Fermionic Exchange Symmetry: Quantifying its Influence beyond Pauli's Exclusion Principle

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Pauli's Exclusion Principle (1925)
Antisymmetry of wave function (Dirac 1926)

Pauli’s Exclusion Principle

What’s beyond

Pauli’s Exclusion Principle

Antisymmetry of wave function
Outlook

1. Generalised Pauli constraints revisited
2. Pauli Exclusion Principle and hierarchy of pinning
3. Quasipinning measure $Q$
4. Relevance of $Q$
5. Study of physical systems
(1)
Generalised Pauli constraints revisited
Generalised Pauli Constraints (GPCs):

N-fermion wave function antisymmetry:
\[ \psi(\vec{x}_1, \ldots, \vec{x}_j, \ldots, \vec{x}_i, \ldots, \vec{x}_N) = -\psi(\vec{x}_1, \ldots, \vec{x}_i, \ldots, \vec{x}_j, \ldots, \vec{x}_N) \]

Further constraints beyond Pauli’s Exclusion Principle (PEP),
\[ 0 \leq \lambda_i \leq 1 \]
on spectrum of 1-particle density operator:
\[ \rho_N \equiv |\Psi\rangle \langle \Psi| \xrightarrow{Tr_{N-1}(\cdots)} \rho_1 \xrightarrow{\text{spec}} \tilde{\lambda} \]

\[ D_j(\tilde{\lambda}) = \kappa_0 + \sum_{i=1}^{d} \kappa_i \lambda_i \geq 0 \quad \text{for} \quad j \in 1 \ldots r_{(N,d)} \]
GPCs: geometrical illustration

Geometrically: Polytope

\[ D_j(\vec{\lambda}) = \kappa_0 + \sum_{i=1}^{d} \kappa_i \lambda_i \geq 0 \]

for \( j \in 1 \ldots r_{(N,d)} \)
Impact of GPCs on Physics beyond PEP

\[ \vec{\lambda}_{HF} \equiv (1, \ldots, 1, 0, \ldots) \]

Here?

Or here?
Example: \((N=3,d=6)\)-setting

Constraints:

\[
\begin{align*}
\lambda_1 + \lambda_6 &= 1 \\
\lambda_2 + \lambda_5 &= 1 \\
\lambda_3 + \lambda_4 &= 1 \\
-\lambda_4 + \lambda_5 + \lambda_6 &\geq 0
\end{align*}
\]
Example: (N=4,d=10)-setting

Pick a constraint:

\[ 3 - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_5 - \lambda_9 \geq 0 \]

Set \( \lambda_1 = 1 \):

\[ 2 - \lambda_2 - \lambda_3 - \lambda_5 - \lambda_9 \geq 0 \]
Do the remaining constraints imply equality?

\[ \text{max}[2 - \lambda_2 - \lambda_3 - \lambda_5 - \lambda_9] = ? \]

such that \( \lambda_1 = 1 \) and \( \lambda_i \geq \lambda_{i+1} \geq 0 \), together with:
(2) Pauli Exclusion Principle and hierarchy of pinning
PEP revisited (1)

- Consider N fermions in d-dimensional 1-particle Hilbert space
- PEP restricts decreasingly ordered $\vec{\lambda}$-vector to the `Pauli Simplex´:

$$\Sigma \equiv \{ \vec{\lambda} \in (\mathbb{R}_0^+)^d \mid 1 \geq \lambda_1 \geq \ldots \geq \lambda_d \land \| \vec{\lambda} \|_1 = N \}$$

Since $\mathcal{P} \subset \Sigma$ one has:

$$\vec{\lambda} \in \mathcal{P} \land \vec{\lambda} \in \partial \Sigma \implies \vec{\lambda} \in \partial \mathcal{P}$$

Sometimes pinning of PEP constraints can imply pinning of GPC(s)!
PEP revisited (2)

- PEP constraints can be written more formally as:

\[ S_{r,s}(\vec{\lambda}) \equiv \sum_{i=1}^{r} (1 - \lambda_i) + \sum_{j=d+1-s}^{d} \lambda_j \geq 0 \]

\[ r \leq N \quad \text{and} \quad s \leq d - N \]

- Introduce the corresponding facets of the Pauli simplex:

\[ \Sigma_{r,s} \equiv \{ \vec{\lambda} \in \Sigma \mid S_{r,s}(\vec{\lambda}) = 0 \} = \Sigma | \lambda_1 = \ldots = \lambda_r = 1 \]

\[ \lambda_{d+1-s} = \ldots = \lambda_d = 0 \]

- Facets obey inclusion relation:

\[ \Sigma_{r,s} \subseteq \Sigma_{r',s'} \iff r \geq r' \land s \geq s' \]
Example: \((N=3,d=6)\)-setting
Hierachy of Pinning (1)

• Crucial Observation: For any pair \((r,s)\) pinning by corresponding PEP imposes pinning for a GPC \(D_j\) IF AND ONLY IF

\[
\mathcal{P} \cap \Sigma_{r,s} \subset F_j \equiv \{ \vec{\lambda} \in \mathcal{P} \mid D_j(\vec{\lambda}) = 0 \}
\]  
(#1)

• Relation (#1) can therefore more easily be written as:

\[
\mathcal{P}^{(N,d)} \cap \Sigma_{r,s} \equiv \mathcal{P}^{(N,d)} \bigg|_{\begin{align*}
\lambda_{d-s+1} = \ldots = \lambda_d &= 0 \\
\lambda_1 = \ldots = \lambda_r &= 1
\end{align*}} \simeq \mathcal{P}^{(N-r,d-r-s)}
\]
Hierachy of Pinning (2)

- Due to inclusion relation of Pauli facets, $\Sigma_{r,s} \subseteq \Sigma_{r',s'}$, natural class structure on the set of GPCs arises:

$$C_{r,s} \equiv \{D_j \mid \mathcal{P} \cap \Sigma_{r,s} \subset F_j\}$$

- $C_{r,s}$ comprises of all GPCs that are pinned whenever PEP $S_{r,s}$ is pinned

- Hierachy of classes and partial ordering on $(r,s)$:

$$C_{r,s} \subseteq C_{r',s'} \iff r \leq r' \land s \leq s'$$

- Determine smallest $(r,s)$ for which GPC $D_j$ is still in class $C_{r,s}$
Example: Classes in the Borland-Dennis Setting (N=3,d=6)

• Recall Borland-Dennis setting:
  \[ D(\tilde{\lambda}) = \lambda_5 + \lambda_6 - \lambda_4 \geq 0 \]
• D contains Hatree-Fock point, i.e. belongs to class \( C_{3,3} \)
• D also contains \( \tilde{\lambda} \in \mathcal{P} \cap \Sigma_{2,2} \) (which is again the Hatree-Fock point), i.e. belongs to class \( C_{2,2} \)
• D further belongs to class \( C_{1,1} \)

Hierarchies in higher dimensional settings become very complex and can be evaluated by linear algorithm
(3) Quasipinning measure $Q$
Quasipinning and distances to facets of constraints

- Pinning by PEP constraints was found to impose pinning of certain related classes of GPCs.
- This can be extended to quasipinning.
- Distance to facet $F_{D_j}$ of GPC $D_j$ is given by:
  \[ \text{dist}_1(\vec{\lambda}, F_{D_j}) = 2D_j(\vec{\lambda}) \]
- Note that the 1-norm is the most natural choice of a distance measure due to the inclusion relation of GPCs and normalisation condition.

Supl. Mat. arXiv1509.00358
Upper bounds on $D_j(\vec{\lambda})$

- Flat geometry of polytope imposes linear upper bounds on the distance to the polytope boundary:

$$D_j(\vec{\lambda}) \leq c_j \text{dist}_1(\vec{\lambda}, \Sigma_{r,s}) = S_{r,s}(\vec{\lambda})$$

$$c_j \equiv \min_{\vec{\lambda} \in \mathcal{P}} \left( \frac{D_j(\vec{\lambda})}{\text{dist}_1(\vec{\lambda}, \Sigma_{r,s})} \right)$$

- Hierarchy of classes $\mathcal{C}_{r,s}$ suggests to use minimal pair $(r,s)$

Compare distances of $\vec{\lambda}$-vector to Pauli facets and GPC facets!
**Q-measure**

- Define Q-measure by:

\[
Q_j(\vec{\lambda}) \equiv -\log_{10}\left[ \frac{D_j(\vec{\lambda})}{c_j \, \text{dist}_1(\vec{\lambda}, \Sigma_{r,s})} \right]
\]

\[
Q(\vec{\lambda}) = \max_j Q_j(\vec{\lambda})
\]

- Minimal distance to polytope boundary is \(10^{Q_j(\vec{\lambda})}\) smaller than could be expected from approximate saturation of PEP!
(4) Operational significance of Q
Structural Simplification of the N-fermion wave function

- Pinning of PEP and GPC constraints allows for a simplified expansion of N-fermion wave functions by a reduced number of Slater determinants:

\[ |\psi\rangle = \sum_{i \in \mathcal{I}_{PEP/GPC}} a_i |i\rangle \]

- Expand:

\[ |\psi\rangle = |\psi_{PEP}\rangle + |\psi_{GPC\setminus PEP}\rangle + |\psi_{rest}\rangle \]

- Q evaluates the ratios of \( L^2 \)-weights:

\[ \beta_- \cdot 10^{-Q_j(\tilde{\lambda})} \leq \frac{1 - \|\Psi_{PEP}\|_{L^2}}{1 - \|\Psi_{GPC}\|_{L^2}} \leq \beta_+ \cdot 10^{-Q_j(\tilde{\lambda})} \]
(5)
Q-measure of Harmonium Ground States
Quasipinning in Harmonium

Hamiltonian:

\[
H_N = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + \frac{m}{2} \frac{\theta_i}{\omega_i} \Omega x_i \right) + \frac{K}{2} \sum_{1 \leq i < j \leq N} (x_i - x_j)^2
\]

Ground states:

\[
\kappa = \frac{KN}{m\omega^2}
\]

Slater determinant \( \times \) physical correlation

\[
\begin{array}{cccc}
\mu^{(2)} \\
2 & \square & \square & \square & \square \\
1 & \bullet & \bullet & \square & \square \\
0 & \bullet & \bullet & \bullet & \square \\
0 & 1 & 2 & 3 & \mu^{(1)} \\
\end{array}
\]

\[
e^{\frac{1}{\hbar} \omega^{(2)}} \times e^{\frac{1}{\hbar} \omega^{(1)}} B \tilde{X}
\]
Previous results: $\kappa^8$-Quasipinning in 3-Harmonium in 1 dimension for weak interactions (CS et al, Phys. Rev. Lett. 110, 040404 (2013))

- More particles?
- Strong interactions?
- Higher dimensions?
- Spinful particles?
- Dimensional crossovers?
N \geq 4 \text{ particles in } d = 1 \text{ dimension}

More particles: \[ D_{min} \sim \kappa^{2N} \text{ for } N \geq 4 \]

Nontriviality: \[ \frac{dist_1(\vec{\lambda}, \partial \mathcal{P})}{dist_1(\vec{\lambda}, \partial \Sigma)} \sim \kappa^2 \]

For d=1, quasipinning increases with the particle number!

Previous results: $δ^8$-Quasipinning in 3-Harmonium in 1 dimension for weak interactions (PRL CS ’12)

More particles? ✓ Strong interactions?
Strong interactions, e.g. for $N=3$ particles in 1 dimension:

Quasipinning extends to intermediate interactions; truncation methods hold even up to ultrastrong couplings!

Concept of Truncation: C. Schilling:
Previous results: $\delta^8$-Quasipinning in 3-Harmonium in 1 dimension for weak interactions (PRL CS ’12)

More particles?

Strong interactions?

Higher dimensions?
3 spinless fermions in 2 dimensions
4 spinless fermions in 3 dimensions

Quasipinning becomes weaker with additional dimensions!
Previous results: $\delta^8$-Quasipinning in 3-Harmonium in 1 dimension for weak interactions (PRL CS ’12)

More particles?

Strong interactions?

Higher dimensions?

Spinful particles?

Dimensional crossovers?
3 spinful fermions in 2 dimensions
Previous results: $\delta^8$-Quasipinning in 3-Harmonium in 1 dimension for weak interactions (PRL CS '12)

- More particles?
- Strong interactions?
- Higher dimensions?
- Spinful particles?
- Dimensional crossovers?
Summary

• Pinning of GPCs can be a consequence of pinning by PEP constraints
• GPCs are seen to be hierachically ordered in classes
• As result of comprehensive geometrical analysis: Q-measure, determining relevance of GPCs beyond PEP
• Application to model system revealed significance of GPCs for Physics

FT, V. Vedral and C. Schilling; arXiv1509.00358
FT, V. Vedral and C. Schilling; forthcoming (2016)