Generator Coordinate Method
and
Symmetries

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GCM and GHW equation 1/2

Trial function

$$|\Psi\rangle = \int_{\mathcal{O}} d\alpha f(\alpha)|\alpha\rangle$$

α= set of generator variables, $|\alpha\rangle$= set of intrinsic generator functions and unknown $f(\alpha)$= weight functions.

Variational principle

$$\delta\langle\Psi|\hat{H}|\Psi\rangle = 0, \text{ where } \langle\Psi|\Psi\rangle = 1.$$

GHW equation

$$\hat{\mathcal{H}}f(\alpha) = E\hat{\mathcal{N}}f(\alpha),$$

One needs to solve the integral equation.

GCM and GHW equation 2/2

Notation:

The integral Hamilton operator

$$\hat{\mathcal{H}} f(\alpha) \equiv \int_{\mathcal{O}} d\alpha' \, \mathcal{H}(\alpha, \alpha') f(\alpha'),$$

where the hamiltonian kernel $\mathcal{H}(\alpha, \alpha') \equiv \langle \alpha | \hat{H} | \alpha' \rangle$.

The overlap operator

$$\hat{\mathcal{N}} f(\alpha) \equiv \int_{\mathcal{O}} d\alpha' \, \mathcal{N}(\alpha, \alpha') f(\alpha'),$$

where the overlap kernel $\mathcal{N}(\alpha, \alpha') \equiv \langle \alpha | \alpha' \rangle$.

GCM as a projection method 1/2

The eigenequation of $\hat{\mathcal{N}}$

$$\hat{\mathcal{N}} w_n(\alpha) = \lambda_n w_n(\alpha).$$

The set of $w_n(\alpha)$ for $\lambda_n \neq 0$ is the basis in the space $\mathcal{K}_w$ of the weight functions f. It allows to construct the basis in the corresponding many-body space $\mathcal{K}$:

The natural states

$$|\psi_n\rangle = \frac{1}{\sqrt{\lambda_n}} \int_{\mathcal{O}} d\alpha \, w_n(\alpha) |\alpha\rangle.$$

This basis allows to **construct the projection operator**

$$P_{\mathcal{K}_{coll}} = \sum_{\lambda_n > 0} |\psi_n\rangle\langle\psi_n|$$

GCM as a projection method 2/2

Standard way – solution of the GHW equation:

- Solve the overlap operator equation, and find: λ_n and $w_n(\alpha)$.
- Construct the natural states.
- Compute

$$\langle\psi_k|\hat{H}|\psi_l\rangle = \frac{1}{\sqrt{\lambda_k\lambda_l}}\int_{\mathcal{O}} d\alpha d\alpha' w_k(\alpha)^\star \langle\alpha|\hat{H}|\alpha'\rangle w_l(\alpha').$$

- Solve the eigenvalue problem $\sum_l H_{kl}h_l = Eh_k$.
- Construct the weight function

$$f(\alpha) = \sum_n \frac{1}{\sqrt{\lambda_n}} h_n w_n(\alpha)$$

Hamiltonian symmetries and GHW equation 1/3

Let G be a symmetry group of the Hamiltonian $\hat{H}$:

$$\hat{g}\hat{H}\hat{g}^{-1} = \hat{H}$$

Fundamental property

$$\hat{H}\phi_n(x) = E_n\phi_n(x) \quad \Rightarrow \quad \hat{H}(\hat{g}\phi_n(x)) = E_n(\hat{g}\phi_n(x)).$$

Assume the GCM ansatz:

$$\phi_n(x) = \int_{\mathcal{O}} d\alpha\, f_n(\alpha)\Phi_0(\alpha; x),$$

where $\Phi_0(\alpha; x) \equiv \langle x|\alpha\rangle$.

Hamiltonian symmetries and GHW equation 2/3

One expects the same property for the GHW equation

$$\hat{\mathcal{H}}(g\, f_n(\alpha)) = E_n \hat{\mathcal{N}}(g\, f_n(\alpha)).$$

Transform the left hand side of the above condition:

$$\begin{aligned}
&\hat{\mathcal{H}}\, g f_n(\alpha) = [\hat{\mathcal{H}}, g] f_n(\alpha) + g \hat{\mathcal{H}} f_n(\alpha) = \\
&[\hat{\mathcal{H}}, g] f_n(\alpha) + E_n g \hat{\mathcal{N}} f_n(\alpha) = \\
&[\hat{\mathcal{H}}, g] f_n(\alpha) + E_n [g, \hat{\mathcal{N}}] f_n(\alpha) + E_n \hat{\mathcal{N}}\, g f_n(\alpha)
\end{aligned}$$

It implies the following condition:

Compatibility condition (CC)

$$[\hat{\mathcal{H}}, g] f_n(\alpha) = E_n [\hat{\mathcal{N}}, g] f_n(\alpha)$$

Hamiltonian symmetries and GHW equation 3/3

If

Practical and sufficient condition (PSC)

$$g\hat{\mathcal{H}}g^{-1} = \hat{\mathcal{H}} \quad \text{and} \quad g\hat{\mathcal{N}}g^{-1} = \hat{\mathcal{N}}$$

the compatibility condition is always fuflfilled.

Are the condition CC and PSC equivalent ? It is an open question.

Symmetry in GCM

A physical system decribed in the GCM formalism has the symmetry of the Hamiltonian $\hat{H}$ if the PSC, or more generally CC condition is fulfilled.

Symmetry group action 1/2

The symmetry group of the Hamiltonian $\hat{H}$ is defined in the many-body space $\mathcal{K}$. One needs to find its realization in the space of weight functions $\mathcal{K}_w$.

A natural symmetry group G action which relates both spaces $\mathcal{K}$ and $\mathcal{K}_w$:

$$\hat{g}|\alpha\rangle = |g\alpha\rangle, \quad \text{for all} \quad g \in \mathrm{G}$$

It implies (the integral should be G-invariant)

$$\hat{g}|\Psi\rangle = \int_{\mathcal{O}} d\alpha\, f(\alpha)|g\alpha\rangle = \int_{\mathcal{O}} d\alpha\, f(g^{-1}\alpha)|\alpha\rangle$$

G action in the weight space

$$gf(\alpha) = f(g^{-1}\alpha)$$

Symmetry group action 2/2

Using this action:

Invariant kernels

$$\hat{g}\hat{\mathcal{A}}\hat{g}^{-1} = \hat{\mathcal{A}} \Leftrightarrow \mathcal{A}(g\alpha, g\alpha') = \mathcal{A}(\alpha, \alpha').$$

The integral has to be G-invariant.

Symmetry conserving GCM: For all $g \in \mathrm{G}$

$$\mathcal{N}(g\alpha, g\alpha') = \mathcal{N}(\alpha, \alpha'), \quad \text{and} \quad \mathcal{H}(g\alpha, g\alpha') = \mathcal{H}(\alpha, \alpha').$$

G compatible intrinsic generating function:

$$|\beta, g\rangle = \hat{g}|\beta\rangle, \text{ where } \hat{g'}|\beta, g\rangle = \text{ either } |\beta, g'g\rangle \text{ or } |\beta, gg'\rangle.$$

An important example: an abelian group 1/2

Let the symetry group G be an abelian group and

$$|\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)\rangle = \hat{g}(\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n))|-\rangle$$

Note that

$$\hat{\mathcal{N}}\chi^{\Gamma}(\alpha) = \int_{\mathrm{G}} d\alpha' \, \langle -|\hat{g}(\alpha)^{\dagger}\hat{g}(\alpha')|-\rangle \chi^{\Gamma}(\alpha') =$$

$$\int_{\mathrm{G}} d\alpha' \, \langle -|\hat{g}(\alpha^{-1}\alpha')|-\rangle \chi^{\Gamma}(\alpha') = \int_{\mathrm{G}} d\alpha' \, \langle -|\hat{g}(\alpha')|-\rangle \chi^{\Gamma}(\alpha\alpha')$$

$$\hat{\mathcal{N}}\chi^{\Gamma}(\alpha) = \left\{ \int_{\mathrm{G}} d\alpha' \, \langle -|\hat{g}(\alpha')|-\rangle \chi^{\Gamma}(\alpha') \right\} \chi^{\Gamma}(\alpha),$$

where $\chi^{\Gamma}(\alpha)$ are characters of the symmetry group G.

An important example: an abelian group 2/2

To this class belongs a series of problems:

Axial symmetry and simplified angular momentum conservation

$$|\alpha\rangle = \exp(-i\alpha\vec{n}\cdot\hat{\vec{J}})$$

Rotations in the space of number of particles and the particle number conservation

$$|\alpha\rangle = \exp(-i\phi\hat{N})$$

and many others.

Remark: GCM as "restoration" of symmetries 1/2

Assume $\tilde{w}_{\nu\Gamma\kappa}(g,\alpha)$ are eigenstates of $\hat{\mathcal{N}}$ and G required symmetry:

$$\mathrm{G} = \mathrm{Sym}(\hat{\mathcal{N}}) \text{ and } \mathrm{G} \neq \mathrm{Sym}(\hat{\mathcal{H}}) \subset \mathrm{G}.$$

$$|\nu\Gamma\kappa\rangle = \frac{1}{\sqrt{\lambda_{\nu\Gamma}}} \int_{\mathrm{G}} dg \int_{\mathcal{O}} d\alpha\, \tilde{w}_{\nu\Gamma\kappa}(g,\alpha)\hat{g}|\alpha\rangle =$$

$$= \int_{\mathcal{O}} d\alpha \sum_{\kappa'} w_{\nu\Gamma\kappa'}(\alpha) P^{\Gamma}_{\kappa\kappa'}|\alpha\rangle$$

where

$$\tilde{w}_{\nu\Gamma\kappa}(g,\alpha) = \dim(\Gamma) \sum_{\kappa'} w_{\nu\Gamma\kappa'}(\alpha) \Delta^{\Gamma}_{\kappa\kappa'}(g)^{\star}.$$

An important note: GCM as "restoration" of symmetries 2/2

Set of generator functions

$$\sum_{\kappa'} w_{\nu\Gamma\kappa'}(\alpha) P^{\Gamma}_{\kappa\kappa'} |\alpha\rangle,$$

where $w_{\nu\Gamma\kappa'}(\alpha)$ can be considered as the weight functions, allows to force ("restore") the required symmetry G of the integral Hamiltonian $\hat{\mathcal{H}}$.

Symmetries in the intrinsic frame

The most important symmetries
are seen ONLY in the
INTRINSIC FRAME of the NUCLEUS

Quantum rotations

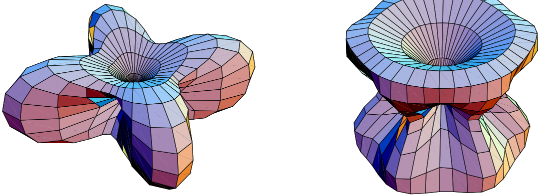

Figure: The rotated body probability spin orientations for the rotator wave functions $\psi \sim D^5_{M2} - D^5_{M,-2}$ (left) and $\psi \sim D^5_{M3} - D^5_{M,-3}$ (right)

Microscopic intrinsic frame 1/3

DEF. Intrinsic Frame (Biedernharn, Louck)

$$\vec{f}_k(\vec{x}_1 + \vec{a}, \vec{x}_2 + \vec{a}, \ldots, \vec{x}_A + \vec{a}) = \vec{f}_k(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A)$$

$$\begin{aligned} \vec{f}_k(\hat{\mathcal{R}}\vec{x}_1, \hat{\mathcal{R}}\vec{x}_2, \ldots, \hat{\mathcal{R}}\vec{x}_A) &= \hat{\mathcal{R}}\vec{f}_k(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A) \\ &= \sum_k \mathcal{R}_{ki}\vec{f}_k(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A) \end{aligned}$$

$$\left(\frac{\partial \vec{f}_i}{\partial x_{n;1}}, \frac{\partial \vec{f}_i}{\partial x_{n;2}}, \frac{\partial \vec{f}_i}{\partial x_{n;3}},\right) \neq \vec{0},$$

for any i and all n.

Microscopic intrinsic frame 2/3

A natural choice of the microscopic intrinsic frame:

The following conditions relate the laboratory $x_{n;l}$ and intrinsic $(y_{n;l}, \Omega)$ coordinates:

$$x_{n;l} = R_l^{CM} + \sum_k D_{kl}(\Omega^{-1}) y_{n;k}$$

Def. of rotational variables

$$\vec{l}_k = R(\Omega^{-1}) \vec{f}_k(\vec{x}_1, \ldots, \vec{x}_A)$$

The center of mass condition

$$\sum_{n=1}^{3A} m_n \, y_{n;k} = 0$$

Microscopic intrinsic frame 3/3

Principal axes frame:

Def. of rotation variables

$$Q_{ij}^{(lab)}(x) = \sum_{i'j'} D_{ii'}(\Omega) Q_{i'j'}(y), D_{j'j}(\Omega^{-1})$$

$$Q_{ij}(y) = \sum_{n=1}^{A} m_n y_{ni} y_{nj}.$$

Principal axes rotating frame

$$Q_{ij}(y) = 0 \text{ for } i \neq j.$$

Intrinsic groups $\overline{\mathrm{G}}$

Jin-Quan Chen, Jialun Ping & Fan Wang: Group Representation Theory for Physicists, World Scientific, 2002.

Def. For each element g of the group G, one can define a corresponding operator $\overline{g}$ in the group linear space $\mathcal{L}_G$ as:

$$\overline{g}S = Sg, \qquad \text{for all } S \in \mathcal{L}_G.$$

The group formed by the collection of the operators $\overline{g}$ is called the intrinsic group of G.

IMPORTANT PROPERTY:

$$[G, \overline{\mathrm{G}}] = 0$$

The groups G and $\overline{\mathrm{G}}$ are antyisomorphic.

Hamiltonian and tranformations 1/3

Hamiltonian in the intrinsic frame

$$\hat{H}(x) \to \bar{H}(y,\Omega) = \bar{H}(y,\bar{J}_x,\bar{J}_y,\bar{J}_z)$$

Possible form: generalized rotor

$$\bar{H}(y,\bar{J}_x,\bar{J}_y,\bar{J}_z) = \bar{H}_0(y) + h_{00}(y)\,\bar{J}^2$$
$$+\sum_{\lambda=1}^{\infty}\left(h_{\lambda 0}(y)\,\hat{T}_0^{\lambda} \;+\; \sum_{\mu=1}^{\lambda}\left(h_{\lambda\mu}(y)\,\hat{T}_{\mu}^{\lambda} + (-1)^{\mu} h_{\lambda\mu}^{\star}(y)\,\hat{T}_{-\mu}^{\lambda}\right)\right),$$

$$\hat{T}_{\mu}^{\lambda} \;=\; \left(\left(\ldots\left(\left(\bar{J}\otimes\bar{J}\,\right)^{\lambda_2=2}\otimes\bar{J}\,\right)^{\lambda_3=3}\otimes\ldots\otimes\bar{J}\,\right)^{\lambda_{n-1}=n-1}\otimes\bar{J}\,\right)_{\mu}^{\lambda=n},$$

Hamiltonian and tranformations 2/3

Laboratory rotations

$$\hat{R}(\omega) \in \mathrm{SO}(3) : \hat{R}(\omega) f(y, \Omega) = f(y, \omega^{-1}\Omega)$$

Rotational invariance

$$\hat{R}(\omega)\hat{H}(x)\hat{R}(\omega^{-1}) = \hat{H}(x)$$

It implies

$$\hat{R}(\omega)\bar{H}(y, \bar{J}_x, \bar{J}_y, \bar{J}_z)\hat{R}(\omega^{-1}) = \bar{H}(y, \bar{J}_x, \bar{J}_y, \bar{J}_z)$$

Hamiltonian and tranformations 3/3

Important classes of transformations in the intrinsic frame:

1. Rotation intrinsic group

$$\bar{R}(\omega) \in \overline{\mathrm{SO}(3)} : \bar{R}(\omega) f(y, \Omega) = f(\bar{\omega} y, \Omega \omega^{-1})$$

It does not change laboratory variables x.

2. Intrinsic transformations of y only

$$\hat{g} \in \mathrm{G}_{vib} : \hat{g} f(y, \Omega) = f(\hat{g}^{-1} y, \Omega)$$

3. Intrinsic transformations of Ω only

$$\hat{g} \in \mathrm{G}_{rot} : \hat{g} f(y, \Omega) = f(y, \Omega g^{-1})$$

Symmetries of the intrinsic Hamiltonian

Intrinsic Hamiltonian symmetries

- $\bar{H}$ is invariant under all laboratory symmetries
- $\bar{H}$ has additional symmetries related to transformations of intrinsic variables

Structure of the symmetry group of $\bar{H}$:

$$\mathrm{G} = \mathrm{G}_{lab} \times \mathrm{G}_{int}$$

Symmetrization group G_s:

$$\mathrm{G}_s = \{g_s : g_s(y, \Omega) = (y', \Omega') \text{ then } x(y', \Omega') = x(y, \Omega)\}.$$

Symmetrization group G_s

To have unique states in the laboratory frame:

State symmetrization

$$g_s \psi(y, \Omega) = \psi(y, \Omega)$$

for all $g_s \in \mathrm{G}_s$

Note: All the transformations $\bar{R}(\omega) \in \overline{\mathrm{SO}(3)}$ which keep structure of the intrinsic variables belong to the symmetrization group G_s.

Example

For the principal axes frame and the intrinsic variables (y, Ω), the symmetrization group is the octahedral group O.

GCM in the intrinsic frame 1/2

Assume: $\hat{H}$ is rotation invariant (lab frame).

General structure of the physical generating functions

$$\Phi_{JM}(\alpha; y, \Omega) = \sum_K \phi_{JK}(\alpha; y) r^J_{MK}(\Omega)$$

where $r^J_{MK}(\Omega) = \sqrt{2J+1} D^{J\star}_{MK}(\Omega) \leftarrow$ (NOTE: it has well determined angular momentum)

GCM ansatz

$$\Psi_{JM}(y, \Omega) = \int_O d\alpha \int_{\mathrm{G}_{int}} dg \, f(\alpha, g) \, \hat{g} \Phi_{JM}(\alpha; y, \Omega)$$

where G_{int} is intrinsic symmetry of the intrinsic Hamiltonian.

GCM in the intrinsic frame 2/2

The weight functions

$$f(\alpha, g) = \dim(\Gamma) \sum_b \Delta^\Gamma_{ab}(g)^\star f^J_{\Gamma b}(\alpha)$$

Δ^Γ i.r. of the intrinsic symmetry group G_{int}.

GHW equation

$$\int_O d\alpha' \sum_{b'} f^J_{\Gamma b'}(\alpha') \langle \alpha; JM | (\bar{H} - E\mathbb{I}) B^\Gamma_{bb'} | \alpha'; JM \rangle = 0$$

where $\langle y, \Omega | \alpha; JM \rangle = \Phi_{JM}(\alpha; y, \Omega)$ and the projector:

$$B^\Gamma_{bb'} = \dim(\Gamma) \int_{\mathrm{G}_{int}} dg \, \Delta^\Gamma_{ab}(g)^\star \hat{g}$$

Example: The symmetry group as a subgroup of the symmetrization group

Example: Let $\mathrm{G} \subset \mathrm{G}_s$

For all $g \in \mathrm{G}_s$

$$\hat{g}\Phi_{JM}(\alpha; y, \Omega) = \Phi_{JM}(\alpha; y, \Omega)$$

then

$$B^{\Gamma}_{bb'}\Phi_{JM}(\alpha; y, \Omega) = \delta_{\Gamma 0}\Phi_{JM}(\alpha; y, \Omega)$$

$\Gamma = 0$ means the scalar representation of G.

GHW equation

$$\int_O d\alpha'\, f^J_{\Gamma=0 b'=0}(\alpha')\langle\alpha; JM|\bar{H} - E\mathbb{I}|\alpha'; JM\rangle = 0$$

Conclusions

- $\mathrm{Sym}(\mathrm{GHW}) = \mathrm{Sym}(\hat{H}) = \mathrm{G}$ if $\mathrm{Sym}(\hat{\mathcal{H}}) = \mathrm{Sym}(\hat{\mathcal{N}}) = \mathrm{G}$.
- For all $g \in \mathrm{G}$ the ket $\hat{g}|\alpha\rangle$ is defined.
  – Required: $|g\alpha\rangle = \hat{g}|\alpha\rangle$ and $f'(\alpha) = gf(\alpha)$, here $f(\alpha)$ is the weight function.
  Solution: $|\alpha\rangle = \hat{g}|\beta\rangle$, here $\alpha = (g, \beta)$.
- If $|\alpha\rangle = \hat{g}|\beta\rangle$ and $\hat{g}\hat{H}\hat{g}^{-1} = \hat{H}$,
  then
  $$\hat{g}\hat{\mathcal{H}}\hat{g}^{-1} = \hat{\mathcal{H}} \text{ and } \hat{g}\hat{\mathcal{N}}\hat{g}^{-1} = \hat{\mathcal{N}}.$$
- GHW in the intrinsic frame
  - LaboratoryFrameForm(GHW)=IntrinsicFrameForm(GHW)
  - The laboratory symmetries automatically implemented (e.g. spherical symmetry – conservation of angular momentum).
  - Additional symmetries – intrinsic symmetries.
  - A lot of open problems related to implementation of physical transformations in the intrinsic frame.

Problems

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