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Beyond the Traditional Shell Model



- relevant valence space
- symmetries
- fundamental and empirical parameters
- Large scale manybody numerical methods

Reactions

 relevant reaction channels

- reaction calculation (kinematics)
- symmetries: unitarity
- decay chain couplings
- New reaction manybody numerical methods

Basic Theory

 $|1\rangle$ - set of "internal" A-nucleon many-body states (*P*-space) $|c; E\rangle$ set of "external" many-body continuum states (*Q*-space) Solve problem:

$$H|\Psi
angle=E|\Psi
angle$$

where

$$|\Psi
angle = \sum_{1} x_{1}|1
angle + \sum_{c} \int dE'\,\chi^{c}(E')|c;E'
angle$$

For structure physics solve for internal coefficients x_1

$$\sum_{2} \left[\underbrace{\langle 1|H|2 \rangle + \sum_{c} \int dE' \frac{\langle 1|H|c;E' \rangle \langle c;E'|H|2 \rangle}{E - E' + i0}}_{\mathcal{H}_{12}(E)} - \delta_{12}E \right] x_{2} = 0$$

[1] C. Mahaux and H. Weidenmüller, Shell-model approach to nuclear reactions, North-Holland Publishing, Amsterdam 1969 $\langle 1|H|2 \rangle$ Usual shell-model Hamiltonian involving intrinsic states

$$\langle 1|H|2 \rangle = H_{12}^{\circ} + V_{12}$$

 $A_1^c(E') = \langle 1|H|c; E' \rangle$ decay amplitude

$$\sum_{c} \int dE' \frac{A_{1}^{c} A_{2}^{c*}}{E - E'} = \sum_{\substack{c \text{ (all)} \\ \Delta(E)}} P \int dE' \frac{A_{1}^{c} A_{2}^{c*}}{E - E'} - i \pi \sum_{\substack{c \text{ (open)} \\ W(E)/2}} A_{1}^{c} A_{2}^{c*}$$

$$\mathcal{H}(E) = H^{\circ} + V + \Delta(E) - \frac{i}{2}W(E)$$

 H° s.p energies V residual inteaction Δ interaction via continuum W non-Hermitian - decay

Continuum Shell Model Hamiltonian

- PHP Internal, one-body + two-body
 - "Original" shell model, adjusted, tested... (USD and others)
 - Exact shell model for bound states E<threshold
- QHQ External, one-body (presently)
 - kinetic energy + long range interaction, (plane waves or Bessel functions, Coulomb functions)
- QHP Cross space, one-body + two-body
 - Responsible for coupling of spaces

One-body continuum state

$$egin{aligned} |c;E
angle_N &= c_j^\dagger(\epsilon_j) |lpha;N-1
angle \ |c;E
angle_N &= c_j^\dagger(\epsilon_j) c_{j\prime}^\dagger(\epsilon_j') |lpha;N-2
angle \end{aligned}$$

Two-body continuum state

One-body decay

- Continuum channel $|c; E\rangle_N = c_j^{\dagger}(\epsilon_j) |\alpha; N-1\rangle$
 - State α in *N*-1 nucleon daughter
 - Particle in continuum state j
 - Energy $E = E_{\alpha} + \varepsilon_{j}$
- Transition Amplitude

Important: W-not a single particle operator

Shell model s.p. transition

s.p. decay

amplitude

 $A_1^c(E_{\alpha} + \epsilon_j) = a^j(\epsilon_j) \langle \alpha; N - 1 | b_j | 1; N \rangle$

Single particle decay-Woods-Saxon potential calculation

$$a^{j}(\epsilon) = \langle 0|c_{j}(\epsilon)Vb_{j}^{\dagger}|0\rangle = \sqrt{\frac{2\mu}{\pi k}} \int_{0}^{\infty} dr F_{l}(r) V(r) u_{l}(r)$$

One-body decay realistic one-body potential

Scattering calculation using Woods-Saxon with size parameters adjusted for ¹⁶O



$$\begin{aligned} & \text{Two-body decay: sequential} \\ & \text{Mediated by s.p. part of QHP} \\ & A^{c}(E) = \langle c, \epsilon_{1}, \epsilon_{2} | H_{s.p.} | 1; N \rangle \\ & \overset{\bullet}{\underset{N=2}{\text{virtual N-1 state from previous solution}}} \\ & \overset{\bullet}{\underset{N=2}{\text{virtual N-1 state from previous solution}} \\ & \overset{\bullet}{\underset{N=2}{\text{virtual N-1 state from previous solution}}} \\ & \overset{\bullet}{\underset{N=2}{\text{virtual N-1 state from previous solution}} \\ & \overset$$

Two-body decay: Direct Mediated by 2-body part of QHP

$$A^{c}(E) = \langle c, \epsilon_{1}, \epsilon_{2} | H_{2body} | 1; N \rangle$$



$$A_1^c(E) = a^{(j_1 j_2)}(\epsilon_1, \epsilon_2) \, \langle \alpha; N - 2 | p_L^{(j_1 j_2)} | 1; N \rangle \,,$$

two-body decay amplitude

Shell model pair removal amplitude

V(r,r') – effective pair potential

$$a^{(j_1j_2)}(\epsilon_1\epsilon_2) = \frac{2\mu}{\pi\sqrt{k_1k_2}} \int_0^\infty dr dr' F_{j_1}(r) F_{j_2}(r') V(r,r') u_{j_1}(r) u_{j_2}(r')$$

Width at low energy

$$\Gamma(E_k) \sim W(E_k) \sim E_k^{l_1 + l_2 + 2}$$

Non-Hermitian eigenvalue problem

Reaction calculation

Traditional Shell Model

Hermitian part of interaction

$$H = H_{\mathcal{PP}} + \Delta$$

Full effective Hamiltonian

Unperturbed Green's function

$$-\Delta \qquad \qquad G(E) = \frac{1}{E - H_{PP} - \Delta(E)}.$$

Inclusion of decay channels

Full Internal propagator

$$\mathcal{H}(E) = H_{\mathcal{PP}} + \Delta(E) - i\pi \mathbf{A}\mathbf{A}^{\dagger} \qquad \qquad \mathcal{G}(E) = \frac{1}{E - \mathcal{H}}$$

Results

Matrix diagonalization

•Hermitian eigenvalues below

thresholds

•Non-Hermitian eigenvalues above threshold

•resonances and widths (need definition)

•R-matrix $R = \mathbf{A}^{\dagger} G \mathbf{A}$

•Dyson Equation

$$\mathcal{G} = G - (i/2)GW\mathcal{G}$$

Transition matrix and cross section

$$T = \frac{R}{1 + i\pi R}, \quad S = \frac{1 - i\pi R}{1 + i\pi R}$$

Complex Energy eigenvalue problem

Eigenvalue problem $\mathcal{H}(E)|\alpha\rangle = E|\alpha\rangle$ has only complex (E>threshold) roots but E is real?

Definitions of resonance

Gamow: poles of scattering matrix H(ε)|α⟩ = ε|α⟩
 Eigenvalue problem with regular w.f. inside outgoing outside boundary condition → discrete resonant states + complex energies ε

$$E_{\text{res}} = Re(\mathcal{E}) \quad \Gamma_{\text{res}} = -2Im(\mathcal{E})$$

- Breit-Wigner: Find roots on real axis $Re\left[\mathcal{H}(E_{\text{res}})\right] = E_{\text{res}}$ $\Gamma_{\text{res}} = -2Im\left[\mathcal{H}(E_{\text{res}})\right]$
- Cross section peaks and lifetimes

$$\frac{d^2 \delta_l(E)}{dE^2} \bigg|_{E=E_{\text{res}}} = 0 \qquad \frac{2}{\Gamma_{\text{res}}} = \frac{d \delta_l(E)}{dE} \bigg|_{E=E_{\text{res}}}$$

Interpretation of complex energies

Observed

Poles in

complex plane

cross section

F

- For isolated narrow resonances all definitions agree
- Real Situation
 - Many-body complexity
 - High density of states
 - Large decay widths
- Result:
 - Overlapping, interference, width redistribution
 - Resonance and width are definition dependent
 - Non-exponential decay
- Solution: Cross section is a true observable (S-matrix)

$$S^{ab}(E) = s_a^{1/2} \left\{ \delta^{ab} - \sum_{12} A_1^{a*} \left(\frac{1}{E - \mathcal{H}} \right)_{12} A_2^b \right\} s_b^{1/2}.$$

Non-Hermitian eigenvalue problem

Reaction calculation

Traditional Shell Model

Hermitian part of interaction

$$H = H_{\mathcal{PP}} + \Delta$$

Unperturbed Green's function

Full Internal propagator

 $\mathcal{G}(E) = \frac{1}{E - \mathcal{H}(E)}$

$$G(E) = \frac{1}{E - H_{\mathcal{PP}} - \Delta}$$

Inclusion of decay channels

Full effective Hamiltonian

$$\mathcal{H}(E) = H_{\mathcal{PP}} + \Delta(E) - i\pi \mathbf{A}\mathbf{A}^{\dagger}$$

Results

Matrix diagonalization

•Hermitian eigenvalues below

thresholds

•Non-Hermitian eigenvalues above threshold

•resonances and widths (need definition)

•R-matrix
$$R(E) = \mathbf{A}^{\dagger} G \mathbf{A}$$

•Dyson Equation

$$\mathcal{G} = G - (i/2)GW\mathcal{G}$$

Transition matrix and cross section

$$T = \frac{R}{1 + i\pi R}, \quad S = \frac{1 - i\pi R}{1 + i\pi R}$$

Calculation Details, Propagator-Strength Function

 $G(E)|\lambda\rangle = \frac{1}{E-H} = -i \int_0^\infty dt \exp(iEt) \exp(-iHt)|\lambda\rangle$ •Scale Hamiltonian so that eigenvalues are in [-1 1] •Expand Using evolution operator in Chebyshev polynomials $\exp(-iHt) = \sum_{n=0}^\infty (-i)^n (2 - \delta_{n0}) J_n(t) T_n(H)$

•Use iterative relation and matrix-vector multiplication to generate

$$\begin{aligned} |\lambda_n\rangle &= T_n(H)|\lambda\rangle \\ |\lambda_0\rangle &= |\lambda\rangle, \quad |\lambda_1\rangle = H|\lambda\rangle, \quad \text{and} \quad |\lambda_{n+1}\rangle = 2H|\lambda_n\rangle - |\lambda_{n-1}\rangle \\ \langle \tilde{\lambda}|\lambda_{m+n}\rangle &= 2\langle \tilde{\lambda}_m|\lambda_n\rangle - \langle \tilde{\lambda}|\lambda_{n-m}\rangle, \quad n \ge m \end{aligned}$$

•Use ⊢⊢ I to find return to energy representation

T. Ikegami and S. Iwata, J. of Comp. Chem. 23 (2002) 310-318

Green's function calculation

- Advantages of the method
- -No need for full diagonalization or inversion at different E
- -Only matrix-vector multiplications
- -Numerical stability*



*W.Press, S. Teukolsky, W. Vetterling, B. Flannery, Numerical Recipes in C++ the art of scientific computing, Cambridge University Press, 2002

Realistic Shell Model Example

- Interaction
 - PHP Shell model Hamiltonian, USD interaction
 - Assume that USD includes Hermitian Δ
 - QHQ and QHP one-body Woods-Saxon potential
 - QHP two-body phenomenological parameterization
- Solution
 - From ⁴He up to ¹⁰He
 - From ¹⁶O up to ²⁸O
 - Given guess energy E for state α , W(E) is constructed by considering all open channels.
 - Non-Hermitian Hamiltonian is solved for iteratively for new E (Breit-Wigner resonance condition)

Continuum Shell Model He isotopes

Cross section and structure within the same formalism
Reaction I=1 polarized elastic channel



References

[1] A. Volya and V. Zelevinsky,
Phys. Rev. Lett 94 (2005) 052501.
[2] A. Volya and V. Zelevinsky,
Phys. Rev. C 67 (2003) 54322



CSM oxygen results

Α	j	mode	EXP	Q	Г	theory	E	Q	Г
17	3/2+	γn	5.085	0.941	96	WS	4.5	1.0	122
18	2+	$\gamma \alpha n$	8.213	0.169	1 ± 0.8	USD	9.465	1.242	200
18	1+	lpha n	8.817	0.773	70 ± 12	USD	10.823	2.600	85
18	4+	$\gamma \alpha n$	8.955	0.911	43 ± 3	USD	8.750	0.526	28
19	5/2+	n	5.148	1.191	3.4 ± 1	USD	5.011	1.121	5.1
19	9/2+		5.384	1.427	~ 0	USD	5.175	1.282	0
19	3/2+	n	5.54	1.58	320	USD	5.529	1.636	290
19	7/2+	n	6.466	2.509	small	USD	6.880	0.808*	63
24	2+	n	?	?	?	HBUSD	4.850	0.489	18
26	0+	2n	0	?	?	HBUSD	0	0.021	0.02
28	0+	2 <i>n</i>	0	?	?	HBUSD	0	0.345	14

Lowest resonant states in the chain of oxygen isotopes. The experimental data on the left, (EXP) - energy of the state (MeV), Q - energy above threshold (MeV), γ - width (keV), are compared to the theoretical results on the right. The decay mode in the second column indicates the decay branches assumed by experimentalists (NNDC)

Continuum Shell Model Oxygen Isotopes



Narrow resonance-spectroscopic factor approximation for sequential decay



Kinematics of sequential 2-body s-wave decay. Example:²⁶O->2n+²⁴O



Interplay of collectivities

Definitionsn - labels particle-hole state ε_n - excitation energy of state n d_n - dipole operator A_n - decay amplitude of n

Model Hamiltonian

$$\mathcal{H}_{nn'} = \epsilon_n \delta_{nn'} + \lambda d_n d_{n'} - \frac{i}{2} A_n A_{n'},$$

Driving GDR externally (doing scattering)





Everything depends on angle between multi dimensional vectors A and d

States and cross section in ²²O

Parameters of the model

Internal shell s-p-sd-pf shell model with WBP interaction
 Decay channels g.s. of ¹⁹O(or ²¹O) + neutron decay from fp
 EM channel: E1 strength from ²⁰O(or ²²O)



Isovector Dipole strength in Oxygen



Summary:

- New theoretical techniques
- First applications and success stories
- Interplay of internal and external, generic features
- Technical problems and solutions
- Toward realistic applications

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Recent publications:

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