Pinning of fermionic occupation numbers: Higher spatial dimensions and spin

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The role of the generalized Pauli constraints (GPCs) in higher spatial dimensions and by incorporating spin degrees of freedom is systematically explored for a system of interacting fermions confined by a harmonic trap. Physical relevance of the GPCs is confirmed by analytical means for the ground state in the regime of weak couplings by finding its vector of natural occupation numbers close to the boundary of the allowed region. Such quasipinning is found to become weaker in the intermediate- and strong-coupling regime. The study of crossovers between different spatial dimensions by detuning the harmonic trap frequencies suggests that quasipinning is essentially an effect for systems with reduced spatial dimensionality. In addition, we find that quasipinning becomes stronger by increasing the degree of spin polarization. Consequently, the number of states available around the Fermi level plays a key role for the occurrence of quasipinning. This suggests that quasipinning emerges from the conflict between energy minimization and fermionic exchange symmetry.

DOI: 10.1103/PhysRevA.94.012120

I. INTRODUCTION

Pauli's exclusion principle (PEP) has been a strong guiding tool for the understanding and description of numerous manyfermion systems. It however does not entirely resemble the exchange antisymmetry of the *N*-fermion wave function. In a number of works [1–5] that property was found to impose greater restrictions on the *one-particle reduced density operator* (1-RDO): The vector $\vec{\lambda} \equiv (\lambda_i)_{i=1}^d$ of its decreasingly ordered eigenvalues λ_i , the so-called *natural occupation numbers* (NONs), is confined to a polytope within the "Pauli simplex" Σ defined by Pauli's exclusion principle $1 \ge \lambda_1 \ge$ $\dots \ge \lambda_d \ge 0$ (see Fig. 1). The corresponding constraints take the form of linear inequalities:

$$D_j(\vec{\lambda}) \equiv \kappa_j^{(0)} + \vec{\kappa}_j \cdot \vec{\lambda} \ge 0, \quad j = 1, 2, \dots, r_{N,d}, \quad (1)$$

and are commonly referred to as *generalized Pauli constraints* (GPCs).

Exploring the physical significance of the GPCs remains to be a challenge that has recently seen a growing interest among physicists and quantum chemists [6–22]. Especially the phenomenon where the λ vector lies close to or on the boundary [23] of the polytope, also known as *quasipinning* [7,11,13] and *pinning* [6], respectively, has stimulated much research since it implies a number of remarkable properties for the corresponding *N*-fermion quantum system [24]. The most striking implication is the resulting structural simplification of the *N*-fermion quantum state. Therefore, studying and understanding (quasi)pinning may provide further insights into concepts such as entanglement [25–29] and correlations [30–33] in few-fermion quantum systems as being recently explored from a quite conceptual and often particularly quantum information theoretical viewpoint.

This paper aims to explore in great detail the scope of (quasi)pinning and to recognize and describe its origin. In Ref. [21], tools and methods required for a sound and conclusive (quasi)pinning analysis have been introduced and applied to the instructive model system of Harmonium in one spatial dimension. In the present paper, we are going to extend these investigations to systems of higher spatial dimensions and to spinful particles. Furthermore, dimensional crossovers will be studied by considering detunings of the external trapping frequencies. Alongside the results in Ref. [21], this will suggest that the structure of the active space around the Fermi level plays a key role in the occurrence of quasipinning and will particularly show that quasipinning is becoming stronger by reducing the spatial dimensionality.

The paper is organized as follows: In Sec. II the model of Harmonium in multiple spatial dimensions will be introduced and its ground state will be determined. The definition, form, and properties of the one-particle reduced density operator and related NONs will be discussed in Sec. III. This is followed by Sec. IV where quasipinning is explored for a quasi-one-dimensional system. The extension to proper two- and three-dimensional systems will be provided in Sec. V by a thorough analysis. Results of (quasi)pinning analyses of different dimensional crossovers will be shown as well. In the sixth section, spin degrees of freedom will be incorporated by considering non-fully-polarized fermions and magnetic crossovers between different spin states. Section VII summarizes and discusses our findings.

II. MODEL AND ITS GROUND STATE

In this section we generalize the model of Ref. [21] to higher spatial dimensions. We discuss in detail the structure of its ground state and define the relevant coupling parameters.

The system we are considering consists of *N* identical (yet spinless) particles of mass *m* that are confined in an *n*-dimensional (not necessarily isotropic) harmonic trapping potential characterized by its trapping frequencies $\{\omega^{(\alpha)}\}_{\alpha=1}^{n}$. In addition to the external potential, a harmonic particle-particle interaction of strength *K* will be taken into account. Consequently, the Hamiltonian reads

$$H_N = \sum_{i=1}^{N} \left(\frac{\vec{p}_i^2}{2m} + \frac{m}{2} \vec{x}_i^{\,t} \Omega \vec{x}_i \right) + \frac{K}{2} \sum_{1 \le i < j \le N} (\vec{x}_i - \vec{x}_j)^2, \quad (2)$$

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FIG. 1. Illustration of the mapping of *N*-fermion quantum states (left) onto their vectors $\vec{\lambda}$ (right) of decreasingly ordered natural occupation numbers, giving rise to a polytope \mathcal{P} (dark grey). \mathcal{P} is a proper subset of the Pauli simplex Σ (grey) defined by $1 \ge \lambda_1 \ge \cdots \ge \lambda_d \ge 0$.

where $\vec{p}_i = (p_i^{(\alpha)})_{\alpha=1}^n$ and $\vec{x}_i = (x_i^{(\alpha)})_{\alpha=1}^n$ represent the momentum and position operators of the *i*th particle, respectively, and $\Omega \equiv \text{diag}(\omega_1^2, \ldots, \omega_n^2)$. In the present paper, the *N*-fermion system associated with this Hamiltonian is referred to as Harmonium.

The Harmonium model arises as an effective model in the harmonic approximation applied to systems of harmonically confined interacting particles [34]. For instance, this approximation works fairly well in the description of quantum dots since the Coulomb interaction between the electrons is screened (see Ref. [35]). Furthermore, Harmonium was used to explore the emergence of shell structures in atoms (see, e.g., Ref. [36]) and nuclei (see, e.g., Ref. [37]). Also for ultracold gases in a trap it plays a role since there the two-body interactions can be tuned [38–40]. In particular, it is possible to change the interactions from repulsive to attractive [41].

Harmonium encompasses an important advantage. In order to analytically investigate the occurrence of quasipinning, a system must permit the *analytical* execution of all of the following steps:

(i) computation of the many-body eigenstates in a system of *interacting fermions* (see, e.g., Refs. [7,42–44]);

(ii) tracing out N - 1 particles [i.e., calculating analytically (N - 1)n integrals];

(iii) diagonalizing the 1-RDO, either analytically in the regime of weak couplings or exact numerically for medium and strong couplings.

While all three steps are possible for Harmonium, none of them is feasible for most continuous physical models.

A priori, the Hamiltonian (2) acts as an operator on the *N*-particle Hilbert space $\mathcal{H}^{(N)} = \bigotimes_{i=1}^{N} \mathcal{H}$, where the one-particle Hilbert space \mathcal{H} is given by $\mathcal{H} = L_2(\mathbb{R}^n)$. When incorporating spin degrees of freedom in Sec. VI, this will be modified to $\mathcal{H} = L_2(\mathbb{R}^n) \otimes \mathbb{C}^2$. Any permutation of particles leaves H_N invariant. In particular, this allows us to treat the *N* particles as indistinguishable fermions and thus restrict the Hamiltonian (2) to the subspace

$$\mathcal{H}_{N}^{(f)} \equiv \wedge^{N}[\mathcal{H}] = \mathcal{A}_{N}\mathcal{H}_{N} \lneq \mathcal{H}_{N} \equiv \mathcal{H}^{\otimes^{N}}$$
(3)

of antisymmetric states. Here, A_N represents the antisymmetrizing operator. In order to derive the set of fermionic eigenstates of the Hamiltonian (2) we therefore initially may derive the set of all *N*-particle eigenstates followed by a projection onto $A_N \mathcal{H}_N$.

In the following we present and describe the fermionic ground state and provide a concise derivation in Appendix A. It turns out to be instructive to first discuss the case of zero interaction, K = 0. Clearly, in that case the corresponding time-independent Schödinger equation for the Hamiltonian (2) effectively simplifies to a one-fermion eigenvalue problem,

$$\left(\frac{\vec{p}^{\,2}}{2m} + \frac{1}{2}m\vec{x}^{t}\Omega\vec{x}\right)\chi = \varepsilon\,\chi\,. \tag{4}$$

The solutions of Eq. (4) are given by the *n*-dimensional Hermite functions denoted by $\phi_{\mu}^{(l)}(\vec{x}) \equiv \prod_{\alpha=1}^{n} \varphi_{\mu}^{(l^{(\alpha)})}(x^{(\alpha)})$ with corresponding energy $\varepsilon_{\mu} = \sum_{\alpha=1}^{n} (\mu^{(\alpha)} + \frac{1}{2})\hbar\omega^{(\alpha)}$. Here, $\varphi_{m}^{(l^{(\alpha)})}$ denotes the *m*th Hermite function in one dimension with natural length scale $l^{(\alpha)} \equiv \sqrt{\frac{\hbar}{m\omega^{(\alpha)}}}$, $\mu \equiv (\mu^{(\alpha)})_{\alpha=1}^{n}$, and $l \equiv (l^{(\alpha)})_{\alpha=1}^{n}$. The fermionic eigenstates of the Hamiltonian (2) for zero interaction are then given by the "configuration states," i.e., by Slater determinants obtained by distributing the *N* particles in *N* different states $\phi_{\mu}^{(l)}$. In particular, the corresponding ground state is then given by filling the *N* one-particle states with lowest one-particle energies ε_{μ} according to Pauli's exclusion principle.

In general, for interacting fermions one cannot expect that the structure of the energy eigenstates can be elegantly described by exploiting the elementary and convenient one-fermion picture. Yet, a bit surprisingly, this is still possible at least for the ground state of Harmonium [45]:

Theorem II.1. The *N*-fermion ground state $\Psi^{(f)}$ of the Harmonium model (2) is given by

$$\Psi^{(f)}(\vec{x}_{1},...,\vec{x}_{N}) = \mathcal{N} \begin{vmatrix} \phi_{\mu_{1}}^{(\tilde{l})}(\vec{x}_{1}) & \cdots & \phi_{\mu_{1}}^{(\tilde{l})}(\vec{x}_{N}) \\ \vdots & \vdots \\ \phi_{\mu_{N}}^{(\tilde{l})}(\vec{x}_{1}) & \cdots & \phi_{\mu_{N}}^{(\tilde{l})}(\vec{x}_{N}) \end{vmatrix} \times e^{\vec{X}' B \vec{X}}, \quad (5)$$

with $\vec{X} \equiv \frac{1}{N}(\vec{x}_1 + \cdots + \vec{x}_N)$ the center-of-mass vector, $\boldsymbol{B} \equiv \text{diag}(\boldsymbol{B}^{(1)}, \dots, \boldsymbol{B}^{(n)}), \qquad \boldsymbol{B}^{(\alpha)} \equiv \frac{N}{2}(\frac{1}{(l^{(\alpha)})^2} - \frac{1}{(l^{(\alpha)})^2}), \qquad \tilde{\omega}^{(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK}{m}}, \quad \tilde{l}^{(\alpha)} \equiv \sqrt{\frac{\hbar}{m\tilde{\omega}^{(\alpha)}}}, \text{ and } \mathcal{N} \text{ is a normalization constant. The quantum number vectors } \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_N \text{ in (5) are chosen such that the energy function}$

$$E_{\boldsymbol{\mu}_1,\dots,\boldsymbol{\mu}_N} \equiv \sum_{i=1}^N \tilde{\varepsilon}_{\boldsymbol{\mu}_i} \tag{6}$$

is minimal, yet respecting Pauli's exclusion principle [46] (i.e., all μ_i are different) and $\tilde{\varepsilon}_{\mu_i} \equiv \sum_{\alpha=1}^n (\mu^{(\alpha)} + \frac{1}{2}) \hbar \tilde{\omega}^{(\alpha)}$.

Since the proof of Theorem II.1 is less trivial we present it in Appendix A. As a caveat, we would like to stress that the excited states are *not* given by filling "boxes" of higher energy and then multiplying the corresponding Slater determinant by the exponential factor as in Eq. (5). Indeed, their structure is more complicated and the single Slater determinant in Eq. (5) would need to be replaced by a linear combination of several Slater determinants, expressing the additional correlations in the system.



FIG. 2. Graphical illustration of the fermionic ground state $|\Psi^{(f)}\rangle$ for the exemplary case of n = 2 spatial dimension and N = 5 fermions. In general, $|\Psi^{(f)}\rangle$ is given by a single Slater determinant, obtained by filling the *N* boxes with lowest energy respecting Pauli's exclusion principle (left), multiplied by a correlation term $e^{\vec{X}'B\vec{X}}$ (right) for the center of mass $\vec{X} \equiv \frac{1}{N}(\vec{x_1} + \cdots \vec{x_N})$. Each box, labeled by $\vec{\mu} = (\mu_1, \dots, \mu_n)$ describes a one-particle orbital given by a harmonic oscillator state in *n* dimensions with corresponding frequencies $\tilde{\omega}^{(\alpha)}$, $\alpha = 1, \dots, n$.

The ground state as stated in Theorem II.1 is graphically illustrated in Fig. 2. It is given by a Slater determinant, obtained by successively distributing fermions in the boxes (energy levels) $\phi_{\mu}^{(\bar{l})}$ with lowest energy $\tilde{\varepsilon}_{\mu}$, respecting Pauli's exclusion principle, multiplied by the term $e^{\vec{X}^{t}B\vec{X}}$. This latter term contains the physical correlations, in contrast to the Slater determinant which contains only exchange correlations. For the example in Fig. 2 of N = 5 and n = 2 the occupied boxes are given by the configuration $C = \{\{0,0\},\{1,0\},\{0,1\},\{2,0\},\{1,1\}\}.$

Consequently, the ground state for finite interaction has some similarity to the ground state for zero interaction. They differ by the correlation term $e^{\vec{X}'B\vec{X}}$ and a change of the natural length scales $\tilde{l}^{(\alpha)}$ of the Hermite functions $\Phi_{\mu}^{(\tilde{l})}$. Furthermore, if the coupling constant K (or some $\omega^{(\alpha)}$) changes, the structure of the ground state can change at some "critical" values: For this, notice that the energy ratios $\tilde{\varepsilon}_{\mu}/\tilde{\varepsilon}_{\mu'}$, i.e., the ratios of the distances between the boxes in different directions $\alpha = 1, \dots, n$ in Fig. 2, depend on the coupling strength. By changing these ratios, the Nth lowest and (N + 1)th lowest energies $\tilde{\boldsymbol{\varepsilon}_{\mu}}$ may cross and the N fermions change their configuration $\{\mu_1, \ldots, \mu_N\}$ to minimize the total energy (6). Such crossings particularly occur when one of the harmonic trap frequencies $\omega^{(\alpha)}$ is increased to very large values implying that all degrees of freedom in the corresponding α dimension are frozen. For instance, in the example presented in Fig. 2 increasing $\omega^{(2)}$ will initially change the ground-state configuration to $\{\{0,0\},\{1,0\},\{2,0\},\{0,1\},\{3,0\}\}$ and eventually to the quasi-one-dimensional case $\{\{0,0\},\{1,0\},\{2,0\},\{3,0\},\{4,0\}\}$.

As it was illustrated in Ref. [21] it is instructive to compare the fermionic ground state $\Psi^{(f)}$ to the bosonic ground state $\Psi^{(b)}$ of the Hamiltonian (2). The bosonic ground state can be described by the "box picture" as well: $\Psi^{(b)}$ is given by distributing all *N* bosons in the lowest energy "box" [defined by $\boldsymbol{\mu} \equiv (0, ..., 0) \equiv \mathbf{0}$] and multiplying the corresponding product state by the same exponential $e^{\vec{X}' B \vec{X}}$ as for fermions [cf. Eq. (5)]. Consequently, we get (see also Appendix A)

$$\Psi^{(b)}(\vec{x}_1, \dots, \vec{x}_N) \sim \left(\prod_{i=1}^N \phi_{\mathbf{0}}^{(\bar{l})}(\vec{x}_i)\right) \times e^{\vec{X}^t B \vec{X}}$$
$$\sim \left(\prod_{i=1}^N e^{-\vec{x}_i A \vec{x}_i}\right) \times e^{\vec{X}^t B \vec{X}}, \qquad (7)$$

where $A \equiv \text{diag}(A^{(1)}, \ldots, A^{(n)})$ and $A^{(\alpha)} \equiv \frac{1}{2(\tilde{l}^{(\alpha)})^2}$.

It is also worth discussing the symmetries of the *N*-Harmonium ground state (5). For all parameters K, $\{\omega^{(\alpha)}\}_{\alpha=1}^{n}$ the Hamiltonian (2) is invariant under simultaneous spatial reflections $P^{(\alpha)}: x_i^{(\alpha)} \to -x_i^{(\alpha)}, i = 1, ..., N$, of the α coordinate of various fermions, i.e.,

$$[\hat{H}, U(P^{(\alpha)})^{\otimes^{N}}] = 0, \tag{8}$$

where U is its unitary representation on the one-particle Hilbert space \mathcal{H} . Consequently, in particular the ground state (5) inherits the corresponding symmetry, $U(P^{(\alpha)})^{\otimes^N} \Psi^{(f)} = \pm \Psi^{(f)}$.

Furthermore, if two trap frequencies are equal, $\omega^{(\alpha)} = \omega^{(\alpha')}$ the Hamiltonian is in addition also invariant under simultaneous spatial rotation $R^{(\alpha,\alpha')}: (x_i^{(\alpha)}, x_i^{(\alpha')})^t \to R(x_i^{(\alpha)}, x_i^{(\alpha')})^t$, $R \in SO(2)$, of the α and α' coordinates of all N fermions. This extends in an elementary way to the case of more than two identical trap frequencies. For the case of isotropic traps, shell structures similar to those in atoms emerge [36].

III. ONE-PARTICLE REDUCED DENSITY OPERATOR AND NATURAL OCCUPATION NUMBERS

In this section, we discuss symmetries of 1-RDOs in general and present specific properties of the 1-RDO of the *N*-Harmonium ground state in particular.

A. General considerations

For pure N-fermion quantum states $|\Psi^{(f)}\rangle$ the 1-RDO is defined by

$$\rho^{(f)} = N \operatorname{tr}_{N-1}[|\Psi^{(f)}\rangle \langle \Psi^{(f)}|]$$
(9)

and is consequently normalized to the particle number N, i.e., $tr[\rho^{(f)}] = N$. Due to the fermionic exchange symmetry the choice of the N - 1 fermions to be traced out does not matter.

It is worth noting that 1-RDOs inherit one-particle symmetries of the corresponding *N*-fermion state [47]. To explain this, consider a one-particle symmetry of the *N*-fermion quantum state $|\Psi^{(f)}\rangle$ generated by the unitary operator $G = g^{\otimes^N}$ with g acting on the one-particle Hilbert space \mathcal{H} ,

$$G|\Psi^{(f)}\rangle = e^{i\zeta}|\Psi^{(f)}\rangle, \qquad (10)$$

with $\zeta \in \mathbb{R}$. Then, due to elementary properties of partial traces, the 1-RDO $\rho^{(f)}$ of $|\Psi^{(f)}\rangle$ inherits this symmetry and it follows

$$[g,\rho^{(f)}] = 0. (11)$$

Equation (11) particularly implies that the 1-RDO expressed as a matrix with respect to the *g*-symmetry-adapted states (eigenstates of *g*) is block diagonal. For instance, for translationally invariant *N*-electron states for one-band lattice models this implies that the natural orbitals, the eigenstates of $\rho^{(f)}$, are given by the Bloch states multiplied by a spin state. In that case, the NONs gain a lot of physical significance [18] since they are not just the eigenvalues of the 1-RDO but the occupancies with respect to physically distinguished one-particle states (Bloch states).

B. One-particle reduced density operator for the Harmonium ground state

Applying the considerations of Sec. III A to the parity symmetries of *N*-Harmonium we can conclude that the 1-RDOs of various eigenstates are block diagonal with respect to each parity symmetry $U(P^{(\alpha)}), \alpha = 1, 2, ..., n$. For instance, for the 1-RDO $\rho^{(f)}$ of the *N*-Harmonium ground state $|\Psi^{(f)}\rangle$ in two spatial dimensions we find

$$\rho^{(f)} = \rho_{ee}^{(f)} \oplus \rho_{eo}^{(f)} \oplus \rho_{oe}^{(f)} \oplus \rho_{oo}^{(f)}, \qquad (12)$$

where the indices e and o denote underlying even and odd parities for the respective dimensions $\alpha = 1,2$. Decomposition structures such as (12) will help us to significantly simplify the calculation of the eigenvalues of the 1-RDO $\rho^{(f)}$.

Similar to the computations in Ref. [21] for the ground state of Harmonium in one spatial dimension we determine the 1-RDO of the ground state in higher spatial dimensions by using the Hubbard-Stratonovitch relation (see Appendix B for more details). Again, it is instructive to relate the fermionic 1-RDO $\rho^{(f)}$ to the 1-RDO $\rho^{(b)}$ of the bosonic ground state (7). By comparing Eqs. (5) and (7) one immediately finds

$$\rho^{(f)}(\vec{x}, \vec{y}) = F(\vec{x}, \vec{y}) \cdot \rho^{(b)}(\vec{x}, \vec{y}), \tag{13}$$

where $F(\vec{x}, \vec{y})$ is a multivariate polynomial and $\rho^{(b)}(\vec{x}, \vec{y})$ is a Gaussian.

Since $\rho^{(b)}$ is a Gaussian state it can be analytically diagonalized (see for instance Ref. [43]). In contrast to $\rho^{(b)}$, this is not possible for the fermionic 1-RDO $\rho^{(f)}$. Yet, similar to Ref. [21], we can diagonalize $\rho^{(f)}$ by numerical means for fixed couplings. We introduce dimensionless coupling strengths for the spatial dimensions $\alpha = 1, 2, ..., n$,

$$\kappa^{(\alpha)} \equiv \frac{NK}{m(\omega^{(\alpha)})^2} = \left(\frac{l^{(\alpha)}}{\tilde{l}^{(\alpha)}}\right)^4 - 1.$$
(14)

Recall that the structure of the Hamiltonian (2) implies that the NONs of any of its eigenstates do not depend on $m(\omega^{(\alpha)})^2$ and *K* separately, but just on their ratios.

In addition, we use again as in Refs. [7,21] a perturbational approach for the regime of weak couplings. This perturbation theoretical approach can be simplified by exploiting a duality of NONs proven in Ref. [48]: By employing the alternative coupling parameters

$$\delta^{(\alpha)} := \ln\left(\frac{l^{(\alpha)}}{\overline{l}^{(\alpha)}}\right) = \frac{1}{4}\ln(1+\kappa^{(\alpha)})$$
$$= \frac{1}{4}\kappa^{(\alpha)} + O((\kappa^{(\alpha)})^2), \qquad (15)$$

with $\alpha = 1, 2, \ldots, n$, this duality reads

$$\vec{\lambda}(\ldots,\delta^{(\alpha)},\ldots) = \vec{\lambda}(\ldots,-\delta^{(\alpha)},\ldots),\tag{16}$$

for each $\alpha = 1, 2, ..., n$. As a consequence, the series expansions of various NONs simplifies since it contains even orders of each $\delta^{(\alpha)}$, only.

We conclude this section by briefly recalling that the exponential factor $\rho^{(b)}$ in the expression (13) implies an exponential decaying behavior of the NONs (for more details we refer the reader to Sec. IV B in Ref. [21]). This allows us to simplify the investigations of possible (quasi)pinning by exploiting the concept of truncation described in Ref. [21]: The infinite spectrum of NONs can be truncated by skipping various NONs which are very close to 1 or 0, respectively, and the (quasi)pinning analysis can be performed within the remaining smaller setting. Any result on possible quasipinning found in the truncated setting translates to quasipinning of the same strength in the infinite setting up to a small truncation error (for more details see Ref. [21]).

In the following sections we explore the occurrence of (quasi)pinning in great detail for various spatial dimensions, different particle numbers, and last but not least by incorporating spin degrees of freedom.

IV. QUASI-ONE-DIMENSIONAL HARMONIUM

Before investigating truly higher-dimensional systems in later sections, we are going to explore the quasipinning behavior in quasi-one-dimensional systems. This will especially allow us to link outcomes of subsequent analyses to the results from Refs. [7,21] for the strictly one-dimensional Harmonium. By quasi-one-dimensional systems we mean systems in which all but one trapping frequencies have been highly detuned. In addition, we assume those detuned frequencies $\omega^{(2)}, \ldots, \omega^{(n)}$ to be identical yielding a hypercylindric trapping potential. In graphical representations of the Harmonium ground state as shown in Fig. 2 this relates to a situation in which the interbox spacings $\hbar \tilde{\omega}^{(\alpha)}$ have severely been increased in all but one dimension, $\tilde{\omega}^{(\alpha)}/\tilde{\omega}^{(1)} \gg 1$ for $\alpha = 2, \ldots, N$. Consequently, only energy levels along the one-axis will be occupied. This resembles the physical situation in which harmonic oscillators in the directions $\alpha \ge 2$ carry no excitations.

Generally, the notion of effective lower dimensionality can be captured more formally as follows. If a configuration has quantum number vectors $\{\boldsymbol{\mu}_i\}_{i=1}^N$ with $\mu_i^{(\alpha)} = 0$ for all $\alpha > n'$ and i = 1...N, the fermionic ground-state function decomposes into a product of the fermionic ground-state function in the first n' dimensions and the bosonic ground-state function in the remaining (n' - n) dimensions,

$$\Psi_{n}^{(f)} = \Psi_{n'}^{(f)} \otimes \Psi_{n-n'}^{(b)}.$$
(17)

Such effective lower dimensionality has structural implications on the fermionic 1-RDO as well: The polynomial *F* in Eq. (13) will not depend on $x_i^{(\beta)}, y_i^{(\beta)}$ with i = 1...N and $\beta > n'$. Hence, the 1-RDO becomes a product of a fermionic 1-RDO in the first *n'* dimensions and the bosonic 1-RDO in remaining n - n' dimensions,

$$\rho_n^{(f)} = \frac{1}{N} \,\rho_{n'}^{(f)} \otimes \rho_{n-n'}^{(b)}.$$
(18)

The factor N originates from the specific normalization of 1-RDOs, $tr[\rho] = N$.

As a consequence of Eq. (18), the spectrum of $\rho_n^{(f)}$ becomes the product of the spectrum of the lower-dimensional fermionic 1-RDO and the spectrum of the bosonic 1-RDO,

$$\vec{\lambda}_n^{(f)} = \frac{1}{N} \left(\vec{\lambda}_{n'}^{(f)} \times \vec{\lambda}_{n-n'}^{(b)} \right)^{\downarrow},\tag{19}$$

where " \downarrow " denotes decreasing ordering.

These considerations can now be applied to quasi-onedimensional Harmonium which is achieved for sufficiently large trapping frequency detunings, namely $\tilde{\omega}^{(\alpha)} > (N - 1)\tilde{\omega}^{(1)}$ for $\alpha \ge 2$. The corresponding vector of ground state NONs is then given by the product of the spectrum $\tilde{\lambda}_1^{(f)}$ of the one-dimensional fermionic 1-RDO and (n - 1) spectra $\tilde{\lambda}_1^{(b)}$ of the (n - 1) decoupled one-dimensional bosonic 1-RDOs. According to Ref. [21], the spectrum of the one-dimensional bosonic 1-RDO with coupling $\overline{\kappa}$ is given by the NONs

$$\lambda_k^{(b)}(\overline{\kappa}) = N(1 - q(\overline{\kappa})) q(\overline{\kappa})^k, \quad k \in \mathbb{N}_0^+,$$
(20)

where

$$q(\overline{\kappa}) = 1 - \frac{2N}{N + \sqrt{N^2 - (N-1)[2 - (1+\overline{\kappa})^2 - 1/(1+\overline{\kappa})^2]}}.$$
(21)

The corresponding coupling strengths $\kappa^{(2)} = \cdots = \kappa^{(n)} \equiv \overline{\kappa}$ for those bosonic spectra can be expressed as a function of $\delta \equiv \delta^{(1)}$ and the trapping frequency ratios $\chi \equiv \omega^{(\alpha)}/\omega^{(1)}, \alpha \ge 2$. It is also worth noticing that with increasing detunings χ , the bosonic spectra approach more and more $(N, 0, 0, \ldots)$.

We apply these general ideas to the exemplary case N = 3and n = 2. The spectrum $\vec{\lambda}_1^{(f)}$ was determined in Ref. [7] and is also listed in Appendix C. Then, we determine the NONs of the corresponding three-Harmonium ground state via Eq. (19). The corresponding quasipinning analysis is slightly involved. The main reason for this is that by varying the parameters δ and χ the hierarchy of NONs in Eq. (19) does change, which changes the quasipinning behavior as well [18]. Even within regimes of noncrossing NONs, providing a closed analytical expression for the minimal distance D_{\min} of $\vec{\lambda}$ to the polytope boundary is often not possible since the GPC which is most saturated may change while changing δ and χ .

This then requires us to split the parameter space into separate regimes where the most relevant NONs do not cross. We consider in the following only the regime which includes particularly the limit $\chi \to \infty$. This regime turns out to be defined by

$$\chi > \chi_{\rm crit}(\delta) \equiv \sqrt[4]{\frac{243}{40}} \frac{1}{\delta^{3/2}},$$
 (22)

where $\delta \ll 1$. A thorough and quite lengthy quasipinning analysis is performed by exploiting the concept of truncation (cf. Ref. [21]). Conclusive results on the occurrence of quasipinning can be found in the truncated setting $\wedge^3[\mathcal{H}_1^{(10)}]$ and the minimal distance to the polytope boundary follows as

$$D_{\min}(\delta,\chi) = \frac{4}{9\chi^4}\delta^2 + \frac{20}{2187}\delta^8 + O(\delta^{10}).$$
 (23)

Note that due to the condition (22) we have $\delta^8 \gtrsim \delta^2 / \chi^4$. The truncation error, given by $\sum_{k=11}^{\infty} \lambda_k(\delta, \chi)$, is of the order $O(\delta^{10})$ which is negligible indeed.

Furthermore, taking the limit $\chi \to \infty$ as a consistency check reveals that

$$\lim_{\chi \to \infty} D_{\min}(\delta, \chi) = \frac{20}{2187} \delta^8 + O(\delta^{10}),$$
(24)

which coincides with the quasipinning found for the strictly one-dimensional three-Harmonium [see Eq. (16) in Ref. [7]].

The result (23) indicates that the strength of quasipinning in one-dimensional systems is only slightly reducing when adding a second spatial dimension. This is not surprising since in general adding additional spatial dimensions, whose degrees of freedom, however, are frozen, should not change physical quantities.

V. FULLY SPIN-POLARIZED HARMONIUM IN HIGHER SPATIAL DIMENSIONS

After having presented an analysis on quasipinning of the Harmonium in quasi-one-dimensional setups in the previous section, we are now going to consider the extension to higher dimensions. Still, we assume a complete alignment of all spins, i.e., freezing out the spin degree of freedom.

A. Two spatial dimensions and corresponding dimensional crossovers

Let us start by considering the weak-coupling regime. In addition we restrict this analysis to the case of an isotropic external trap, i.e., $\omega^{(2)} = \omega^{(1)}$. According to the definitions (14) and (15), we have $\kappa \equiv \kappa^{(1)} = \kappa^{(2)}$ and $\delta \equiv \delta^{(1)} = \delta^{(2)}$, respectively. Due to the simplifications following from the duality of NONs (16) we determine Taylor series of various NONs in the mathematically more convenient parameter δ . First, we discuss in more detail the case of three fermions. The corresponding unique ground state is given by Theorem II.1 and its configuration follows as $C = \{\{0,0\},\{1,0\},\{0,1\}\}$. The perturbational expansion of its NONs leads to the following results up to corrections of the order $O(\delta^{(8)})$:

$$\lambda_{1}(\delta) = 1 - \frac{32\delta^{4}}{81} + \frac{224\delta^{6}}{729} + O(\delta^{8}),$$

$$\lambda_{2}(\delta) = \lambda_{3}(\delta) = 1 - \frac{4\delta^{2}}{9} + \frac{4\delta^{4}}{27} - \frac{152\delta^{6}}{3645} + O(\delta^{8}),$$

$$\lambda_{4}(\delta) = \lambda_{5}(\delta) = \frac{4\delta^{2}}{9} - \frac{8\delta^{4}}{27} + \frac{16\delta^{6}}{135} + O(\delta^{8}),$$

$$\lambda_{6}(\delta) = \lambda_{7}(\delta) = \frac{4\delta^{4}}{27} - \frac{88\delta^{6}}{729} + O(\delta^{8}),$$

$$\lambda_{8}(\delta) = \lambda_{9}(\delta) = \frac{4\delta^{4}}{27} - \frac{40\delta^{6}}{243} + O(\delta^{8}),$$

$$\lambda_{10}(\delta) = \frac{8\delta^{4}}{81} - \frac{16\delta^{6}}{243} + O(\delta^{8}),$$

$$\lambda_{i \ge 11}(\delta) = O(\delta^{6}).$$
(25)

Note that some NONs are degenerate in pairs. This is a direct consequence of the substructure of the 1-RDO as given by Eq. (12) since spec[$\rho_{1,ee}^{(f)}$] = spec[$\rho_{1,ee}^{(f)}$] in the case of an isotropic trap. It should be also stressed that the extension of the perturbation series to deformed anisotropic traps is a bit more tedious but can be carried out in a similar fashion.

TABLE I. For the *N*-Harmonium ground states in n = 2 spatial dimensions we present the 'active space structures' by considering NONs with corrections to the values 1 or 0 up to the orders δ^2 , δ^4 , and δ^6 , respectively. The results on quasipinning are presented (D_{\min}) as well as its 'nontriviality,' quantified by the *Q* parameter (see text).

(N,n)	δ^2	δ^4	δ^6	D_{\min}	10-2
(3,2)	$\wedge^2[\mathcal{H}_1^{(4)}]$	$\wedge^3[\mathcal{H}_1^{(10)}]$	$\wedge^3[\mathcal{H}_1^{(14)}]$	$\propto \delta^4$	$\propto \delta^0$
(4,2)	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^4[\mathcal{H}_1^{(13)}]$	$\wedge^4[\mathcal{H}_1^{(20)}]$	$\propto \delta^4$	$\propto \delta^2$
(5,2)	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^5[\mathcal{H}_1^{(20)}]$	$\propto \delta^4$	$\propto \delta^0$
(6,2)	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^5[\mathcal{H}_1^{(21)}]$	$\propto \delta^6$	$\propto \delta^0$
(7,2)	$\wedge^4[\mathcal{H}_1^{(9)}]$	$\wedge^6[\mathcal{H}_1^{(17)}]$	$\wedge^7[\mathcal{H}_1^{(24)}]$	$\propto \delta^6$	$\propto \delta^0$

Since the spectrum $\overline{\lambda}(\delta)$ is infinite we exploit again the concept of truncation. By considering the truncated setting $\wedge^{3}[\mathcal{H}_{1}^{(10)}]$ we find a minimal distance $D_{\min}(\delta)$ of $[\lambda_{k}(\delta)]_{k=1}^{10}$ to the boundary of the corresponding polytope $\mathcal{P}_{3,10}$, given by

$$D_{\min}(\delta) = \frac{8}{27}\delta^4 + O(\delta^6).$$
 (26)

Since the neglected NONs are of smaller order, $O(\delta^6)$, this truncated (quasi)pinning analysis is conclusive: For weak coupling the ground-state NONs $\vec{\lambda}(\delta)$ in the infinite-dimensional setting $(N,d) = (3,\infty)$ are not exactly on, but very close to the boundary of the allowed region $\mathcal{P}_{3,\infty}$. This distance is indeed smaller by two orders in δ than the distance D_{HF} of $\vec{\lambda}(\delta)$ to the Hartree-Fock point $\vec{\lambda}_{HF} \equiv (1,1,1,0,\ldots)$,

$$D_{HF}(\delta) = \frac{8}{9}\delta^2 + \frac{8}{81}\delta^4 + O(\delta^6).$$
(27)

On the other hand, comparing these results on quasipinning of the three-Harmonium ground state in two dimensions to the remarkable result of δ^8 quasipinning ($D_{\min} \sim \delta^8$) found in one dimension [7] indicates that reduced spatial dimensionality seems to be essential for the occurrence of strong quasipinning.

In the same way as for N = 3 particles we study ground states of the Harmonium model for N > 3 and determine Taylor series for the corresponding NONs. We present the results in Table I for the cases of N = 4,5,6,7. There, in the second, third, and fourth columns we present the active space structures by taking into account different orders in δ . An active space structure $\wedge^{N'}[\mathcal{H}_1^{(d')}]$ on the scale $O(\delta^r)$ means that exactly N' NONs, $\lambda_{N-N'+1}, \ldots, \lambda_N$, and d' - N' NONs, $\lambda_{N+1}, \ldots, \lambda_{N+d'-N'}$, have corrections on the scales $\delta^s, s \leq r$ to the maximal value 1 and the minimal value 0, respectively. It is particularly remarkable that such well-pronounced hierarchies of actives spaces exist for the Harmonium model and can even be proven analytically. In addition, it should be stressed that such hierarchies are very convenient for the (quasi)pinning analysis. For any scale of interest, we can choose the coupling such that the higher orders are sufficiently small and the corresponding truncation error becomes negligible. In the secondto-last column we present the strength of the quasipinning by stating the minimal distance D_{\min} of $\lambda(\delta)$ to the boundary of $\mathcal{P}_{N,\infty}$, determined by exploiting the concept of truncation. For the cases N = 4.5 we find again quasipinning of the strength δ^4 which increases for N = 6,7 to δ^6 quasipinning. This increase of the quasipinning strength by adding more fermions to the trap suggests the existence of a "Pauli pressure," created by the additional particles, pressing λ closer to the polytope boundary. For the case of the corresponding one-dimensional system discussed in Ref. [21] the active space hierarchy was even more well pronounced due to missing degenerate angular degrees of freedom (which typically reduce the Pauli pressure) in agreement with the much stronger quasipinning of the order

 δ^{2N} for $N \ge 4$ particles found there. As can be inferred from the inclusion relation $\mathcal{P} \subset \Sigma$, illustrated in Fig. 1, and as has been carefully explored in Ref. [19], quasipinning by GPCs can in some cases be just a consequences of quasipinning by PEP constraints. For instance, the distance of $\overline{\lambda}$ to the polytope boundary is bounded from above by $1 - \lambda_1$, the distance of $\overline{\lambda}$ to the corresponding facet $\lambda_1 = 1$ of the Pauli simplex Σ . Hence, it is not only important to explore and quantify quasipinning by GPCs on an absolute scale but also relative to possible quasipinning by PEP constraints. In Ref. [19] a measure for such nontriviality of quasipinning by GPCs was constructed, the so-called *O*-parameter: $\vec{\lambda}$ is $10^{Q(\vec{\lambda})}$ times closer to the polytope boundary than one may expect from a possibly small distance of λ to the boundary of the Pauli simplex Σ . The results for the Q parameter are shown in the last column of Table I. The quasipinning found for various particle numbers is in all cases, except N = 4, "trivial." It follows already from the approximate saturation of PEP constraints, typically $1 - \lambda_1 \ge 0$. Only in the case of four fermions the quasipinning by GPCs is nontrivial, by two orders in δ . Comparing this to the results for N fermions in one spatial dimension [21], namely $10^{-Q(\bar{\lambda}(\delta))} \sim \delta^2$ for all N, suggests that the GPCs are particularly relevant in lower spatial dimensions (one dimension). In the following we find further evidence for this by comparing dimensional crossovers by ramping up one of the two trap frequencies to approach more and more the effectively one-dimensional regime.

We parametrize the coupling regime by $\kappa \equiv \kappa_1 \ge 0$ [recall Eq. (14)] and the detuning $\chi = \omega_2/\omega_1 \ge 1$ of the trap frequencies. We consider the case of three fermions. For smaller detunings, the ground state takes the configuration $\mu =$ $\{\{0,0\},\{1,0\},\{0,1\}\}$. For larger detunings, the ground state becomes effectively one dimensional, $\mu' = \{\{0,0\},\{1,0\},\{2,0\}\}$ (see remarks at the end of Sec. II). Variation of χ while keeping κ fixed therefore allows one to study the crossover from two to one spatial dimension. In the κ - χ parameter plane, the transition line between the two ground-state configurations is given by $\kappa_{\rm crit} = -\frac{4}{3} + \frac{1}{3}\chi^2$. Following Sec. III, the truncated 1-RDO has been analytically computed. For a logarithmically distributed set of data points in the κ - χ parameter plane, the NONs of truncated 1-RDOs have then been numerically evaluated and used to determine $D_{\min}(\kappa, \chi)$ and $Q(\kappa, \chi)$. The results are displayed in Fig. 3. For all coupling parameters considered there, as well as in the figures of subsequent sections, the concept of truncation was used and the truncation errors turned out to be negligible. The transition line between the two state configurations μ and μ' is marked by a solid line. In addition, there are shown two dashed lines indicating crossings of some specific (nonordered) NONs [49]. In principle, there are many more crossings but according to the



FIG. 3. Quasipinning results for the three-Harmonium ground state in two spatial dimensions with external trap frequencies ω_1, ω_2 and coupling strength κ . Minimal distance D_{\min} of $\vec{\lambda}$ to polytope boundary is shown on the left and its nontriviality is quantified on the right. The solid line represents the boundary $\kappa_{\rm crit}(\chi)$ in between the two different ground-state configurations with the effectively one-dimensional one on the right. Dashed lines mark relevant crossing of NONs (see text for more details).

concept of truncation only the crossings of the largest few NONs can change the quasipinning behavior considerably.

As a first qualitative result we observe that D_{\min} monotonically decreases under the reduction of the fermion-fermion coupling strength κ . This is not surprising since this reduces the correlations in the system and $\overline{\lambda}$ approaches the Hartree-Fock point. For the case $\omega_1 = \omega_2$ the numerical results for the whole κ regime [0,10] are well described by the analytic perturbation-theoretical result (26) since $\delta = 1$ corresponds to $\kappa \approx 55$. We further learn that by narrowing the trap, i.e., by increasing ω_2/ω_1 , D_{\min} decreases as well. This provides further evidence for the existence of a Pauli pressure, supposed to increase whenever the number of available states around the Fermi level reduces. It should be stressed (not shown here) that even the state with configuration $\boldsymbol{\mu} = \{\{0,0\},\{1,0\},\{0,1\}\},\$ being an excited state for too large detunings, begins to exhibit stronger and stronger quasipinning by increasing the detuning.

The relevance of the quasipinning beyond the Pauli exclusion principle as measured by the Q parameter, however, shows a more complex and a different behavior than D_{\min} . For $\kappa \lesssim 1$ fixed, the system undergoes multiple changes from trivial quasipinning (green) to highly nontrivial quasipinning (red). Between different regimes \mathcal{R}_i within the effectively onedimensional state configuration, we observe sharp gradients in both the Q parameter as well as the minimal distance D_{\min} . To explore those transitions further we present fixed κ sections in Fig. 4. While the change of the ground-state configuration does not have a tremendous influence on the absolute quasipinning this is different for the first dashed line (in Fig. 3), where λ_4 and λ_5 are coming together: Within a short ω_2/ω_1 interval, the quasipinning increases by several orders for the two exemplary cases $\kappa = 1/10, 1/50$. In addition this quasipinning changes from trivial to highly nontrivial. Also crossings of smaller eigenvalues lead to nonanalytic behavior of D_{\min} and Q(see, e.g., the black circles) which, however, according to the concept of truncation does not change the quasipinning behavior significantly. Finally, we conclude that for the small coupling $\kappa = 1/50$ (red curve) detunings even larger than $\omega_2/\omega_1 = 1000$ are required to reproduce the quasipinning results for the one-dimensional system.



FIG. 4. Top: Minimal distance D_{\min} of $\vec{\lambda}$ to the polytope boundary as a function of the trap frequency detuning $\chi \equiv \omega_2/\omega_1$ for fixed particle-particle interaction strengths κ . Bottom: Relevance of the quasipinning by GPCs beyond Pauli's exclusion principle as measured by the Q parameter.

The case of four particles in two spatial dimensions is contained in the next section, analyzing dimensional crossovers for N = 4 in three spatial dimensions.

B. Three spatial dimensions and corresponding dimensional crossovers

The analytic results for an isotropic harmonic trap in three spatial dimensions for the regime of weak couplings δ and N = 3,4,5,6 are presented in Table II. In the second, third, and fourth columns we present the active space structures by taking into account the orders $O(\delta^2)$, $O(\delta^4)$, and $O(\delta^6)$,

TABLE II. For the *N*-Harmonium ground states in n = 3 spatial dimensions we present the 'active space structures' by considering NONs with corrections to the values 1 or 0 up to the orders δ^2 , δ^4 , and δ^6 , respectively. The results on quasipinning are presented (D_{\min}) as well as its 'nontriviality,' quantified by the *Q* parameter. A question mark indicates that no analysis was possible due to too large active spaces.

(N,n)	δ^2	δ^4	δ^6	D_{\min}	10^{-Q}
(3,3)	$\wedge^3[\mathcal{H}_1^{(8)}]$	$\wedge^3[\mathcal{H}_1^{(18)}]$	$\wedge^3[\mathcal{H}_1^{(32)}]$	$O(\delta^4)$	$O(\delta^2)$
(4,3)	$\wedge^3[\mathcal{H}_1^{(8)}]$	$\wedge^4[\mathcal{H}_1^{(20)}]$	$\wedge^4[\mathcal{H}_1^{(34)}]$	$\propto \delta^4$	$\propto \delta^0$
(5,3)	$\wedge^4[\mathcal{H}_1^{(12)}]$	$\wedge^5[\mathcal{H}_1^{(26)}]$	$\wedge^5[\mathcal{H}_1^{(45)}]$	$O(\delta^4)$?
(6,3)	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^6[\mathcal{H}_1^{(29)}]$	$\wedge^5[\mathcal{H}_1^{(49)}]$	$O(\delta^4)$?



FIG. 5. Quasipinning results for the four-Harmonium ground state in three dimensions with external trap frequencies $\omega_1, \omega_2, \omega_3$ and coupling strength κ . Minimal distance D_{\min} of λ to polytope boundary is shown in the upper diagram and its nontriviality Q is quantified in the lower diagram (see text for details). The left and right solid curves indicate a change of the ground-state configuration.

respectively. Comparing those active spaces with those for two spatial dimensions, shown in Table I, confirms that the additional angular degrees of freedom in n = 3 dimensions increase significantly the dimensions of the active spaces and therefore reduce the Pauli pressure. This increase of the dimension reduces the chances for a conclusive (quasi)pinning analysis. Indeed, as we can infer from the last two columns this is only possible for N = 4. A conclusive (quasi)pinning analysis for the larger particle numbers N = 5.6 would require the knowledge of the GPCs at least for the settings (N,d) = (4,12) and (5,14), respectively. For the cases N = 3.4 we find quasipinning of the strength δ^4 which might be even stronger for N = 3 since the truncation error is of the same order, $O(\delta^4)$. For N = 3, as quantified by the Q parameter, this quasipinning by GPCs is nontrivial by at least two orders in δ . For N = 4, however, it follows already from quasipinning by PEP constrains, $1 - \lambda_1(\delta) \sim \delta^4$. For N = 5.6we can determine only lower bounds on the strength of the quasipinning (upper bounds on D_{\min}): Since $1 - \lambda_1 \sim \delta^4$ we can conclude quasipinning by GPCs of order 4 or larger in δ .

To further explore the role of the spatial dimension for quasipinning we study dimensional crossovers for the exemplary case of four fermions. The results are shown in Fig. 5. We first start with the isotropic trap, $\omega_1 = \omega_2 = \omega_3$ and ramp up continuously ω_3 to the value $\omega_3 = 1000 \,\omega_1$ while fixing $\omega_2 = \omega_1$. In particular, this induces a change of the ground-state configuration (first solid line) from $\mu = \{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{0,0,1\}\}\$ to $\{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{2,0,0\}\}\$. Then, we approach the effectively one-dimensional regime by also ramping up ω_2 relative to ω_1 , inducing in particular another change of the ground-state configuration (last solid line) to $\{\{0,0,0\},\{1,0,0\},\{2,0,0\},\{3,0,0\}\}\$. To keep the error of the truncated (quasi)pinning analysis [performed in the largest known setting (N,d) = (4,10)] sufficiently small we need to restrict ourselves to the coupling regime $\kappa \in [0,1]$. Recall that in two spatial dimensions we could conclusively explore quasipinning up to couplings $\kappa = 10$. This was due to the fact that the active spaces in two spatial dimensions are smaller and that the GPCs for N = 3 (as analyzed in Fig. 3) are already known for d = 11.

In Fig. 5 we observe that the minimal distance D_{\min} of λ to the polytope boundary monotonically decreases with decreasing κ , essentially reflecting the fact of reducing correlations. For every fixed state configuration μ , increasing the anisotropy of the trap increases the strength of the quasipinning as well. Intriguingly, however, at the boundaries of these regimes, the quasipinning strength drops by several orders of magnitude, which has not been the case for N = 3 particles in two spatial dimensions (see Fig. 3).

The most striking aspect of the (quasi)pinning analysis of this system, however, is revealed by a comparison of D_{\min} and Q in the effectively one-dimensional configuration. While D_{\min} decreases with smaller κ and larger ω_2/ω_1 , the Q parameter shows that the quasipinning becomes trivial in parameter regions with small D_{\min} (cf. lower-right corner of the diagram and that it becomes highly nontrivial in parameter regions with large D_{\min} (cf. upper-right corner of the diagram). This irrefutably demonstrates the importance to quantify quasipinning by GPCs *beyond* quasipinning by PEP constraints.

Let us add a closing remark on degeneracies of the eigenspaces of Harmonium in higher dimensions. The box picture (see Fig. 2) reveals the occurrence of shell structures in Harmonium systems where an additional rotational symmetry is given whenever two or more trapping frequencies will be equal. For example N = 4 particles in two-dimensional Harmonium with $\omega_1 = \omega_2$ will have a threefold degenerate ground-state space. The obvious question whether superpositions of these states may experience a different quasipinning has been addressed by considering various superpositions, including the rotational symmetry adapted eigenstates. The quasipinning behavior of these states was found to show the same scaling as the one for nonsymmetry adapted states. They therefore have not separately been displayed in the Tables I and II.

VI. SPIN

In the previous sections and in Refs. [7,21] the Harmonium model was studied for spinless or fully polarized fermions, only, due to a good reason: By considering spinful particles with spin *S*, each spatial orbital gets a multiplicity of factor 2S + 1. This significantly reduces the Pauli pressure which is expected to reduces the relevance of the GPCs as well. In addition, the spin degeneracies make an interpretation of possible quasipinning more challenging. In this section we eventually consider non-fully-polarized systems. This will also allow us to induce changes of the quantum state and thus of quasipinning by ramping up an external magnetic field. In that sense, we provide conceptual ideas for experimental realizations of the quasipinning phenomenon.

Besides taking spin degrees into account, by extending the *N*-fermion Hilbert space to $\wedge^{N}[L_{2}[\mathbb{R}^{n}] \otimes \mathbb{C}^{2}]$ by assuming S = 1/2, we couple the spins to an external homogeneous magnetic field \vec{B} , described by the Zeeman term $-c/\hbar \sum_{i=1}^{N} \vec{s}_i \cdot \vec{B}$, added to the Hamiltonian (2), where *c* is a coupling constant [50].

Since the Zeeman term commutes with the remaining part of the Hamiltonian, Theorem II.1 and the box picture can easily be extended to the spinful case: Each orbital $\phi_{\mu_i}^{(l)}(\vec{x}_i)$ in the Slater determinant in Eq. (5) is multiplied by a spin state $|\sigma_j\rangle = |\uparrow\rangle, |\downarrow\rangle$, defined with respect to the quantization axis \vec{B}/B . The box picture is modified by considering two "box arrays," one for $|\uparrow\rangle$ and one for $|\downarrow\rangle$. These two box arrays are energetically displaced by the energy difference g|B|between $|\uparrow\rangle$ and $|\downarrow\rangle$ due to the external magnetic field B. Then, the ground-state configuration $\mu = (\mu^{\uparrow}, \mu^{\downarrow})$ follows again by distributing the N fermions into the N energetically lowest boxes and the ground state is given by the modified Eq. (5). For instance, the ground state of N = 4 particles in an isotropic two-dimensional trap with frequencies $\omega_1 = \omega_2 \equiv \omega$ with an external magnetic field $\hbar\omega\sqrt{1+\kappa}/c < |B| < 2\hbar\omega\sqrt{1+\kappa}/c$ is described by $\mu^{\downarrow} = \{\{0,0\},\{1,0\},\{0,1\}\}$ and $\mu^{\uparrow} = \{\{0,0\}\}.$

We first investigate quasipinning for the one-dimensional case. For the regime of weak coupling δ we determine for N = 3,4 and for each spin sector the corresponding ground state. For N = 3, depending on the field strength *B* of the magnetic field and the coupling parameter δ , the ground state can have the magnetic quantum number $M = \pm \frac{3}{2}, \pm \frac{1}{2}$ and for N = 4 the magnetic quantum number $M = \pm 2, \pm 1,0$, respectively. A thorough and conclusive (quasi)pinning analysis by using the concept of truncation shows the following universal quasipinning behavior:

$$D_{\min}(\delta) \sim \delta^{4+2|M|}.$$
 (28)

This remarkable result for N = 3,4 strongly supports the relevance of the proposed Pauli pressure for the occurrence of quasipinning: The larger the degree of polarization, |M|, the stronger the conflict between energy minimization and fermionic exchange symmetry and the stronger the quasipinning according to Eq. (28).

We briefly comment on the nontriviality of the quasipinning (28) by comparing it to quasipinning by PEP constraints. For N = 3 and both values $|M| = \frac{3}{2}, \frac{1}{2}$ the quasipinning by GPCs is nontrivial by two orders in δ . The same holds of course for N = 4 in case of full polarization [21]. Yet, for not-fully-polarized fermions, |M| = 0, 1, quasipinning by GPCs turns out to be trivial. In contrast to the case $M = \pm 1$, this is obvious for the case M = 0 [51]: It is well known [52] that for spin-singlet states the only constraints on the NONs are the PEP constraints. In other words, by restricting the *N*-fermion Hilbert space to spin-singlet states the corresponding GPCs coincide with the PEP constraints and therefore do not facilitate any nontrivial quasipinning by GPCs.

As an example for higher spatial dimension we consider the case of three fermions in two dimensions. We exploit the physically more relevant coupling parameter $\kappa \equiv \kappa_1$ [recall Eq. (14)] and the detuning $\chi \equiv \omega_2/\omega_1 \ge 1$. We start with $\chi = 1$ and choose the magnetic field such that $\hbar\omega\sqrt{1+\kappa} < c|B| < 2\hbar\omega\sqrt{1+\kappa}$. This leads to a ground state with index sets $\mu^{\uparrow} = \{\{0,0\},\{1,0\},\{0,1\}\}$ and $\mu^{\downarrow} = \emptyset$. Increasing ω_2 while keeping ω_1 constant induces a dimensional crossover to an effectively one-dimensional configuration with index sets $\mu^{\uparrow} = \{\{0,0\},\{0,1\}\}$ and $\mu^{\downarrow} = \{\{0,0\}\}$. The results of a



FIG. 6. Quasipinning results for the non-fully-spin-polarized three-Harmonium ground state in two spatial dimensions with external trap frequencies ω_1, ω_2 , coupling strength κ , and some fixed homogeneous magnetic field *B* fulfilling $\hbar\omega\sqrt{1+\kappa} < c|B| < 2\hbar\omega\sqrt{1+\kappa}$. Minimal distance D_{\min} of λ to polytope boundary is shown in the left diagram and its nontriviality is quantified in the right diagram by the *Q* parameter. The solid line marks the boundary between the effectively two- and one-dimensional ground-states configuration.

(quasi)pinning analysis are shown in Fig. 6. Whereas the minimal distance D_{\min} of λ to the polytope boundary becomes smaller when reducing κ and increasing $\chi = \omega_2/\omega_1$, the behavior of the Q parameter is more complex and shows similarities to the fully spin-polarized case in Sec. V. Again, the crossing of NONs induces different regimes leading to a high-low-high transition of the Q values when increasing χ for a fixed interaction strength κ . This once more proves the significance of the Q parameter as it unveils the importance of GPCs beyond the Pauli exclusion principle in parameter ranges with attributed moderate minimal distances D_{\min} . In the regime of the two-dimensional ground-state configuration, i.e., left to the solid black line, the quasipinning is trivial (green).

VII. SUMMARY AND CONCLUSION

By studying the Harmonium system, we have thoroughly explored how the spatial dimension, the particle number, the total spin, and the coupling strength affect the physical relevance of the generalized Pauli constraints (GPCs). First, in the form of Theorem II.1, we succeeded in finding a compact analytical form for the ground state of this interacting Nfermion system. This then allowed us to determine the natural occupation numbers analytically by perturbation theory for the regime of small coupling strengths δ and by an exact numerical approach for medium- and strong-coupling strengths.

Given the set $\vec{\lambda} \equiv (\lambda_k)_{k=1}^{\infty}$ of NONs for the ground state of some Harmonium system and a fixed coupling we have explored whether $\vec{\lambda}$ (approximately) saturates some of the GPCs. Since such (quasi)pinning, as quantified by the minimal distance D_{\min} of $\vec{\lambda}$ to the boundary of the allowed region (polytope \mathcal{P}), has remarkable physical consequences, this would then confirm the physical relevance of the GPCs. Since the GPCs are known so far only for one-particle Hilbert spaces of dimension d < 11 we exploited the concept of truncation: All occupation numbers sufficiently close to 1 or 0 can be neglected and possible (quasi)pinning is then explored in the truncated setting. It turned out that for most Harmonium systems and not too strong couplings the corresponding active spaces are sufficiently low dimensional to facilitate a conclusive analysis of (quasi)pinning. In addition, since the GPCs imply the Pauli exclusion principle (PEP) constraints (whose relevance is already well known) we quantify the quasipinning by GPCs *beyond* quasipinning by PEP constraints by using the Q parameter [19].

In general, for the regime of small coupling strengths $\delta \ll 1$ we found that the active spaces in two and three spatial dimensions are significantly larger than for the one-dimensional case studied in Ref. [21]. This is due to the additional degenerate orbital degrees of freedom. Moreover, similar to the one-dimensional case, there are well-pronounced hierarchies of active spaces defined by considering corrections of different orders $O(\delta^r)$ of the NONs to 1 and 0, respectively. These specific shell structures make the concept of truncation even more powerful for the Harmonium systems.

For the case of n = 2 spatial dimensions and spinless fermions we found for N = 3,4,5 fermions quasipinning of strength $D_{\min} \sim \delta^4$ which increased to δ^6 quasipinning for N = 6,7. Comparing this quasipinning by GPCs to quasipinning of the less-restrictive PEP constraints shows that our findings are only nontrivial for N = 4, namely by two orders in δ . For the case of three spatial dimensions the active space dimensions increase even further which does not allow us anymore to perform a conclusive quasipinning analysis for several N. For N = 3,4 we find again δ^4 quasipinning which might, at least in principle, be even stronger for N = 3 since the corresponding truncation error is of the same order, $O(\delta^4)$. The quasipinning turns out to be trivial for N = 4 but nontrivial by at least two orders in δ for N = 3.

It is also instructive to compare those findings for two and three spatial dimensions to those in one dimension, showing quasipinning described by $D_{\min} \sim \delta^8$ for N = 3 [7] and $D_{\min} \sim \delta^{2N}$ for $N \ge 4$ [21]. The increase of quasipinning by reducing the spatial dimension or by adding more fermions to the trap suggests that quasipinning emerges from a Pauli pressure. Such Pauli pressure, which still needs to be formally defined and carefully worked out, describes for ground states the conflict of energy minimization and fermionic exchange symmetry (antisymmetry) from the one-particle picture's viewpoint. Indeed, this conflict reduces by increasing the spatial dimension (leading to additional degenerate orbital degrees of freedom) and increases by adding more fermions to the trap.

By detuning the trap frequencies we explored crossovers between Harmonium systems of different effective spatial dimensions allowing us to also analyze quasipinning for "intermediate" dimensions. From a qualitative viewpoint, we found further evidence for the Pauli pressure being the origin of quasipinning: The stronger the detuning between the trap frequencies and the smaller the fermion-fermion coupling, the stronger the quasipinning. While the absolute quasipinning, as measured by the minimal distance D_{\min} of $\overline{\lambda}$ to the polytope boundary, behaves mainly monotonically as function of the detunings and the coupling strength, the Q parameter shows a much more complex behavior: While keeping the coupling strength constant, ramping up the detuning can lead to multiple crossovers between nontrivial and trivial quasipinning. Although such less monotone behavior seems to be more difficult to understand it clearly shows the importance of the Q parameter for a genuine quantification of the relevance of GPCs in concrete systems.

In the final section, Sec. VI, we eventually included the spin degree of freedom as well. By varying an external magnetic-field coupling to the spins of the uncharged fermions we can induce transitions between states of different spin polarization. The main result, for not to strong couplings δ and N = 3.4 states $D_{\min} \sim \delta^{4+2|M|}$ [Eq. (28)]: The larger the total magnetization (*M*) the stronger the quasipinning. This remarkable universal relation confirms again the role of the Pauli pressure for quasipinning since increasing the degree of polarization reduces the effective number of available states around the Fermi level.

The findings on the spinful fermions provide a general idea for an experimental realization and verification of (quasi)pinning. In a first step, a Harmonium-like system of spinful fermions shall be prepared in its ground state exhibiting quasipinning. Then, by coupling this system to an external oscillating magnetic field the system's ground state and its corresponding vector $\vec{\lambda}$ of NONs are perturbed. Due to the strong quasipinning of λ to the polytope boundary this perturbation $\Delta \lambda$ can be directed for any choice of the perturbation (here, e.g., the field polarization) only parallel but not perpendicular to the polytope boundary (see also Ref. [18]). Without the knowledge of the GPCs and the corresponding polytope \mathcal{P} such behavior of λ restricted to a hyperplane looks magical. This is conceptually very similar to the prohibited decay of valence electrons to lower-lying energy shells in atoms due to the more elementary Pauli exclusion principle.

ACKNOWLEDGMENTS

We gratefully acknowledge financial support from the Friedrich-Naumann-Stiftung and Christ Church Oxford (F.T.), the Oxford Martin School, the NRF (Singapore), the MoE (Singapore), and the EU Collaborative Project TherMiQ (Grant Agreement No. 618074) (V.V.), the Swiss National Science Foundation (Grant No. P2EZP2 152190), and the Oxford Martin Programme on Bio-Inspired Quantum Technologies (C.S.).

APPENDIX A: DERIVATION OF THE HARMONIUM GROUND STATE

In this appendix we provide an elegant proof of Theorem II.1, i.e., we derive the explicit form of the ground state(s) of Harmonium (2).

First, we consider the Hamiltonian (2) on the *N*-particle Hilbert space $\mathcal{H}_N \equiv L_2[\mathbb{R}^n]^{\otimes^N}$, i.e., without any exchange symmetry. On that space, it can easily be diagonalized by decoupling the harmonic oscillators by introducing center of mass $(y_1^{(\alpha)})$ and "relative" coordinates $(y_k^{(\alpha)}, k = 2, ..., N)$ for all *n* spatial dimensions $\alpha = 1, ..., n$ (see, e.g., Ref. [43] for the case n = 1). The corresponding eigenstates follow as

$$\Phi_{\boldsymbol{v}}^{(\omega,K)}(\vec{x}_{1},\ldots,\vec{x}_{N})$$

$$= \mathcal{N}_{\boldsymbol{v}}^{(\omega,K)} \left[\prod_{\alpha=1}^{n} \varphi_{\nu_{1}^{(\alpha)}}^{(l^{(\alpha)})} (y_{1}^{(\alpha)}(x_{1}^{(\alpha)},\ldots,x_{N}^{(\alpha)})) \right]$$

$$\times \left[\prod_{\alpha=1}^{n} \prod_{k=2}^{N} \varphi_{\nu_{k}^{(\alpha)}}^{(l^{(\alpha)})} (y_{k}^{(\alpha)}(x_{1}^{(\alpha)},\ldots,x_{N}^{(\alpha)})) \right], \quad (A1)$$

with $\mathbf{v} \equiv (v_k^{(\alpha)}), v_k^{(\alpha)} \in \mathbb{N}_0, k = 1, ..., N, \alpha = 1, ..., n, \omega \equiv (\omega^{\alpha}), \mathbf{K} \equiv (K^{(\alpha)}), \text{ and } \mathcal{N}_{\mathbf{v}}^{(\omega, \mathbf{K})}$ a normalization constant. Since the dependence of $\Phi_{\mathbf{v}}^{(\omega, \mathbf{K})}$ on the couplings $(\boldsymbol{\omega}, \mathbf{K})$ becomes relevant below we made it explicit. We also introduced for each spatial dimension α the corresponding length $l^{(\alpha)} = \sqrt{\frac{\hbar}{m\omega^{(\alpha)}}}$ for the center of mass and the lengths $\tilde{l}^{(\alpha)} = \sqrt{\frac{\hbar}{m\tilde{\omega}^{(\alpha)}}}$ for the relative motion between the particles. The corresponding frequencies are given by

$$\tilde{\omega}^{(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}}.$$
 (A2)

For the following, it will be crucial that the center-of-mass coordinates $y_1^{(\alpha)}(x_1^{(\alpha)}, \ldots, x_N^{(\alpha)})$ are symmetric in the physical coordinates $x_1^{(\alpha)}, \ldots, x_N^{(\alpha)}$ and the precise form of the relative coordinate functions $y_k^{(\alpha)}, k = 2, \ldots, N$ will not be relevant. The corresponding energy of the eigenstates (A1) are given (up to a constant energy shift) by

$$E_{\boldsymbol{\nu}}^{(\boldsymbol{\omega},\boldsymbol{K})} = \sum_{\alpha=1}^{n} \hbar \omega^{(\alpha)} v_{1}^{(\alpha)} + \sum_{\alpha=1}^{n} \hbar \tilde{\omega}^{(\alpha)} \sum_{k=2}^{N} v_{k}^{(\alpha)}.$$
 (A3)

By introducing the corresponding coupling parameter space

$$\Omega \equiv \{ (\boldsymbol{\omega}, \boldsymbol{K}) \in (\mathbb{R}^+)^n \times \mathbb{R}^n \, | \, \forall \alpha : N K^{(\alpha)} > -m(\omega^{(\alpha)})^2 \},$$
(A4)

we observe that most of the energy branches $E_{\nu}^{(\omega,K)}$ are degenerate on Ω . Accordingly, we introduce equivalence classes $[\nu]$ by identifying the index sets ν and ν' of quantum numbers whenever their energies values (A3) are identical on Ω . Moreover, we introduce the corresponding eigenspace,

$$\mathcal{H}_{[\boldsymbol{\nu}]}^{(\boldsymbol{\omega},K)} \equiv \operatorname{span}\left(\left\{\Phi_{\boldsymbol{\nu}'}^{(\boldsymbol{\omega},K)} \mid \boldsymbol{\nu}' \in [\boldsymbol{\nu}]\right\}\right),\tag{A5}$$

which are all finite dimensional and depend analytically on $(\omega, K) \in \Omega$.

In order to find the fermionic ground state for arbitrary but fixed $(\omega, K) \in \Omega$ one may consider the projection of the set of *N*-particle eigenstates (A1) onto the fermionic subspace,

$$\mathcal{H}_{N}^{(f)} \equiv \wedge^{N} [L_{2}[\mathbb{R}^{n}]] \lneq \mathcal{H}_{N} \equiv L_{2}[\mathbb{R}^{n}]^{\otimes^{N}}.$$
(A6)

More precisely, one needs to determine the index set $\boldsymbol{\nu}$ which minimizes the energy function (A3) while still having nonvanishing support on $\mathcal{H}_N^{(f)}$, i.e., $\mathcal{A}_N \mathcal{H}_{[\nu]}^{(\omega,K)} \neq 0$.

nonvanishing support on $\mathcal{H}_N^{(f)}$, i.e., $\mathcal{A}_N \mathcal{H}_{[\nu]}^{(\omega,K)} \neq 0$. Due to the nontrivial dependency of the relative coordinates $y_i^{(\alpha)}$ on the physical coordinates $x_j^{(\alpha)}$ it proves to be challenging to simplify the resulting expression of the action of the antisymmetrization operator \mathcal{A}_N on the *N*-particle eigenstates of Eq. (A1). In the following we present an elegant, systematic way for determining the fermionic ground state:

(1) Due to the specific structure (A1), separating symmetric center-of-mass coordinates from relative coordinates, the fermionic ground state lies in an eigenspace $\mathcal{H}_{[(\vec{v}_1,...,\vec{v}_N)]}^{(\omega,K)}$ with zero center-of-mass excitations, i.e., $\vec{v}_1 = \vec{0}$.

(2) The main idea is now to relate the fixed coupling $(\boldsymbol{\omega}, \boldsymbol{K})$ to another one with zero interaction $(\boldsymbol{\omega}', \boldsymbol{K}') \equiv (\boldsymbol{\omega}', \boldsymbol{0})$ such that

$$\omega^{\prime(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}}, \quad \alpha = 1, \dots, n.$$
 (A7)

The coupling parameters $(\boldsymbol{\omega}', \mathbf{0})$ are chosen in such a way that they lead to the same frequencies for the relative motion as $(\boldsymbol{\omega}, \boldsymbol{K})$. Indeed, since $K'^{(\alpha)} = 0$ we find

$$\tilde{\omega}^{\prime(\alpha)} = \sqrt{(\omega^{\prime\alpha})^2 + \frac{NK^{\prime(\alpha)}}{m}} = \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}} = \tilde{\omega}^{(\alpha)},$$

$$\alpha = 1, \dots, n.$$
(A8)

This then implies for the energies

$$E_{(\vec{0},\vec{\nu}_{2},...,\vec{\nu}_{N})}^{(\boldsymbol{\omega},K)} = E_{(\vec{0},\vec{\nu}_{2},...,\vec{\nu}_{N})}^{(\boldsymbol{\omega}',0)}, \quad \forall \vec{\nu}_{2},\ldots,\vec{\nu}_{N}.$$
(A9)

Moreover, due to the specific structure of the eigenstates (A1) we can relate the corresponding eigenspaces as well,

$$\mathcal{H}_{[(\vec{0},\vec{v}_{2},...,\vec{v}_{N})]}^{(\boldsymbol{\omega},\boldsymbol{K})} = G^{(\boldsymbol{\omega},\boldsymbol{K})} \mathcal{H}_{[(\vec{0},\vec{v}_{2},...,\vec{v}_{N})]}^{(\boldsymbol{\omega},\boldsymbol{0})},$$
(A10)

where $G^{(\omega,K)}$ describes the multiplication by the Gaussian factor $\exp\left[-\frac{N}{2}\sum_{\alpha=1}^{n}\left(\frac{1}{(l^{(\alpha)})^{2}}-\frac{1}{(l^{(\alpha)})^{2}}\right)(X^{(\alpha)})^{2}\right]$ (see Ref. [43]) and $X^{(\alpha)} \equiv y_{1}^{(\alpha)} \equiv \frac{1}{N}\left(x_{1}^{(\alpha)}+\cdots+x_{N}^{(\alpha)}\right)$ is the center-of-mass coordinate in the α direction.

(3) Since $(\omega', \mathbf{K}') = (\tilde{\omega}, \mathbf{0})$ describes noninteracting fermions we can easily determine the fermionic ground state for this case. The corresponding Schrödinger equation turns into an effectively one-fermion equation describing a single harmonic oscillator in *n*-spatial dimensions with frequencies $\tilde{\omega}^{(\alpha)}$ and with *n*-dimensional Hermite functions $\phi_{\mu}^{(\bar{l})}(\vec{x}) \equiv \prod_{\alpha=1}^{n} \varphi_{\mu^{(\alpha)}}^{(l^{(\alpha)})}(x^{(\alpha)})$ as eigenstates with corresponding energy $\varepsilon_{\mu} = \sum_{\alpha=1}^{n} (\mu^{(\alpha)} + \frac{1}{2})\hbar\tilde{\omega}^{(\alpha)}$. The corresponding fermionic ground state for $(\tilde{\omega}, \mathbf{0})$ is then given by the "configuration state," i.e., by the Slater determinant obtained by distributing the *N* particles in *N* energetically lowest states $\phi_{\mu}^{(\bar{l})}$. By denoting the corresponding sets of quantum numbers by $\mu_1 = \mathbf{0}, \dots, \mu_N$, the ground state reads

$$\Psi_{gs}^{(\tilde{\boldsymbol{\omega}},\mathbf{0})} = \phi_{\mu_1}^{(\tilde{l})} \wedge \dots \wedge \phi_{\mu_N}^{(\tilde{l})}.$$
 (A11)

It should be also stressed that for generic couplings $(\boldsymbol{\omega}, \boldsymbol{K}) \in \Omega$ the ground state for $(\tilde{\boldsymbol{\omega}}, \boldsymbol{0})$ is unique because the frequencies $\tilde{\omega}^{(\alpha)}$ are generically incommensurate.

(4) Equation (A11) allows us to find the ground state for (ω, K) as well. This is based on the previous points, essentially Eqs. (A9) and (A10), implying

$$\Psi_{gs}^{(\tilde{\omega},\mathbf{0})} \in \mathcal{H}_{[(\vec{0},\vec{v}_{2},...,\vec{v}_{N})]}^{(\tilde{\omega},\mathbf{0})} \Leftrightarrow \Psi_{gs}^{(\omega,K)} \in \mathcal{H}_{[(\vec{0},\vec{v}_{2},...,\vec{v}_{N})]}^{(\omega,K)}.$$
 (A12)

Hence,

$$\mathcal{A}_{N}\mathcal{H}_{[(\vec{0},\vec{\nu}_{2},...,\vec{\nu}_{N})]}^{(\boldsymbol{\omega},\boldsymbol{K})} = \mathcal{A}_{N}G^{(\boldsymbol{\omega},\boldsymbol{K})}\mathcal{H}_{[(\vec{0},\vec{\nu}_{2},...,\vec{\nu}_{N})]}^{(\boldsymbol{\tilde{\omega}},\boldsymbol{0})}$$
$$= G^{(\boldsymbol{\omega},\boldsymbol{K})}\mathcal{A}_{N}\mathcal{H}_{[(\vec{0},\vec{\nu}_{2},...,\vec{\nu}_{N})]}^{(\boldsymbol{\tilde{\omega}},\boldsymbol{0})}$$
(A13)

and therefore

$$\Psi_{\varrho_s}^{(\omega,K)} = G^{(\omega,K)} \Psi_{\varrho_s}^{(\tilde{\omega},0)},\tag{A14}$$

which is nothing else than Eq. (5) in Theorem II.1. It should be also stressed that the same conclusions also hold in the case of degenerate fermionic ground states. Notice also that Theorem II.1 and Eq. (5) do not hold for the excited fermionic states. The subtle difference between the ground state and excited states is that in the case of ground states we can assume zero center-of-mass excitations, $\vec{v} = 0$, in contrast to excited states. In the latter case, by following the same derivation the energy eigenspace for couplings $(\tilde{\omega}, \mathbf{0})$ has additional degeneracies coming from center-of-mass excitations.

APPENDIX B: DERIVATION OF THE FERMIONIC 1-RDO OF *N* HARMONIUM IN *n* SPATIAL DIMENSIONS

Starting with the general form of the ground-state wave function of N Harmonium in n spatial dimensions, Eq. (5), the partial trace over (N - 1) fermions of the N-particle density operator $\rho_N = \Psi^* \Psi$ will be computed by integrating over the particle positions $\vec{x}_i \in \mathbb{R}^n$ with labels i = 2, ..., N. Using the Hubbard-Stratonovich relation for each spatial dimension $\gamma = 1, ..., n$,

$$\exp\left[a^{(\gamma)} \left(x_{1}^{(\gamma)} + \dots + x_{N}^{(\gamma)}\right)^{2}\right]$$

= $\sqrt{\frac{a^{(\gamma)}}{\pi}} \int dy^{(\gamma)} \exp\left[-a^{(\gamma)} (y^{(\gamma)})^{2} + 2a^{(\gamma)} y^{(\gamma)} (x_{1}^{(\gamma)} + \dots + x_{N}^{(\gamma)})\right],$ (B1)

yields (see Ref. [43])

$$\rho_{1}^{(f)}(\vec{x};\vec{x}') = |\mathcal{N}|^{2} \cdot \underbrace{\prod_{\gamma=1}^{d} \left\{ \exp\left[\left(\frac{1}{N^{2}} B^{(\gamma)} + C^{(\gamma)} - A^{(\gamma)} \right) [(x^{(\gamma)})^{2} + (x^{\prime(\gamma)})^{2}] + 2C_{N}^{(\gamma)} x^{(\gamma)} x^{\prime(\gamma)} \right] \right\}}_{\rho_{1}^{(b)}(\vec{x};\vec{x}')} \times \underbrace{\sum_{i=1}^{N} \left(\prod_{\gamma=1}^{d} \int du_{\gamma} \left\{ e^{-u_{\gamma}^{2}} \frac{H_{\mu_{i}^{(\gamma)}}(p_{\gamma}u_{\gamma} + r_{\gamma}(x^{(\gamma)}, x^{\prime(\gamma)})) H_{\mu_{i}^{(\gamma)}}(p_{\gamma}u_{\gamma} + r_{\gamma}(x^{\prime(\gamma)}, x^{(\gamma)})) H_{\mu_{i}^{(\gamma)}}(p_{\gamma}u_{\gamma} + r_{\gamma}(x^{\prime(\gamma)}, x^{(\gamma)})) }_{2^{\mu_{i}^{(\gamma)}}(\mu_{i}^{(\gamma)})!} \right\} \right)}_{\equiv F(\vec{x};\vec{x}')}$$
(B2)

In this expression, $H_{\mu_i^{(\gamma)}}$ denotes the Hermite polynomial of degree $\mu_i^{(\gamma)}$, where $\{\mu_i\}_{i=1}^N$ is the set of quantum number vectors introduced in Sec. II. The quantities $A^{(\gamma)}, B^{(\gamma)}, C^{(\gamma)}$, p, and $r(\cdot, \cdot)$ are given by

$$A^{(\gamma)} = \frac{1}{2(\tilde{l}^{(\gamma)})^2},$$
(B3)

$$B^{(\gamma)} = \frac{N}{2} \left(\frac{1}{(\tilde{l}^{(\gamma)})^2} - \frac{1}{(l^{(\gamma)})^2} \right),\tag{B4}$$

$$C^{(\gamma)} = \frac{(N-1)(B^{(\gamma)})^2}{2N^2[N^2A^{(\gamma)} - (N-1)B^{(\gamma)}]},$$
(B5)

$$p_{\gamma} = \sqrt{\frac{B^{(\gamma)}}{N^2 A^{(\gamma)} - B^{(\gamma)}(N-1)}},$$
 and (B6)

$$r_{\gamma}(v,w) = \sqrt{2A^{(\gamma)}} \left(v - \frac{B^{(\gamma)}}{2[N^2 A^{(\gamma)} - (N-1)B^{(\gamma)}]} (v+w) \right), \tag{B7}$$

where we suppressed the index N of $A^{(\gamma)}$, $B^{(\gamma)}$, and $C^{(\gamma)}$. $l^{(\gamma)}$ and $\tilde{l}^{(\gamma)}$ denote again the length scale in the γ direction for the center of mass and the relative motion, respectively.

The 1-RDO associated with the ground state of Harmonium for spinful fermions can be derived by tracing out spin and spatial degrees of freedom by applying the same ideas to the spatial part as in the case of fully spin-polarized Harmonium Eq. (B2):

$$\begin{split} \rho_{1}^{(f)}(\vec{x},\sigma;\vec{x}',\sigma') &= |\mathcal{N}|^{2} \cdot \underbrace{\prod_{\gamma=1}^{d} \left\{ \exp\left[\left(\frac{1}{N^{2}} B^{(\gamma)} + C^{(\gamma)} - A^{(\gamma)} \right) [(x^{(\gamma)})^{2} + (x'^{(\gamma)})^{2}] + 2C^{(\gamma)} x^{(\gamma)} x'^{(\gamma)} \right] \right\}}_{\rho_{1}^{(b)}(\vec{x};\vec{x}')} \\ &\times \left[\underbrace{\sum_{i=1}^{N^{\dagger}} \left(\prod_{\gamma=1}^{d} \int du_{\gamma} \left\{ e^{-u_{\gamma}^{2}} \frac{H_{\mu_{i}^{\uparrow(\gamma)}}(p_{\gamma}u_{\gamma} + r_{\gamma}(x^{(\gamma)}, x'^{(\gamma)})) H_{\mu_{i}^{\uparrow(\gamma)}}(p_{\gamma}u_{\gamma} + r_{\gamma}(x'^{(\gamma)}, x^{(\gamma)}))}{2^{\mu_{i}^{\uparrow(\gamma)}}(\mu_{i}^{\uparrow(\gamma)})!} \right\} \right)}_{=F^{\dagger}(\vec{x};\vec{x}')} \right] \uparrow \rangle \langle \uparrow |$$



In this expression, the μ_i^{\uparrow} and μ_j^{\downarrow} quantum number vectors represent the set of particles with spins parallel and antiparallel to the external magnetic field.

APPENDIX C: NATURAL OCCUPATION NUMBERS FOR THE THREE-HARMONIUM GROUND STATE IN ONE DIMENSION

For the sake of self-containedness of this work we recall the natural occupation numbers for the three-Harmonium ground state presented in Ref. [7]. They are given by the following series up to corrections of the order $O(\delta^{10})$, where the coupling

- R. E. Borland and K. Dennis, The conditions on the one-matrix for three-body fermion wavefunctions with one-rank equal to six, J. Phys. B 5, 7 (1972).
- [2] A. Klyachko, Quantum marginal problem and N-representability, J. Phys. Conf. Ser. 36, 72 (2006).
- [3] M. Altunbulak and A. Klyachko, The Pauli principle revisited, Commun. Math. Phys. 282, 287 (2008).
- [4] M. Altunbulak, The Pauli principle, representation theory, and geometry of flag varieties, Ph.D. thesis, Bilkent University, 2008.
- [5] M. B. Ruskai, Connecting *N*-representability to Weyl's problem: the one-particle density matrix for N = 3 and R = 6, J. Phys. A **40**, F961 (2007).
- [6] A. Klyachko, The Pauli exclusion principle and beyond, arXiv:0904.2009.
- [7] C. Schilling, D. Gross, and M. Christandl, Pinning of Fermionic Occupation Numbers, Phys. Rev. Lett. 110, 040404 (2013).
- [8] A. Klyachko, The Pauli principle and magnetism, arXiv:1311.5999.
- [9] C. Benavides-Riveros, J. Gracia-Bondia, and M. Springborg, Quasipinning and entanglement in the lithium isoelectronic series, Phys. Rev. A 88, 022508 (2013).
- [10] R. Chakraborty and D. A. Mazziotti, Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules, Phys. Rev. A 89, 042505 (2014).
- [11] C. Schilling, Quantum marginal problem and its physical relevance, Ph.D. thesis, ETH-Zürich, 2014.
- [12] R. Chakraborty and D. A. Mazziotti, Sufficient condition for the openness of a many-electron quantum system from the violation of a generalized Pauli exclusion principle, Phys. Rev. A 91, 010101(R) (2015).
- [13] C. Schilling, Quasipinning and its relevance for *N*-fermion quantum states, Phys. Rev. A 91, 022105 (2015).

parameter δ is defined in Eq. (15),

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

- [14] C. L. Benavides-Riveros and M. Springborg, Quasipinning and selection rules for excitations in atoms and molecules, Phys. Rev. A 92, 012512 (2015).
- [15] I. Theophilou, N. N. Lathiotakis, M. A. L. Marques, and N. Helbig, Generalized Pauli constraints in reduced density matrix functional theory, J. Chem. Phys. 142, 154108 (2015).
- [16] A. Lopes, Pure univariate quantum marginals and electronic transport properties of geometrically frustrated systems, Ph.D. thesis, University of Freiburg, 2015.
- [17] R. Chakraborty and D. A. Mazziotti, Structure of the oneelectron reduced density matrix from the generalized Pauli exclusion principle, Int. J. Quantum Chem. 115, 1305 (2015).
- [18] C. Schilling, Hubbard model: Pinning of occupation numbers and role of symmetries, Phys. Rev. B 92, 155149 (2015).
- [19] F. Tennie, V. Vedral, and C. Schilling, Generalized Pauli constraints: Hierarchy of pinning and quasipinning-measure, arXiv:1509.00358.
- [20] C. L. Benavides-Riveros and C. Schilling, Natural extension of Hartree-Fock through extremal 1-fermion information: Overview and application to the lithium atom, Z. Phys. Chem. 230, 703 (2016).
- [21] F. Tennie, D. Ebler, V. Vedral, and C. Schilling, Pinning of fermionic occupation numbers: General concepts and one spatial dimension, Phys. Rev. A 93, 042126 (2016).
- [22] R. Chakraborty and D. A. Mazziotti, Role of the generalized Pauli constraints in the quantum chemistry of excited states, Int. J. Quantum Chem. 116, 784 (2016).
- [23] Here and in the following, boundary refers only to that part of the mathematical boundary $\partial \mathcal{P}_{N,d}$ of the polytope $\mathcal{P}_{N,d}$ which corresponds to saturation of a GPC. The part of $\partial \mathcal{P}_{N,d}$ corresponding to saturation of an ordering constraint, $\lambda_i \lambda_{i+1} \ge 0$ or $\lambda_d \ge 0$ will not play any role.

- [24] C. Schilling, The quantum marginal problem, in *Mathematical Results in Quantum Mechanics* (World Scientific, Singapore, 2014), Chap. 1, pp. 165–176.
- [25] P. Lévay and P. Vrana, Three fermions with six single-particle states can be entangled in two inequivalent ways, Phys. Rev. A 78, 022329 (2008).
- [26] G. Sárosi and P. Lévay, Entanglement classification of three fermions with up to nine single-particle states, Phys. Rev. A 89, 042310 (2014).
- [27] L. Chen, J. Chen, D. Djokovic, and B. Zeng, Universal subspaces for local unitary groups of fermionic systems, Commun. Math. Phys. 333, 541 (2014).
- [28] L. Chen, D. Djokovic, M. Grassl, and B. Zeng, Canonical form of three-fermion pure-states with six single particle states, J. Math. Phys. 55, 082203 (2014).
- [29] P. Lévay, S. Nagy, J. Pipek, and G. Sárosi, The coupled cluster method and entanglement, arXiv:1506.06914.
- [30] A. D. Gottlieb and N. J. Mauser, New Measure of Electron Correlation, Phys. Rev. Lett. 95, 123003 (2005).
- [31] A. D. Gottlieb and N. J. Mauser, Properties of nonfreeness: An entropy measure of electron correlation, Int. J. Quantum Inf. 05, 815 (2007).
- [32] A. D. Gottlieb and N. J. Mauser, Nonfreeness and related correlation functionals for many-fermion states, arXiv:1510.04573.
- [33] A. D. Gottlieb, N. J. Mauser, and J. M. Zhang, Concise configuration interaction expansions for three fermions in six orbitals, arXiv:1602.00578.
- [34] P. Kościk and R. Maj, Note on the harmonic approximation in the treatment of entanglement: *N* cold trapped ions, Few-Body Syst. 55, 1253 (2014).
- [35] N. F. Johnson and M. C. Payne, Exactly Solvable Model of Interacting Particles in a Quantum Dot, Phys. Rev. Lett. 67, 1157 (1991).
- [36] H. R. Post, Many-particle systems: Derivation of a shell model, Proc. Soc. A 66, 649 (1953).
- [37] N. T. Zinner and A. S. Jensen, Nuclear α-particle condensates: Definitions, occurrence conditions, and consequences, Phys. Rev. C 78, 041306 (2008).
- [38] M. Weidemüller and C. Zimmermann, Interactions in Ultracold Gases: From Atoms to Molecules (John Wiley & Sons, New York, 2011).

- [39] I. Bloch, J. Dalibard, and W. Zwerger, Many-body physics with ultracold gases, Rev. Mod. Phys. 80, 885 (2008).
- [40] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Feshbach resonances in ultracold gases, Rev. Mod. Phys. 82, 1225 (2010).
- [41] G. Zürn, F. Serwane, T. Lompe, A. N. Wenz, M. G. Ries, J. E. Bohn, and S. Jochim, Fermionization of Two Distinguishable Fermions, Phys. Rev. Lett. **108**, 075303 (2012).
- [42] Z.-L. Wang, A. M. Wang, Y. Yang, and X. C. Li, Exact eigenfunctions of *N*-body system with quadratic pair potential, Commun. Theor. Phys. 58, 639 (2012).
- [43] C. Schilling, Natural orbitals and occupation numbers for harmonium: Fermions versus bosons, Phys. Rev. A 88, 042105 (2013).
- [44] J. R. Armstrong, N. T. Zinner, D. V. Fedorov, and A. S. Jensen, Analytic harmonic approach to the *N*-body problem, J. Phys. B 44, 055303 (2011).
- [45] The case of an isotropic trap, $\omega^{(1)} = \cdots = \omega^{(n)}$, was already discussed in Ref. [42] but no constructive proof was presented.
- [46] Strictly speaking, this is not exactly the Pauli exclusion principle since it is not applied to the total quantum state $\Psi^{(f)}$ but just to one of its two factors. In a similar way, one should understand the term distributing *N* fermions in *N* shells more as an analogy.
- [47] E. R. Davidson, *Reduced Density Matrices in Quantum Chem*istry (Academic, New York, 1976).
- [48] C. Schilling and R. Schilling, Duality of reduced density matrices and their eigenvalues, J. Phys. A 47, 415305 (2014).
- [49] The left dashed line describes $\lambda_4 = \lambda_5$ and the right one $\lambda_6 = \lambda_7$.
- [50] We skip the coupling of the magnetic field to the angular momentum of the fermions by assuming them to be uncharged. One could in principle extend our model to charged fermions which, however, would significantly complicate the description of the ground state for nonisotropic traps.
- [51] For the Harmonium ground state, M = 0 always means that every occupied box is doubly occupied and therefore closed. Hence, the total spin for such a configuration is S = 0.
- [52] D. W. Smith, *N*-representability problem for fermion density matrices. II. The first-order density matrix with *N* even, Phys. Rev. 147, 896 (1966).