s. with schematic FF:
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$$\Rightarrow$$
 mDCE $\sim \langle k'|FF^2|k\rangle$

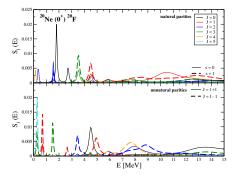


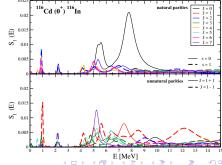


Microscopic form factors: QRPA calculations

- Realistic calculations: microscopic FF from QRPA (with HIDEX code)
 - Difficult to isolate contributions for each state
 - Excitation energies do not match experimental ones
 - Main contributions at larger values of E

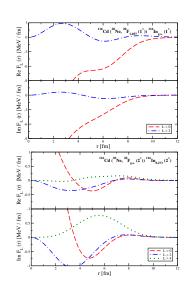
$$S_l(E) = \int dr r^2 \left(\delta
ho_l(r,E)\right)^2 \qquad \delta
ho_l(r,E) \equiv \mathsf{QRPA} \; \mathsf{transition} \; \mathsf{densities}$$





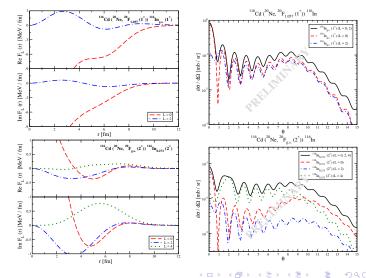
SCEX reaction ¹¹⁶Cd (²⁰Ne, ²⁰F)¹¹⁶In: results

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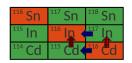
- Isolate CEX contribution from cross section
 - ⇒ description of competing processes (2N-transfer)
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 - \Rightarrow no probe of V_{NN} responsible for **F** and **GT** response
 - SCEX vs transfer for intermediate mass nuclei:

QUESTION

What is the role of **transfer** processes at i**ntermediate** E for **heavier** colliding systems

Lenske H., Wolter H.H., Bohlen H.G., PRL62 (1989).1

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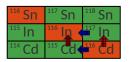
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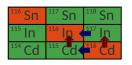
Direct process dominant at energy E~100 Alwev
 Important contribution of both at intermediate B

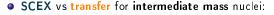
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What is the role of **transfer** processes at ntermediate E for heavier colliding system

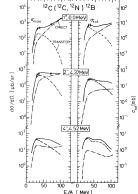
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- ullet Direct process **dominant** at energy E ${\sim}100$ AMeV
 - Important contribution of both at intermediate E



QUESTION

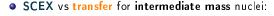
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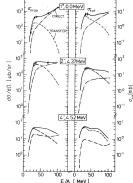


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12C (12C, 12N) 12B

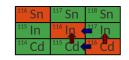
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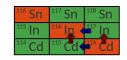


- Preliminary tests ⇒ **DWBA** calculations (**FRESCO** code)



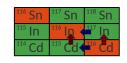
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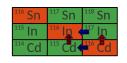
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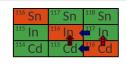
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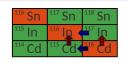
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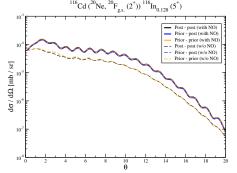


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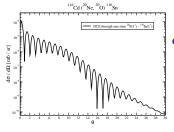
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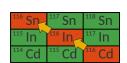
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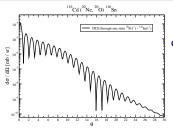
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- Two-step process:
 - One state only ($^{116} ln_{g.s.}$) $\Rightarrow 0.3 nb (exp. 50 nb)$
 - Several intermediate states
 - Contribution of continuum

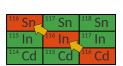


- 3rd order processes:
- Accurate evaluation of NO
 - \Rightarrow work in progress
- 4th order processes:
- No implementation yet of NO



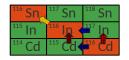
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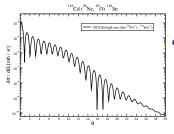


3	rd ord	er pro	cesses:
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Accurate evaluation of NO ⇒ work in progress

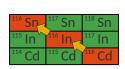


¹¹⁶ Sn ♦	¹¹⁷ ₄Sn	¹¹⁸ Sn
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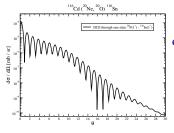
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114 Cd	115 Cd	¹¹⁶

¹¹⁶ Sn ♦	¹¹⁷ ₄Sn	¹¹⁸ Sn
115 In 💠	iln_	¹¹⁷ In
¹¹⁴ Cd	115 Cd	116 Cd

- 4th order processes:
 - No implementation yet of NO
 - Exp. c.s. reproduced for 2n/2p transfer (sim + seq)
 - ⇒ Good performances of FRESCO

116 Sn	Sn (¹¹⁸ S n
¹¹⁵ In	¹¹⁶ In	¹¹⁷ Jn
¹¹⁴ Cd	¹¹⁵ Cd	¹¹⁶ Cd

116 S n	¹¹⁷ Sn	¹¹⁸ Sn
115	¹¹⁶ In	¹¹⁷ In
¹¹⁴ Cd.	¹¹⁵ Cd∢	116 Cd



Two-step process:

- One state only ($^{116}In_{g.s.}$) \Rightarrow 0.3 nb (exp. 50 nb)
- Several intermediate states
- Contribution of continuum

116 Sn	¹¹⁷ Sn	¹¹⁸ Sn
¹¹⁵ In	¹¹⁶ In	¹¹⁷ In
¹¹⁴ Cd	115 Cd	¹¹⁶ Cd

3rd order processes:

Accurate evaluation of NO
 ⇒ work in progress

116 Sn	¹¹⁷ Sn	¹¹⁸ Sn
¹¹⁵ In	¹¹⁶ ln •	¹¹⁷ ln
114 Cd	115 Cd	¹¹⁶

¹¹⁶ Sn•	¹¹⁷ ₄Sn	¹¹⁸ Sn
115 In 🔇	¹¹¹° " In <mark>√</mark>	¹¹⁷ In
¹¹⁴ Cd	115 Cd	116 Cd

4th order processes:

- No implementation yet of NO
- Exp. c.s. reproduced for 2n/2p transfer (sim + seq)
 - ⇒ Good performances of FRESCO

¹¹⁶ Sn	¹¹⁷ Sn	¹¹⁸ Sn
¹¹⁵ In	¹¹⁶ In	¹¹⁷ In
¹¹⁴ Cd	¹¹⁵ Cd	¹¹⁶ Cd

¹¹⁶ Sn	¹¹⁷ Sn	¹¹⁸ Sn
¹¹⁵ In	¹¹⁶ In	¹¹⁷ In
¹¹⁴ Cd ⁴	¹¹⁵ Cd∢	116 Cd

Back-up

Double Charge Exchange (DCE) as a 2-step process: analogies with 2v double beta decay

Transition matrix element

 $\rightarrow M^{(2\nu)}(DGT)$

$$_za+_ZA \rightarrow_{z\pm 2}b+_{Z\mp 2}B$$

$$M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{bB}, \mathbf{k}_{\alpha}) = \langle \chi_{\beta}^{(-)}, bB | T_{NN} \mathcal{G}^{(+)}(\omega) T_{NN} | aA, \chi_{aA}^{(+)} \rangle.$$

► `` nuclear interaction

$$\mathcal{G}(\omega) = \sum_{\gamma = c,C} |\gamma\rangle G_{\gamma}(\omega_{\alpha}) \langle \gamma|, \qquad \Longrightarrow \text{ (intermediate states)}$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

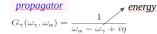
$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$

$$\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) = \sum_{c,C} \int \frac{d^{3}k_{\gamma}}{(2\pi)^{3}} M_{bB,cC}^{(SCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\gamma}) G_{cC}(\omega_{\gamma},\omega_{\alpha}) \tilde{M}_{cC,\alpha A}^{(SCE)}(\mathbf{k}_{\gamma},\mathbf{k}_{\alpha}),$$





40 K

2v double beta decay

 $= \sum_{m} \frac{\langle 0_{g.s.}^{(f)} \| \sum_{k} \sigma_{k} \tau_{k}^{-} \| 1_{m}^{+} \rangle \langle 1_{m}^{+} \| \sum_{k} \sigma_{k} \tau_{k}^{-} \| 0_{g.s.}^{(f)} \rangle}{\frac{1}{2} Q_{\beta\beta} (0_{g.s.}^{(f)}) + E_{x} (1_{m}^{+}) - E_{0}}$



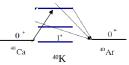
Within standard model



Back-up

DCE Transition matrix element

- $\rightarrow M_{\alpha\beta}^{(DCE)}(\mathbf{k}_{bB}, \mathbf{k}_{\alpha}) = \langle \chi_{\beta}^{(-)}, bB | T_{NN} \mathcal{G}^{(+)}(\omega) T_{NN} | aA, \chi_{\alpha A}^{(+)} \rangle.$
 - Single state dominance (ex: $0^+ \searrow 1^+ \searrow 0^+$)



$$\frac{\textit{small momentum transfer}}{dE d\Omega} = \frac{E_{\alpha} E_{\beta}}{(2\pi \hbar c)^4} \frac{k_{\beta}}{k_{\alpha}} k_{\omega}^2 \mu_{\omega}^2 |K^{(SCE)}(\mathbf{q}_{\alpha\omega})|^2 |K^{(SCE)}(\mathbf{q}_{\omega\beta})|^2} \mathbf{f}_{BD}$$

Product of beta decay strengths associated with the two steps

Closure approximation (one-step process)

$$\bar{M}_{\beta\alpha}^{(DCE)}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}) \simeq \sum_{SM,S:\,S} (-)^{S_{1}+S_{2}-S+M} M_{(S_{1}S_{2})S-M}^{(ba)\dagger}(\mathbf{q}_{\alpha\beta}) M_{(S_{1}S_{2})S-M}^{(BA)}(\mathbf{q}_{\alpha\beta}) V_{S_{2}S_{1}}(\mathbf{k}_{\beta},\mathbf{k}_{\alpha}).$$

 $\sim F^2(r)$

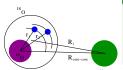
$$\rightarrow M_{(S_1,S_2)SM}^{(f)}(\mathbf{q}_{\alpha\beta}) = \langle \mathbf{k}_{\beta}, f | e^{i\mathbf{q}_{S^{\alpha}}\mathbf{r}} S_{(S_2S_1)SM}(1,2)\tau_{\pm}(2)\tau_{\pm}(1) | \mathbf{k}_{\alpha}i \rangle.$$

$$V_{S_2S_1}(\mathbf{k}_{\beta}, \mathbf{k}_{\alpha}) = \int \frac{d^3k_{\gamma}}{(2\pi)^3} \frac{t_{S_2T}(q_{\beta\gamma}^2)t_{S_1T}(q_{\gamma\alpha}^2)}{(2\pi)^3}$$

$$V_{S_2S_1}(\mathbf{k}_{\beta}, \mathbf{k}_{\alpha}) = \int \frac{d^3k_{\gamma}}{(2\pi)^3} \frac{t_{S_2T}(q_{\beta\gamma}^2)t_{S_1T}(q_{\gamma\alpha}^2)}{(2\pi)^3}$$
Two-body transition operator, similar to DGT

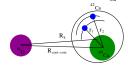


The Schrödinger Equation



Set of Coupled Equations:

$$\langle \phi_j | \mathcal{H} - E | \phi_j \rangle \psi_j(R_j) + \sum_{i \neq j} \langle \phi_j | \mathcal{H} - E | \phi_i \rangle \psi_i(R_i) = 0$$



Distorted Wave:

$$\langle \phi_j | \mathcal{H} - E | \phi_j \rangle \chi_j(R_j) = 0$$

$$A + b \rightarrow a + B$$

Plane Wave:

$$\langle \phi_i | \mathcal{K} - E | \phi_i \rangle e^{-i\vec{k}\cdot\vec{R}_j}(R_i) = 0$$

Distorted Wave Born Approximation

1. $i \rightarrow j \rightarrow k$:

$$\begin{split} &\langle \phi_i | \mathcal{H} - E | \phi_i \rangle \chi_i(R_i) \approx 0 \\ &\langle \phi_j | \mathcal{H} - E | \phi_j \rangle \psi_j(R_j) \approx -\langle \phi_j | \mathcal{H} - E | \phi_i \rangle \chi_i(R_i) \\ &\langle \phi_k | \mathcal{H} - E | \phi_k \rangle \psi_k(R_k) \approx \\ &- \langle \phi_k | \mathcal{H} - E | \phi_i \rangle \chi_i(R_i) - \langle \phi_k | \mathcal{H} - E | \phi_j \rangle \psi_j(R_j) \end{split}$$

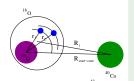
2. T_{ki} amplitudes:

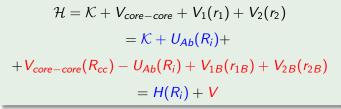
$$T_{ki}^{(1)} = \langle \chi_k^{(-)} \phi_k | \mathcal{H} - E | \phi_i \chi_i^{(+)} \rangle$$

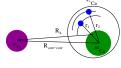
$$T_{ki}^{(2)} = \langle \chi_k^{(-)} \phi_k | \mathcal{H} - E | \phi_j \psi_j^{(+)} \rangle$$
$$T_{ki}^{(2)} = \langle \chi_k^{(-)} | \langle \phi_k | \mathcal{H} - E | \phi_j \rangle G_j^{(+)} \langle \phi_j | \mathcal{H} - E | \phi_i \rangle | \chi_i^{(+)} \rangle$$

The Hamiltonian

Prior







$$A + b \rightarrow a + B$$

Post

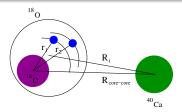
$$\mathcal{H} = \mathcal{K} + V_{core-core} + V_1(r_1) + V_2(r_2)$$

$$= \mathcal{K} + U_{aB}(R_k) +$$

$$+V_{core-core}(R_{cc}) - U_{aB}(R_k) + V_{1A}(r_{1A}) + V_{2A}(r_{2A})$$

$$= H(R_k) + V$$

Prior vs. Post

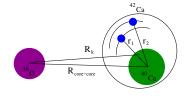


Evaluating the previous brakets: $\langle \phi_i | \mathcal{H} - E | \phi_i \rangle = H_i - E_i$;

prior

$$= \langle \phi_j | V_i | \phi_i \rangle + \langle \phi_j | \phi_i \rangle [H_i - E_i]$$

$$=V_{ii}^{prior}+K_{ji}[H_i-E_i]$$



post

$$= \langle \phi_j | V_j | \phi_i \rangle + [H_j - E_j] \langle \phi_j | \phi_i \rangle$$

$$= V_{ii}^{post} + [H_j - E_j] K_{ji}$$

 $\langle \phi_i | \mathcal{H} - E | \phi_i \rangle =$

$$[H_i - E_i]\chi(R_i) = 0$$

$$K_{ji} = \langle \phi_j | \phi_i \rangle$$

! Prior/Post and NO

$$T_{ki}^{(1)} = \langle \chi_k^{(-)} \phi_k | \mathcal{H} - E | \phi_i \chi_i^{(+)} \rangle$$

prior

$$T_{ki}^{(1)} = \langle \chi_k^{(-)} | V_{ki}^{prior} + K_{ki} [H_i - E_i] | \chi_i^{(+)} \rangle$$

$$T_{ki}^{(1)} = \langle \chi_k^{(-)} | V_{ki}^{prior} | \chi_i^{(+)} \rangle$$

post

$$T_{ki}^{(1)} = \langle \chi_k^{(-)} | V_{ki}^{post} + [H_k - E_k] K_{ki} | \chi_i^{(+)} \rangle T_{ki}^{(1)} = \langle \chi_k^{(-)} | V_{ki}^{post} | \chi_i^{(+)} \rangle$$

m !! Prior and post give the same in $m 1^{st}$ order if converged

! Prior/Post and NO

$$T_{kj}^{(2)} = \langle \chi_k^{(-)} | \langle \phi_k | \mathcal{H} - E | \phi_j \rangle G_j^{(+)} \langle \phi_j | \mathcal{H} - E | \phi_i \rangle | \chi_j^{(+)} \rangle$$

prior-prior

$$T_{ki}^{(2)} = \langle \chi_{k}^{(-)} | (V_{kj}^{prior} + K_{kj}[H_{j} - E_{j}]) G_{j} (V_{ji}^{prior} + K_{ji}[H_{i} - E_{i}]) | \chi_{i}^{(+)} \rangle =$$

$$= \langle \chi_{k}^{(-)} | V_{kj}^{prior} G_{j} V_{ji}^{prior} | \chi_{i}^{(+)} \rangle + \langle \chi_{k}^{(-)} | K_{kj}[H_{j} - E_{j}] G_{j} V_{ji}^{prior} | \chi_{i}^{(+)} \rangle$$

prior-post

$$\begin{split} T_{ki}^{(2)} &= \langle \chi_k^{(-)} | (V_{kj}^{post} + [H_k - E_k] K_{kj}) G_j (V_{ji}^{prior} + K_{ji} [H_i - E_i]) | \chi_i^{(+)} \rangle = \\ &= \langle \chi_k^{(-)} | V_{kj}^{post} G_j V_{ji}^{prior} | \chi_i^{(+)} (R_i) \rangle + 0 \end{split}$$

!! Prior-post has zero NO term

$$T_{ki}^{(2)} = \langle \chi_k^{(-)} | \langle \phi_k | \mathcal{H} - E | \phi_j \rangle G_j^{(+)} \langle \phi_j | \mathcal{H} - E | \phi_i \rangle | \chi_i^{(+)} \rangle$$

post-post

$$T_{ki}^{(2)} = \langle \chi_k^{(-)} | (V_{kj}^{post} + [H_k - E_k] K_{kj}) G_j (V_{ji}^{post} + [H_j - E_j] K_{ji}) | \chi_i^{(+)} \rangle =$$

$$= \langle \chi_k^{(-)} | V_{kj}^{post} G_j V_{ji}^{post} | \chi_i^{(+)} (R_i) \rangle + \langle \chi_k^{(-)} | V_{kj}^{post} G_j [H_j - E_j] K_{ji} | \chi_i^{(+)} \rangle$$

post-prior

$$\begin{split} T_{ki}^{(2)} &= \langle \chi_k^{(-)} | (V_{kj}^{prior} + K_{kj} [H_j - E_j]) G_j (V_{ji}^{post} + [H_j - E_j] K_{ji}) | \chi_i^{(+)} \rangle = \\ &= \langle \chi_k^{(-)} | V_{kj}^{prior} G_j V_{ji}^{post} | \chi_i^{(+)} (R_i) \rangle + \langle \chi_k^{(-)} | K_{kj} [H_j - E_j] G_j V_{ji}^{post} | \chi_i^{(+)} \rangle \\ &+ \langle \chi_k^{(-)} | V_{kj}^{prior} G_j [H_j - E_j] K_{ji} | \chi_i^{(+)} \rangle + \\ &+ \langle \chi_k^{(-)} | K_{kj} [H_j - E_j] G_j [H_j - E_j] K_{ji} | \chi_i^{(+)} \rangle \end{split}$$

! Post-post and prior-prior in a full bases

$$T_{ki}^{(2)} = \langle \chi_k^{(-)} | \langle \phi_k | \mathcal{H} - E | \phi_j \rangle G_j^{(+)} \langle \phi_j | \mathcal{H} - E | \phi_i \rangle | \chi_i^{(+)} \rangle$$

In the limit
$$\epsilon \to 0$$

 $G_j^{(+)}\langle \phi_j|(\mathcal{H} - E) = G_j^{(+)}\langle \phi_j|V - \langle \phi_j|$

$$T_{ki}^{NO,post-post} = -\langle \chi_k^{(-)} \phi_k | V^{post} | \phi_j \rangle \langle \phi_j | \phi_i \chi_i^{(+)} \rangle$$

If
$$\sum |\phi_j\rangle\langle\phi_j|\approx I$$

$$T_{ki}^{NO,post-post} = -T_{ki}^{(1,post)}$$

And same for prior-prior