



Pinning of Fermionic Occupation Numbers

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The Pauli exclusion principle is a constraint on the natural occupation numbers of fermionic states. It has been suspected since at least the 1970s, and only proved very recently, that there is a multitude of further constraints on these numbers, generalizing the Pauli principle. Here, we provide the first analytic analysis of the physical relevance of these constraints. We compute the natural occupation numbers for the ground states of a family of interacting fermions in a harmonic potential. Intriguingly, we find that the occupation numbers are almost, but not exactly, pinned to the boundary of the allowed region (quasipinned). The result suggests that the physics behind the phenomenon is richer than previously appreciated. In particular, it shows that for some models, the generalized Pauli constraints play a role for the ground state, even though they do not limit the ground-state energy. Our findings suggest a generalization of the Hartree-Fock approximation.

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Introduction.—In 1925, the study of atomic transitions led to Pauli’s exclusion principle [1]. It states that for identical fermions the occupation number for any quantum state cannot exceed the value 1. By 1926, Dirac [2] and Heisenberg [3] had identified the exclusion principle as a consequence of a much deeper statement: the antisymmetry of the many-fermion wave function. While antisymmetry allows one to find the correct solutions to the full many-fermion Schrödinger equation, it does not render the exclusion principle obsolete: in many situations, the latter is sufficient to predict the qualitative behavior of fermionic systems without the need to resort to (often computationally intractable) *ab initio* methods. The Aufbau principle for elements in the periodic table serves as a prime example.

This observation motivates the study of generalizations of the exclusion principle, which, maybe surprisingly, exist and exhibit an extremely rich structure [4]. To set the scene, note that the Pauli constraint can be stated succinctly as

$$0 \leq \lambda_i \leq 1 \quad \forall i, \quad (1)$$

in terms of the natural occupation numbers λ_i , which are the eigenvalues of the 1-particle reduced density operator (1-RDO) ρ_1 , normalized to the particle number N . The utility of the exclusion principle is grounded in the fact that in the ground states of many-fermion systems, one often observes $\lambda_i \approx 0$ or $\lambda_i \approx 1$, which is equivalent to stating that the Hartree-Fock approximation works fairly well in these systems.

It had been observed in the 1970s that there are further linear inequalities respected by the natural occupation numbers as a result of global antisymmetry [5–7]. One particular example is the so-called Borland-Dennis setting $\wedge^3[\mathcal{H}_6]$ of three fermions and a six-dimensional 1-particle

Hilbert space \mathcal{H}_6 [7]. Here, the set of constraints is given by

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1, \quad (2)$$

$$D^{(6)} := \lambda_5 + \lambda_6 - \lambda_4 \geq 0, \quad (3)$$

on the ordered eigenvalues $\lambda_i \geq \lambda_{i+1}$.

In a ground-breaking work building on recent progress in invariant theory and representation theory, Klyachko exhibited an algorithm for computing all such Pauli-like constraints [4,8]. In fact, his work is part of a more general effort in quantum information theory addressing the quantum marginal problem which asks when a given set of single-site reduced density operators (marginals) is compatible in the sense that they arise from a common pure global state (see also Refs. [9–12]). The global state may be subject to certain symmetry constraints—one obtains the fermionic case (commonly known as the N -representability problem [13,14]) by requiring total antisymmetry under particle exchange. Klyachko showed that for fixed particle number N and dimension d of the 1-particle Hilbert space, the generalized Pauli constraints amount to affine inequalities of the form

$$\kappa_0 + \kappa_1 \lambda_1 + \cdots + \kappa_d \lambda_d \geq 0. \quad (4)$$

Geometrically, these constraints define a convex polytope $\mathcal{P}_{N,d} \subset \mathbb{R}^d$ of possible spectra (for more details see the Supplemental Material [15]). In general, if a spectral inequality such as (1) or (4) is (approximately) saturated, we say that the corresponding spectrum is (quasi)pinned to its extremum.

The natural question arises whether ground states of relevant many-body models saturate some of those inequalities. Strong numerical evidence supporting this conjecture has been presented in Ref. [16]. The problem

is challenging to address analytically, as one has to not only compute the ground state, but also determine and diagonalize the corresponding 1-RDO.

Here, we present for the first time an analytic analysis. For the ground state of a model of interacting fermions in a harmonic potential, the natural occupation numbers are calculated. We obtain several results. We confirm that for this very natural model, the natural occupation numbers lie, indeed, close to the boundary of the set of allowed ones. The analytic analysis enables us to track the “trajectory” of eigenvalues as a function of the interaction strength between the fermions. What is conceptually also important, is the fact that the eigenvalues never lie exactly on the boundary. To see why one could expect the opposite, note that the ground state energy of a Hamiltonian $H = \sum_{i,j} h^{(i,j)}$ with two-particle terms $h^{(i,j)}$ can be represented as a constrained optimization problem

$$E_{\min} = \min_{\rho_2^{(i,j)}} \sum_{i,j=1}^N \text{tr}[h^{(i,j)} \rho_2^{(i,j)}],$$

where the $\rho_2^{(i,j)}$ are 2-particle density operators that are compatible in the sense that they are the reduced densities of some N -fermion state [13,14]. Since the energy functional is linear, it does not possess an unconstrained minimum. Therefore, E_{\min} will be achieved on the boundary of the set of compatible density operators, where at least one of the compatibility constraints is active in the sense that any further minimization would violate it. One way of understanding why a “pinning” effect for the natural occupation numbers is observed, is to posit that the generalized Pauli constraints are among the active physical constraints. While this effect may well occur, we show in this Letter that quasipinning appears in natural fermionic systems: the eigenvalue constraints seem to play a role, but are not active in the above sense. The finding suggests that the physics of the phenomenon is richer than previously appreciated. We will return to the physical consequences quasipinning has on the structure of wave functions after presenting the calculations for our model system.

The model.—In order to analyze possible pinning effects analytically, we consider a model of N identical fermions subject to a harmonic external potential and a harmonic interaction term

$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i,j=1}^N (x_i - x_j)^2. \quad (5)$$

The corresponding energy eigenvalue problem without any symmetry constraint can easily be solved by transforming the Hamiltonian to the one of decoupled harmonic oscillators. Two eigenfrequencies appear: a nondegenerate one describing the center of mass motion and another $(N - 1)$ -fold degenerate frequency associated with the relative

motion. The natural length scales corresponding to these eigenmodes are

$$l := \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{l} := \sqrt{\frac{\hbar}{m\omega\sqrt{1 + ND/(m\omega^2)}}}$$

By rescaling the energy and the length scale, the fermion-fermion coupling constant D can be absorbed by the term $m\omega^2$. Hence, the spectrum λ of a 1-RDO corresponding to an eigenstate of H depends only on the relative fermion-fermion interaction strength $\frac{ND}{m\omega^2} = \left(\frac{l}{\tilde{l}}\right)^4 - 1$. In fact, it will prove slightly more convenient to parametrize the coupling using

$$\delta := \ln\left(\frac{l}{\tilde{l}}\right) = \frac{1}{4} \ln\left(1 + \frac{ND}{m\omega^2}\right). \quad (6)$$

Then, in the regime of weak interaction, D and δ are in leading order proportional, $D = \frac{4m\omega^2}{N} \delta + O(\delta^2)$.

To study the physical relevance of the generalized Pauli constraints we restrict the Hamiltonian H to the fermionic Hilbert space $\Lambda^N[\mathcal{H}_\infty]$, with $\mathcal{H}_\infty = L^2(\mathbb{R})$; i.e., we are treating the N particles as fermions (without spin). In Ref. [17], H has been diagonalized and the ground state reads in spatial representation $[\vec{x} = (x_1, \dots, x_N)]$

$$\Psi_N(\vec{x}) = \text{const} \times \prod_{1 \leq i < j \leq N} (x_i - x_j) \times \exp\left[-\frac{1}{2N} \left(\frac{1}{l^2} - \frac{1}{\tilde{l}^2}\right) (x_1 + \dots + x_N)^2 - \frac{1}{2} \frac{1}{\tilde{l}^2} \vec{x}^2\right]. \quad (7)$$

(Note its structural similarity to Laughlin’s ground state wave function describing the fractional quantum Hall effect [18]. Moreover, the polynomial in front of the exponential function is the Vandermonde determinant and by omitting it we obtain the ground state in the bosonic N -particle Hilbert space.)

The spectrum and its properties.—We now outline the calculation of the spectrum $\lambda(\delta)$ as a function of the coupling. We omit details of this tedious but mostly straightforward computation, presenting the final result, together with some conceptual insights obtained along the way.

The 1-RDO is calculated by integrating out $N - 1$ coordinates of the N -fermion state $\rho_N(\vec{x}, \vec{x}') = \Psi_N^*(\vec{x}) \Psi_N(\vec{x}')$. An exercise in Gaussian integration and integration by parts yields

$$\rho_1(x, x') = p(x, x') \exp[-\alpha(x^2 + x'^2) + \beta x x'],$$

where p is a symmetric polynomial of degree $2(N - 1)$ in the variables x, x' originating from the Vandermonde determinant in (7), and α and β some constants depending on l, \tilde{l} and N .

If the fermions do not interact with each other, the ground state $|\Psi_N\rangle$ is a single Slater determinant and the spectrum of its 1-RDO is trivial, i.e.,

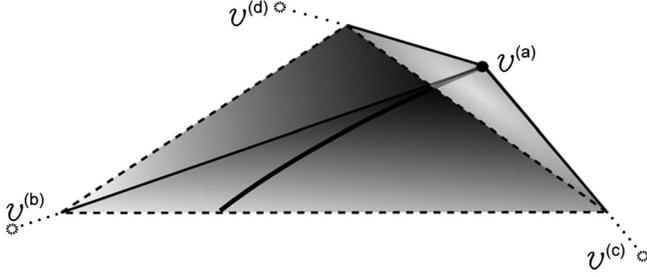


FIG. 1. Spectral “trajectory” $v(\delta)$ (thick line, partially covered by facet, schematic) up to correction of order δ^8 and small part of the polytope \mathcal{P} around vertex $v^{(a)}$ obtained by cutting \mathcal{P} along the dashed lines.

$$\lambda(\delta = 0) = (\underbrace{1, \dots, 1}_N, 0, \dots). \quad (8)$$

The regime of weak interaction can be characterized by the condition $|D| \ll m\omega^2$ or, equivalently, $\delta \approx 0$. We thus employ degenerate perturbation theory to obtain $\lambda(\delta)$ around $\delta = 0$. The reason we employ the parameter δ is that one can prove a duality

$$\lambda_k(\delta) = \lambda_k(-\delta) \quad \forall k, \quad (9)$$

relating the spectra for attractive ($\delta < 0$) and repulsive ($\delta > 0$) fermion-fermion interaction (interestingly, that this duality holds is not obvious on the level of ground-state wave functions). This immediately implies that the expansion $\lambda(\delta)$ contains only even order terms, simplifying the perturbation theory.

The solution for $N = 3$ reads:

$$\begin{aligned} 1 - \lambda_1 &= \frac{40}{729} \delta^6 - \frac{1390}{59049} \delta^8 + O(\delta^{10}), \\ 1 - \lambda_2 &= \frac{2}{9} \delta^4 - \frac{232}{729} \delta^6 + \frac{3926}{10935} \delta^8 + O(\delta^{10}), \\ 1 - \lambda_3 &= \frac{2}{9} \delta^4 - \frac{64}{243} \delta^6 + \frac{81902}{295245} \delta^8 + O(\delta^{10}), \\ \lambda_4 &= \frac{2}{9} \delta^4 - \frac{64}{243} \delta^6 + \frac{73802}{295245} \delta^8 + O(\delta^{10}), \\ \lambda_5 &= \frac{2}{9} \delta^4 - \frac{232}{729} \delta^6 + \frac{3976}{10935} \delta^8 + O(\delta^{10}), \\ \lambda_6 &= \frac{40}{729} \delta^6 - \frac{2200}{59049} \delta^8 + O(\delta^{10}), \\ \lambda_7 &= \frac{80}{2187} \delta^8 + O(\delta^{10}), \\ \lambda_8 &= O(\delta^{10}), \\ &\vdots \quad \vdots \end{aligned} \quad (10)$$

Similar results follow for $N = 2$. Note the nontrivial hierarchy of the eigenvalues,

$$\lambda_k = c_k \delta^{2k-6} + O(\delta^{2k-4}), \quad (11)$$

for all $k \geq 5$. Moreover, the spectrum λ for δ not too large is very close to the one of a single Slater determinant. For instance, λ_i , $i = 1, 2, 3$ deviate from 1 and λ_j , $j \geq 4$ from 0 only by at most 1 percent if $|\delta| \leq 0.5$. This emphasizes the relevance of the Pauli constraints (1).

Quasipinning by generalized Pauli constraints.— Equipped with the explicit solution (10), we can proceed to analyze whether the generalized Pauli constraints play a role for the ground state. While the underlying 1-particle Hilbert space \mathcal{H}_∞ is infinite dimensional, the scaling (11) implies that the spectrum is strongly concentrated on a low-dimensional subspace, at least for small δ . One can use this fact to deduce statements about the position of the total eigenvalues from truncated information alone.

This can be understood from simple geometric considerations. Let $d < d' < \infty$. Because a d -dimensional 1-particle Hilbert space can be imbedded into any (larger) d' -dimensional one, one sees that the convex polytope $\mathcal{P}_{N,d}$ is nothing but the intersection between $\mathcal{P}_{N,d'}$ and the set of spectra with only d nonzero eigenvalues (see also Ref. [15]). Hence, any facet of $\mathcal{P}_{N,d}$ arises from the intersection of some facet of $\mathcal{P}_{N,d'}$ with the subspace of said spectra. Formally, a facet F' of $\mathcal{P}_{N,d'}$ consists of points saturating a generalized Pauli constraint

$$D'(\lambda) = \kappa_0 + \sum_{i=1}^d \kappa_i \lambda_i + \sum_{i=d+1}^{d'} \kappa_i \lambda_i \geq 0. \quad (12)$$

Denote the first two summands by $D(\lambda^{\text{tr}})$, where $\lambda^{\text{tr}} = (\lambda_i)_{i=1}^d$ is the truncated spectrum. Clearly, $D(\lambda^{\text{tr}}) = 0$ describes the restriction of the facet to the d -dimensional setting. Now assume the truncated spectrum $\lambda^{\text{tr}}(\delta)$ is not pinned, i.e., $D[\lambda^{\text{tr}}(\delta)] > 0$, then the hierarchical scaling (11) implies

$$D'(\lambda(\delta)) = D(\lambda^{\text{tr}}(\delta)) + O(\delta^{2d-4}), \quad (13)$$

which is positive for δ small enough. Hence the full spectrum λ' also fails to be pinned. The case $d' = \infty$ works in the same way, up to some mild assumptions (see Ref. [15]).

We will now apply these considerations to our model. First, we truncate to six dimensions, which has the advantage that the spectral polytope corresponding to $\Lambda^3[\mathcal{H}_6]$ is three dimensional and can thus be visualized. In a second step, we take a seventh eigenvalue into account. This setting turns out to be strong enough to establish all statements we have mentioned above—namely that the total spectrum is not exactly pinned, but does lie close to the boundary (quasipinned).

The simplest nontrivial setting $\Lambda^3[\mathcal{H}_6]$ becomes an appropriate description if $\lambda_7, \lambda_8, \dots \approx 0$. By (11), this condition is fulfilled if δ is small enough that contributions of order δ^8 can be neglected. Choosing λ_4, λ_5 , and λ_6 as free parameters according to (2), the corresponding polytope $\mathcal{P}_{3,6}$ effectively reduces [16] to a three-dimensional polytope $\mathcal{P} \subset \mathbb{R}^3$ with vertices,

$$\begin{aligned} \mathbf{v}^{(a)} &= (0, 0, 0), & \mathbf{v}^{(b)} &= \left(\frac{1}{2}, \frac{1}{2}, 0\right), \\ \mathbf{v}^{(c)} &= \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right), & \mathbf{v}^{(d)} &= \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right). \end{aligned} \quad (14)$$

Hence the vertex $\mathbf{v}^{(a)}$ corresponds to single Slater determinants and the 2-facet spanned by $\mathbf{v}^{(a)}$, $\mathbf{v}^{(b)}$, and $\mathbf{v}^{(c)}$ is defined by $D^{(6)} = 0$, which is here the one of interest and represents exact pinning by constraint (3). We first illustrate schematically our result (10) in Fig. 1. There, the spectral “trajectory,”

$$\mathbf{v}(\delta) = (\lambda_4(\delta), \lambda_5(\delta), \lambda_6(\delta)),$$

is shown as a thick line (neglecting effects of order δ^8 and higher). It starts at the vertex $\mathbf{v}^{(a)}$ which corresponds to the noninteracting situation $\delta = 0$. When increasing the fermion-fermion interaction, $\mathbf{v}(\delta)$ leaves the vertex $\mathbf{v}^{(a)}$ and moves along the edge $(\mathbf{v}^{(a)}, \mathbf{v}^{(b)})$, the distance to $\mathbf{v}^{(a)}$ growing as δ^4 . On the finer scale δ^6 , $\mathbf{v}(\delta)$ also moves away from the edge but is still pinned to the boundary of the polytope, lying on the 2-facet spanned by $\mathbf{v}^{(a)}$, $\mathbf{v}^{(b)}$, and $\mathbf{v}^{(c)}$. This is the bottom area in Fig. 1, corresponding to the constraint (3).

The pinning seems to disappear if we consider higher orders. From (10), we can infer that the distance to the 2-facet $(\mathbf{v}^{(a)}, \mathbf{v}^{(b)}, \mathbf{v}^{(c)})$ increases as δ^8 ,

$$D^{(6)}(\delta) = \zeta^{(6)} \delta^8 + O(\delta^{10}), \quad (15)$$

with $\zeta^{(6)} = \frac{4510}{59049}$. However, this calculation is inconclusive, as the distance to the boundary is of the same order, δ^8 , as the truncation error [recall (13)].

To resolve the issue, we take another eigenvalue, λ_7 , into account. We thus work in the setting $\Lambda^3[\mathcal{H}_7]$ with four constraints $D_i^{(7)} \geq 0$ for $i = 1, \dots, 4$ [4]. This setting is valid as long as $\lambda_8, \lambda_9, \dots \approx 0$ or in other words we neglect terms of order δ^{10} or higher (but in contrast to the setting $\Lambda^3[\mathcal{H}_6]$ we include δ^8 -terms). Since the polytope is now six dimensional we cannot present our results graphically anymore. The results (10) lead to $(i = 1, 2, 3, 4)$

$$D_i^{(7)} = \zeta_i^{(7)} \delta^8 + O(\delta^{10}), \quad (16)$$

with $\zeta_1^{(7)} = \frac{20}{2187}$, $\zeta_2^{(7)} = \frac{10}{243}$, $\zeta_3^{(7)} = \frac{50}{2187}$, $\zeta_4^{(7)} = \frac{2890}{59049}$. Here in the $\Lambda^3[\mathcal{H}_7]$ analysis, the new result is that all four distances $D_i^{(7)}$ are nonzero to a smaller order, δ^8 , than the error of spectral truncation, δ^{10} . Together with the comments at the beginning of this section, this shows that the absence of pinned spectra is genuine, rather than an artifact of the truncation. Given this, the quasipinning found here is surprisingly strong. In particular, it exceeds by four additional orders the (quasi)pinning by Pauli’s exclusion principle constraints (1),

$$0 \leq 1 - \lambda_2(\delta), \quad 1 - \lambda_3(\delta), \quad \lambda_4(\delta), \quad \lambda_5(\delta) = \frac{2}{9} \delta^4 + O(\delta^6). \quad (17)$$

Generalizing Hartree-Fock.—In this section, we discuss what conclusions can be drawn about the N -fermion state $|\Psi\rangle$ itself, given information just about the position of the eigenvalues of the corresponding 1-RDO relative to the boundary of the spectral polytope. In this way, quasipinned spectra are endowed with a physical significance. To this end, recall the basic fact that the spectrum $\lambda_{\text{Sl}} = (1, \dots, 1, 0, \dots, 0)$ can only arise from a Slater determinant $|\Psi\rangle = |1, \dots, N\rangle$. It is well-known that this statement is stable under small deviations: if $\lambda \approx \lambda_{\text{Sl}}$, then $|\Psi\rangle$ is well approximated by a Slater determinant (see Ref. [19] or Ref. [15]).

For exactly pinned spectra, there is a simple generalization of these observations. In Ref. [16], it is stated that constraint (3) can be saturated only by states of the form

$$|\Psi\rangle = \alpha|1, 2, 3\rangle + \beta|1, 4, 5\rangle + \gamma|2, 4, 6\rangle,$$

a fact is dubbed “selection rule” for Slater determinants (see also Ref. [15]). The general statement reads: if $D(\lambda) \geq 0$ is a generalized Pauli constraint, then $D(\lambda) = 0$ can only be achieved by states $|\Psi\rangle$ which are superpositions of those Slater determinants whose (unordered) spectra also saturate D .

What is more important, a stable version of this statement applying to quasipinned states can be found—at least for specific situations. In Ref. [15], we show that for the Borland-Dennis setting, spectra in the vicinity of the facet corresponding to constraint (3) are approximately of the form above. In particular, quasipinned states are close to states containing fairly low amounts of multipartite entanglement as quantified by the Schmidt number [20]. We believe that these findings open up a potentially significant avenue for investigating the structure of fermionic ground states via their natural occupation numbers—generalizing a program that has long been carried out for the Hartree-Fock case [19].

We close by speculating that these insights could give rise to improved numerical procedures. The idea is to replace the ground state ansatz of one single Slater determinant by the states corresponding to the points lying on the (quasi)pinning polytope facet. In contrast to the configuration interaction methods in quantum chemistry, which improve the Hartree-Fock approximation by adding several arbitrary Slater determinants to the Hartree-Fock state, our method would add only a few, but carefully chosen, additional Slater determinants.

Conclusions.—For a natural model of interacting fermions in a harmonic trap we analytically calculated the leading orders of the eigenvalues of the 1-RDO corresponding to the fermionic ground state as a function of δ , a measure for the fermion-fermion interaction strength.

The investigation of the generalized Pauli constraints has shown that none of them is completely saturated, which might be a generic property of all continuous models of interacting fermions. In particular, the findings show that it is likely extremely challenging to use numerical methods to distinguish between genuinely pinned and mere quasi-pinned states. This underscores the need for analytical analyses, first provided here. On the other hand the pinning up to corrections of order δ^8 we found here is surprisingly strong. In particular, it exceeds the one by the Pauli exclusion principle constraints (1), which are pinning up to corrections of order δ^4 only.

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