Microscopic folding potentials for negative and positive single-nucleon energies

Hugo F. Arellano
Department of Physics, U Chile-FCFM

In collaboration with G. Blanchon (CEA)

ECT Towards consistent approaches for nuclear structure and reaction*
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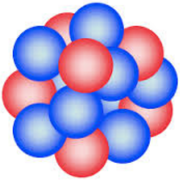
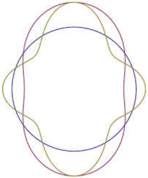
Itinerary

1. Introduction
2. Folding models
3. An application
4. Concluding remarks

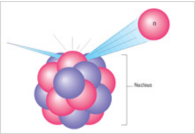
Structure and reactions...



Structure

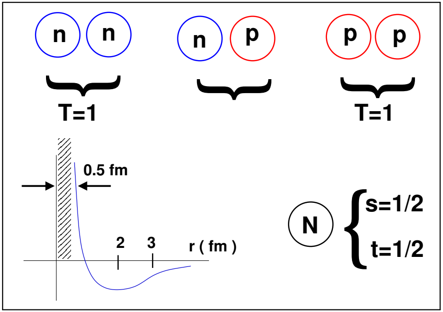


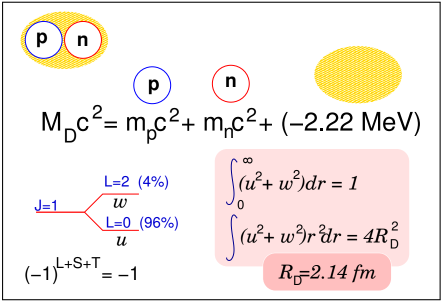
Excitations



Collisions and reactions

$\textit{Ab-initio} \leftrightarrows V_{NN}, V_{NNN}, \ldots \rightarrow$ nuclear matter





- Deuteron (pn), only known bound state in free space: $T = 0$; $S = 1$; $J^\pi = 1^+$.
- Phase-shifts $\delta_L(E)$ for $E/2 \lesssim m_\pi c^2$
- Static properties ^3H, etc.

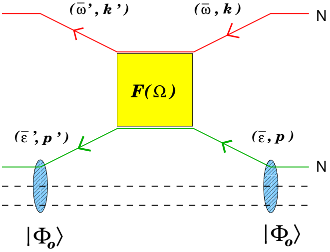
Problem & motivation

- Can we provide a reasonable description of both nucleus g.s. and nucleon-nucleus collisions by extending folding models to negative energies, based *solely* on bare internucleon potentials: $V_{NN}, V_{NNN}, \cdots$?
- Take advantage of BBG effective interaction: $V|\Psi\rangle = G|\phi\rangle$.
- Folding structure for expectation values of one-body operators appear 'universal': Feshbach P Q operators; KMT optical model; ...
- *Caveat:* this attempt lacks rigorous link $1+1 \to A$. Explore feasibility and soundness of the idea.

General considerations

- Non-relativistic
- Realistic bare *NN* interaction:
  AV18, Paris, Nijmegen I and II, N3LO, N3LO+N2LO(3N), etc.
- Lowest order in BHF

Microscopic NA optical potential



$$U_A(\mathbf{k}', \mathbf{k}; E) = \int d\mathbf{p}\, d\mathbf{p}' \underbrace{\rho(\mathbf{p}', \mathbf{p})}_{HF} \underbrace{\langle \mathbf{k}'\, \mathbf{p}' \,|T(E)|\, \mathbf{k}\, \mathbf{p} \rangle_{\mathscr{A}}}_{NN}$$

$$(\hat{K} + \hat{U}_A(E))\,|\,\Psi\rangle = E\,|\,\Psi\rangle$$

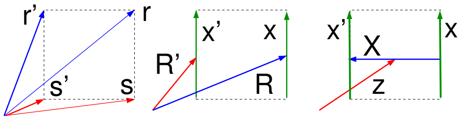
General considerations

Let F a two-body operator and examine its momentum- and coordinate-space structure.

$$\langle \mathbf{r}'\, \mathbf{s}' \mid F \mid \mathbf{r}\, \mathbf{s} \rangle = F(\mathbf{r}'\, \mathbf{s}'; \mathbf{r}\, \mathbf{s}) \to F_{\mathbf{R}'\mathbf{R}}(\mathbf{x}', \mathbf{x})$$

where

$$\mathbf{R}' = \tfrac{1}{2}(\mathbf{r}' + \mathbf{s}')\,; \qquad \mathbf{R} = \tfrac{1}{2}(\mathbf{r} + \mathbf{s})\,; \qquad \mathbf{x}' = \mathbf{r}' - \mathbf{s}'\,; \qquad \mathbf{x} = \mathbf{r} - \mathbf{s}\,.$$



In momentum space we define

$$\langle \mathbf{k}'\,\mathbf{p}' \mid F \mid \mathbf{k}\,\mathbf{p}\rangle \equiv \tilde{F}(\mathbf{k}'\,\mathbf{p}';\mathbf{k}\,\mathbf{p}) \rightarrow F(\mathbf{W}',\mathbf{W};\mathbf{b}',\mathbf{b})$$

We have demonstrated Arellano-Bauge, PRC76,014613 (2007).

$$\langle \mathbf{k}'\,\mathbf{p}' \mid F \mid \mathbf{k}\,\mathbf{p}\rangle = \frac{1}{(2\pi)^3}\int d\mathbf{z}\; e^{i\mathbf{z}\cdot(\mathbf{W}'-\mathbf{W})}\; F_{\mathbf{z}}[\tfrac{1}{2}(\mathbf{W}'+\mathbf{W});\mathbf{b}'\,\mathbf{b}]\,.$$

with

$$\mathbf{z} = (\mathbf{R}'+\mathbf{R})/2$$

and

$$\mathbf{W}' = \mathbf{k}'+\mathbf{p}'\,; \qquad \mathbf{b}' = (\mathbf{k}'-\mathbf{p}')/2\,;$$

$$\mathbf{W} = \mathbf{k}+\mathbf{p}\,; \qquad \mathbf{b} = (\mathbf{k}-\mathbf{p})/2\,.$$

Model

$$U_A(\mathbf{k}',\mathbf{k};E) = \int d\mathbf{p}\, d\mathbf{p}'\, \rho(\mathbf{p}',\mathbf{p})\, \frac{1}{(2\pi)^3} \int d\mathbf{z}\, e^{i\mathbf{z}\cdot(\mathbf{W}'-\mathbf{W})} \underbrace{F_{\mathbf{z}}[\tfrac{1}{2}(\mathbf{W}'+\mathbf{W});\mathbf{b}'\,\mathbf{b}]}_{\text{Model?}}\,.$$

Particular (well established) limits

- F_z translational invariant with $\hat{\rho}$ Slater representation
  $\rightarrow$ mass operator for infinite nuclear matter (JLM)
- F_z translational invariant with $\hat{\rho}$ finite nucleus
  $\rightarrow$ full-folding optical model potentials (KMT)
- F_z local
  $\rightarrow$ density dependent local effective interaction (Melbourne)

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Special cases

1. Free t matrix:
   $F \to t_{free} \Rightarrow z-$independent $\Rightarrow$

$$\langle \mathbf{k}'\,\mathbf{p}' \mid F \mid \mathbf{k}\,\mathbf{p}\rangle = \delta(\mathbf{k}'+\mathbf{p}'-\mathbf{k}-\mathbf{p})\; t(\mathbf{k}+\mathbf{p};\mathbf{b}'\,\mathbf{b})\;.$$

2. BHF g matrix

$$F_{\mathbf{z}}\left[\tfrac{1}{2}(\mathbf{W}'+\mathbf{W});\mathbf{b}'\,\mathbf{b}\right] \to g_E\left[\rho_z;\tfrac{1}{2}(\mathbf{W}'+\mathbf{W});\mathbf{b}'\,\mathbf{b}\right]$$

- BHF: g: infinite nuclear matter g matrix

$$g(E) = V_{NN} + V_{NN}\frac{Q_F}{E+i\eta-\hat{h}_1-\hat{h}_2}\,g(E)$$

- Each $z \Rightarrow \rho_z \quad \Rightarrow \quad g[\rho_z]$.
- Zero-density limit $g \to t$:

$$t(E) = V_{NN} + V_{NN}\frac{1}{E+i\eta-\hat{k}_1-\hat{k}_2}\,t(E)$$

The 'unabridged folding'

$$U_A(\mathbf{k}',\mathbf{k};E) = \frac{1}{(2\pi)^3}\int \underbrace{d\mathbf{Q}\; d\mathbf{P}\; d\mathbf{z}}_{9D!}\; e^{i\mathbf{z}\cdot(\mathbf{Q}-\mathbf{q})}\rho_A(\mathbf{Q};\mathbf{P})\; \mathbf{g_E}\left(\rho_\mathbf{z};\mathbf{K}+\mathbf{P};\kappa_-,\kappa_+\right)\;,$$

where

$$\mathbf{K} = (\mathbf{k}'+\mathbf{k})/2\;;\quad \mathbf{q} = \mathbf{k}-\mathbf{k}'\;;\quad \mathbf{P} = (\mathbf{p}'+\mathbf{p})/\mathbf{2}\;;\quad \mathbf{Q} = \mathbf{p}'-\mathbf{p}\;.$$

and

$$\kappa_\pm = \tfrac{1}{2}(\mathbf{K}-\mathbf{P}) \pm \tfrac{1}{4}(\mathbf{Q}+\mathbf{q}).$$

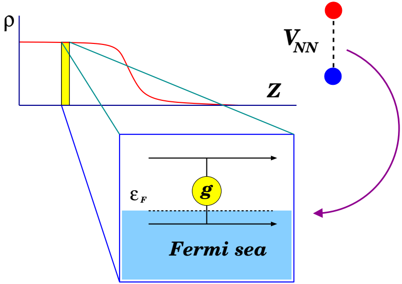
Fermi motion accounted for by:
$\mathbf{Q} = \mathbf{p}'-\mathbf{p}$ (mtum transfer), and
$\mathbf{P} = \frac{1}{2}(\mathbf{p}'+\mathbf{p})/2$ (struck-nucleon 'current')
First calculation reported in PRC84, 034606 (2011).
Uses wavefunctions $\{\phi_\alpha\}$.

Approximations

- Localize the interaction: $g(\vec{k}', \vec{k}) \to \tilde{v}(\vec{k}' - \vec{k}) \to v(r)$
  - K. Amos *et al.* (2000+)
  - H. von Geramb (80s)
  - Brieva-Rook (mid 70s)
- Assume free t matrix $\to$ 'full-folding' (early 90s: Elster+, Crespo+ and Arellano+.) adequate at intermediate energies
- *In-medium* full-folding (mid 90's)
  Include medium effects + simplify momentum dependence and take Slater approximation for mixed density (Arellano-Brieva-Love):

$$U_A(\mathbf{k}', \mathbf{k}; E) \approx \int d\mathbf{z}\, e^{-i\mathbf{z}\cdot\mathbf{q}}\, \rho(z)\, \langle\, g[\,\rho_z\,]\,\rangle_{\mathscr{A}}$$

BHF



$$g(\Omega) = V + V \frac{Q}{\Omega - \hat{h}_1 - \hat{h}_2} g(\Omega)$$

In this work...

$$U_A(\vec{k}',\vec{k};E) = \sum_\alpha \int d\vec{P}\hat{\rho}_\alpha(\vec{q};\vec{P})\mathbf{t}_{Free}(E+\varepsilon_\alpha) \tag{1}$$

$$-\frac{1}{6\pi^2}\int d\vec{Q}\,d\vec{P}\sum_\alpha \hat{\rho}_\alpha(\vec{Q};\vec{P})\int_0^\infty z^3 dz \left[\frac{3j_1(z|\vec{Q}-\vec{q}|)}{z|\vec{Q}-\vec{q}|}\right]\frac{\partial g[\rho(z);E+\varepsilon_\alpha]}{\partial z} \tag{2}$$

Shorthand $\rightarrow U_A(E)$.

Unleash E: $-\infty < E < \infty$

To get $U_A(E)$ need $\{\varphi_\alpha\}$.

Calculate eigenenergies and eigenvectors from $[\hat{K}+\hat{U}_A(\varepsilon)] \mid \varphi\rangle = \varepsilon \mid \varphi\rangle$.

How do we do so? $\rightarrow \det[1-G_0(\varepsilon)U_A(\varepsilon)] = 0$

About the sp wavefunctions

- Lehmann spectral representation for the T matrix $\Rightarrow$

$$\lim_{\eta\to 0} i\eta\, T(\varepsilon_\alpha + i\eta) = U_A(\varepsilon_\alpha) \mid \varphi_\alpha\rangle\langle\varphi_\alpha \mid U_A(\varepsilon_\alpha)\,.$$

  where

$$T(\varepsilon) = U_A(\varepsilon) + U_A(\varepsilon) G_0(\varepsilon) T(\varepsilon)\,.$$

- sp wavefunction:

$$\varphi_\alpha(q) = \langle q \mid \varphi_\alpha\rangle = \frac{\langle q \mid U_A(\varepsilon_\alpha) \mid \phi_\alpha\rangle}{\varepsilon_\alpha - q^2/2m}$$

Results and comparison with data

Self-consistency means

$$[\hat{K} + U_A(\varepsilon_\alpha)]|\phi_\alpha\rangle = \varepsilon_\alpha|\phi_\alpha\rangle \;,$$

Eigenenergies: $\varepsilon_{nlj} \equiv \varepsilon_\alpha$
Expectation values:

$$t_\alpha = \frac{\langle\phi_\alpha|\hat{K}|\phi_\alpha\rangle}{\langle\phi_\alpha|\phi_\alpha\rangle}$$

$$u_\alpha = \frac{\langle\phi_\alpha|U_A(\varepsilon_\alpha)|\phi_\alpha\rangle}{\langle\phi_\alpha|\phi_\alpha\rangle}$$

$$\varepsilon_\alpha = t_\alpha + u_\alpha$$

Ground-state energy:

$$E_0 = \sum_{occ} t_\alpha + \frac{1}{2}\sum_{occ} u_\alpha = E_{sp} - \frac{1}{2}\sum_{occ} u_\alpha \,.$$

The sp energies per nucleon:

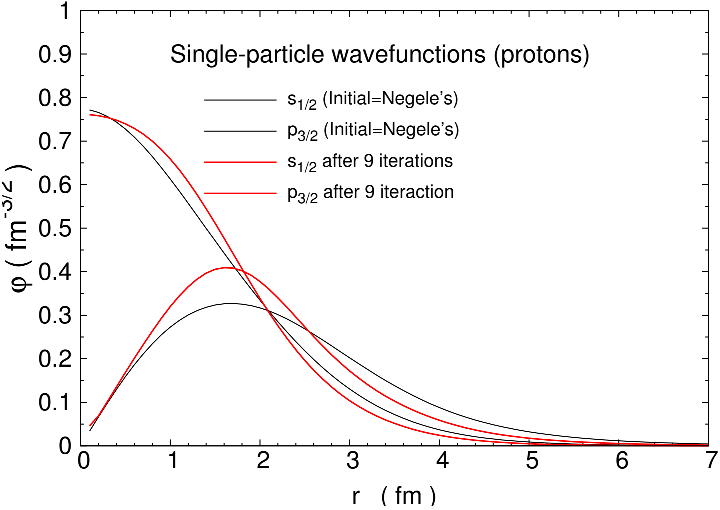
$$E_{sp}^{(p)}/Z = \sum_{prot}(2j+1)\varepsilon_{nlj}/Z \,, \qquad E_{sp}^{(n)}/N = \sum_{neut}(2j+1)\varepsilon_{nlj}/N \,.$$

Results for C12 based on AV18 and N3LO3N

Ground-state sp levels

	Protons				Neutrons				
Force	n	l	j	ε_{nlj} (MeV)	n	l	j	ε_{nlj} (MeV)	Obs.
Negele's	1	0	0.5	-32.81	1	0	0.5	-35.75	
	1	1	1.5	-12.53	1	1	1.5	-15.17	
BHF + AV18	1	0	0.5	-48.02	1	0	0.5	-51.57	
(9 iterations)	1	1	1.5	-21.75	1	1	1.5	-25.03	
BHF + N3LO3N	1	0	0.5	-52.51	1	0	0.5	-56.41	
(9 iterations)	1	1	1.5	-23.54	1	0	0.5	-27.12	

Wavefunctions...



Radii

Bare v_{NN}	RMS radii (fm)			
	Proton	Neutron	Matter	Charge
Negele	2.56	2.54	2.55	2.68
BHF+AV18	2.18	2.16	2.17	2.32
BHF+N3LO3N	2.14	2.12	2.13	2.28

sp levels based on AV18 after 9 iterations

Protons			Neutrons		
ε_{nlj}	l	j	ε_{nlj}	l	j
-48.02	0	0.5	**-51.57**	0	0.5
-21.75	1	1.5	**-25.03**	1	1.5
-16.62	1	0.5	-19.79	1	0.5
-1.83	0	0.5	-4.40	0	0.5
-1.25	2	2.5	-4.14	2	2.5

Hughenholtz-Van Hove (HvH) theorem

General result: Fermi energy *versus* mean energy of bound systems

$$\frac{E}{N} + \frac{p}{\rho} = E_F \,.$$

Equilibrium $p = 0 \quad \rightarrow \quad B/A = E_F$
Infinite NM within BHF violates HvH theorem by (AV18) ∼17.9 MeV.

$$\begin{aligned} k_F^{sat} &= 1.50\,\mathrm{fm}^{-1} \\ B/A &= -16.78\,\mathrm{MeV} \\ E_F &= -34.71\,\mathrm{MeV} \end{aligned} \tag{3}$$

Test HvH for BHF+AV18 (*ab-initio*) calculations (MeV units)

Nucleus	E_0/N	E_F	ΔE
C12 - p	-4.21	-23.54	19.33
C12 - n	-5.57	-27.12	21.55
O16 - p	-6.78	-25.21	18.43
O16 - n	-8.68	-29.37	20.69
Ca40 - p	-11.55	-33.78	22.23
Ca40 - n	-13.42	-37.02	23.60

Issues, current and pending work...

- Ongoing work
- Order of sp states is the correct one. (not obvious!).
- HvH theorem and rearrangement corrections:
  Grange, Cugnon and Lejeune [NPA473, 365(1987)]: Nuclear mean fields with correlations at finite T. Study at normal density. The expansion for the mass operator includes $M(k,E) = M_1(k,E) + M_2(k,E) + \cdots$.
  Zuo, Bombaci and Lombardo [PRC60, 024605(1999)]: Extended BHF for asymmetric nuclear matter.
  Czerski, De Pace and Molinari [PRC65, 044317(2002)] 'empirical' procedure to include rearrangement,
- Gram matrix: $\langle \phi_\alpha \mid \phi_\beta \rangle \neq \delta_{\alpha\beta} \rightarrow \hat{\rho} = ?$
- Center of mass motion
- Scattering?