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Quantum Three-Body System: A Century-Old Problem Revisited

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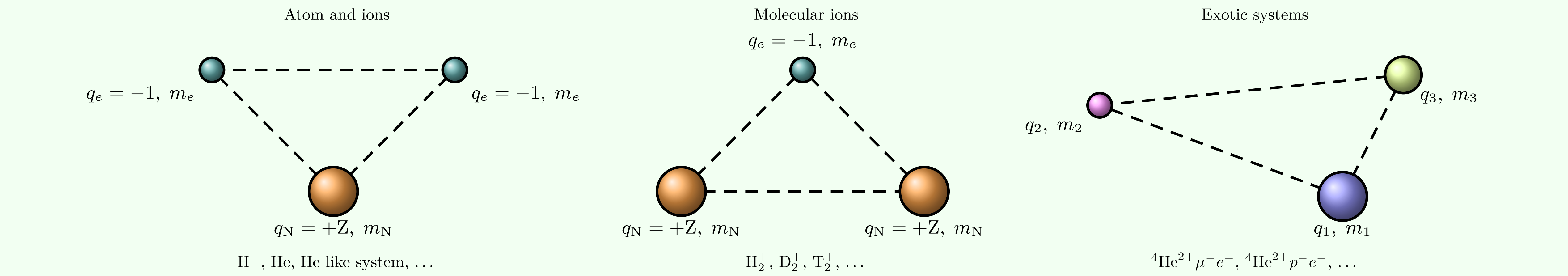
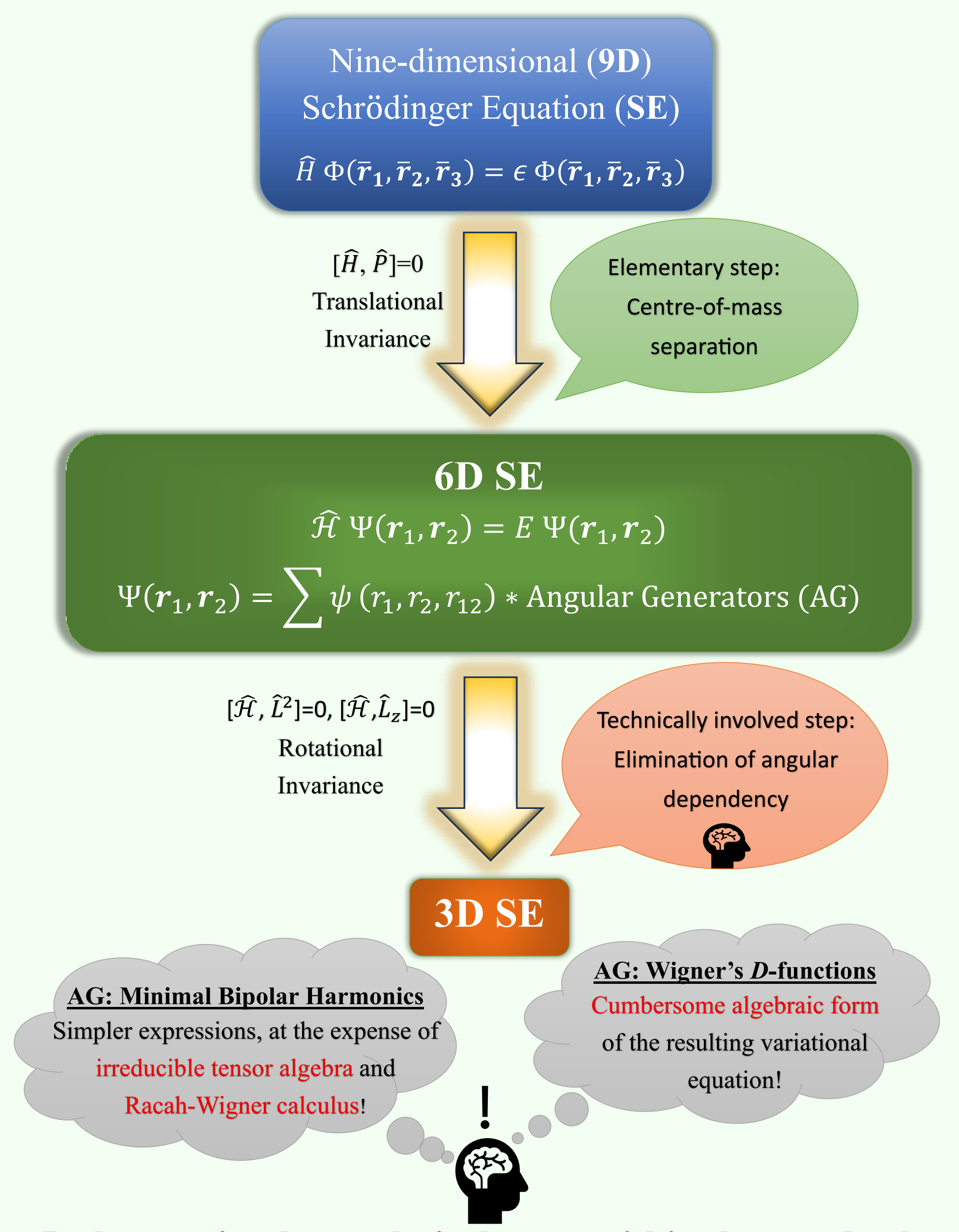
A. Quantum Three-Body Systems (TBS)



B. Conventional Hylleraas-Coordinate Treatment of TBS with Arbitrary Angular Momentum



Is there a simpler analytical route within the standard approach?

C. An Alternative Implementation of the Standard Approach

YES!

After a rigorous analytical treatment, we arrive at

- **Simple expressions**.
- A straightforward procedure to eliminate the angular dependency from the SE, **without using irreducible tensor algebra (ITA)**.
- A simple and novel process for evaluation of the angular integrals **without the use of Racah-Wigner calculus (RWC)**.

D. Brief Overview of the Analytical Approach

- **Wave function**

$$\Psi^{LM\pi}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_{l=d}^{L}\underbrace{\psi_l^{L\pi}(r_1,r_2,r_{12})}_{\text{PWC}}\ \underbrace{\boldsymbol{\Omega}_l^{LM\pi}(\boldsymbol{r}_1,\boldsymbol{r}_2)}_{\text{AG}}$$

PWC: Partial wave components; L : Angular momentum quantum number; M : Projection of L on the laboratory axis; π : Parity.

$$d=\begin{cases}0 & \text{for } \pi=n\equiv\ (-1)^L \quad \text{(natural parity)}\\ 1 & \text{for } \pi=u\equiv-(-1)^L \quad \text{(unnatural parity)}\end{cases}$$

- **AG: Solid Minimal Bipolar Harmonics (SMBH)**

SMBH are expressed in terms of minimal bipolar harmonics (MBH) $\Omega_l^{LL\pi}(\theta_1,\phi_1,\theta_2,\phi_2)$ as:

$$\boldsymbol{\Omega}_l^{LM\pi}(\boldsymbol{r}_1,\boldsymbol{r}_2)=r_1^l r_2^{L-l+d}\ \Omega_l^{LL\pi}(\theta_1,\phi_1,\theta_2,\phi_2)$$

$$\Omega_l^{LL\pi}(\theta_1,\phi_1,\theta_2,\phi_2)=\sum_{\mu}\mathrm{CG}\ Y_\mu^l(\theta_1,\phi_1)\ Y_{M-\mu}^{L-l+d}(\theta_2,\phi_2)$$

– Choosing $M=L$ leads to a substantial simplification of SMBH.

– Further simplified Cartesian representation of the SMBH for $M=L$

$$\boldsymbol{\Omega}_l^{LL\pi}(\boldsymbol{r}_1,\boldsymbol{r}_2)=N_l^{L\pi}\sum_{\kappa=0}^{d}\left(\frac{x_1}{r_1}+\boldsymbol{i}\frac{y_1}{r_1}\right)^{l-\kappa}\left(\frac{z_1}{r_1}\right)^{\kappa}\left(\frac{x_2}{r_2}+\boldsymbol{i}\frac{y_2}{r_2}\right)^{L-l+\kappa}\left(\frac{z_2}{r_2}\right)^{d-\kappa}$$

renders the action of the Hamiltonian operator particularly straightforward.

– Does not require ITA to separate the angular dependence from the SE.

- **Hamiltonian**

$$\hat{\mathcal{H}}=-\frac{\nabla_1\cdot\nabla_1}{2\mu_1}-\frac{\nabla_2\cdot\nabla_2}{2\mu_2}-\frac{\nabla_1\cdot\nabla_2}{m_3}+\frac{q_1q_2}{r_{12}}+\frac{q_1q_3}{r_1}+\frac{q_2q_3}{r_2}$$

acting on the wave function yields a structured tridiagonal matrix representation of the 6D SE:

$$\left(\boldsymbol{\Omega}_d^{LL\pi}\ \boldsymbol{\Omega}_{d+1}^{LL\pi}\cdots\ \boldsymbol{\Omega}_L^{LL\pi}\right)\left[\begin{pmatrix}\hat{\mathcal{H}}_{d,d}^{L\pi} & \hat{\mathcal{H}}_{d,d+1}^{L\pi} & 0 & \cdots & 0\\ \hat{\mathcal{H}}_{d+1,d}^{L\pi} & \hat{\mathcal{H}}_{d+1,d+1}^{L\pi} & \ddots & \ddots & \vdots\\ 0 & \ddots & \ddots & \ddots & 0\\ \vdots & \ddots & \ddots & \hat{\mathcal{H}}_{L-1,L-1}^{L\pi} & \hat{\mathcal{H}}_{L-1,L}^{L\pi}\\ 0 & \cdots & 0 & \hat{\mathcal{H}}_{L,L-1}^{L\pi} & \hat{\mathcal{H}}_{L,L}^{L\pi}\end{pmatrix}-E\mathbb{I}\right]\begin{pmatrix}\psi_d^{L\pi}\\ \psi_{d+1}^{L\pi}\\ \vdots\\ \vdots\\ \psi_L^{L\pi}\end{pmatrix}=0$$

- **Elimination of Angular Dependency**

A two step process

1. Left-multiplication of the 6D SE by Hermitian-conjugate $\left(\boldsymbol{\Omega}_d^{LL\pi}\ \boldsymbol{\Omega}_{d+1}^{LL\pi}\ldots\ \boldsymbol{\Omega}_L^{LL\pi}\right)^\dagger$,
2. Integration over the Euler angles (α,β,γ),

yields an explicit matrix form of the 3D SE or the reduced Schrödinger equation (RSE):

$$\begin{pmatrix}\mathscr{W}_{dd}^{L\pi} & \mathscr{W}_{d+1,d}^{L\pi} & \cdots & \mathscr{W}_{Ld}^{L\pi}\\ \mathscr{W}_{d,d+1}^{L\pi} & \mathscr{W}_{d+1,d+1}^{L\pi} & & \vdots\\ \vdots & & \ddots & \vdots\\ \mathscr{W}_{dL}^{L\pi} & \cdots & \cdots & \mathscr{W}_{LL}^{L\pi}\end{pmatrix}\left[\begin{pmatrix}\hat{\mathcal{H}}_{d,d}^{L\pi} & \hat{\mathcal{H}}_{d,d+1}^{L\pi} & 0 & \cdots & 0\\ \hat{\mathcal{H}}_{d+1,d}^{L\pi} & \hat{\mathcal{H}}_{d+1,d+1}^{L\pi} & \ddots & \ddots & \vdots\\ 0 & \ddots & \ddots & \ddots & 0\\ \vdots & \ddots & \ddots & \hat{\mathcal{H}}_{L-1,L-1}^{L\pi} & \hat{\mathcal{H}}_{L-1,L}^{L\pi}\\ 0 & \cdots & 0 & \hat{\mathcal{H}}_{L,L-1}^{L\pi} & \hat{\mathcal{H}}_{L,L}^{L\pi}\end{pmatrix}-E\mathbb{I}\right]\begin{pmatrix}\psi_d^{L\pi}\\ \psi_{d+1}^{L\pi}\\ \vdots\\ \vdots\\ \psi_L^{L\pi}\end{pmatrix}=\begin{pmatrix}0\\ 0\\ \vdots\\ \vdots\\ 0\end{pmatrix}$$

- **Angular Integrals (AI) $\mathscr{W}_{ll'}^{L\pi}$**

$$\mathscr{W}_{ll'}^{L\pi}(r_1,r_2,\theta)=r_1^{l+l'}r_2^{2L-l-l'+2d}\int_0^{2\pi}d\alpha\int_0^{\pi}\sin\beta\,d\beta\int_0^{2\pi}d\gamma\,\left(\Omega_{l'}^{LL\pi}\right)^*\Omega_l^{LL\pi}$$

E. MBH in terms of Wigner's $\mathcal{D}$-functions

$$\Omega_l^{LM\pi}(\theta_1,\phi_1,\theta_2,\phi_2)=\sum_{K=-L}^{L}\Lambda_{Kl}^{L\pi}(\theta)\,\mathcal{D}_L^{MK}(\alpha,\beta,\gamma)$$

Closed analytic form of expansion coefficients (M independent)

$$\Lambda_{Kl}^{L\pi}(\theta)=\int_0^{2\pi}d\alpha\int_0^{\pi}\sin\beta\,d\beta\int_0^{2\pi}d\gamma\,\left(\mathcal{D}_L^{MK}\right)^*\Omega_l^{LM\pi}$$

are evaluated and available in our paper.

F. AI Evaluation (without RWC)

Considering Sec. E, it can be shown that

$$\mathscr{W}_{ll'}^{L\pi}=r_1^{l+l'}r_2^{2L-l-l'+2d}\sum_{K=-L}^{L}\left(\Lambda_{Kl'}^{L\pi}\right)^*\Lambda_{Kl}^{L\pi}$$

and in terms of Chebyshev polynomials $T_n(\cos\theta)$

$$\mathscr{W}_{ll'}^{L\pi}=r_1^{l+l'}r_2^{2L-l-l'+2d}\sum_{\kappa=d}^{L}\sum_{j,j'=0}^{\kappa}\mathcal{C}_{ll'jj'}^{L\kappa\pi}\ T_{|-l+l'+2j-2j'|}(\cos\theta)$$

Closed form of $\mathcal{C}_{ll'jj'}^{L\kappa\pi}$ are evaluated and available in our paper.

G. Results

Estimated nonrelativistic energies of helium atom corresponding to $L\leq7$ for natural parity ($d=0$) and $L\leq3$ for unnatural parity ($d=1$) states, validate the formalism, agreeing with the best available results.

arXiv link

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