Many-body Hilbert space is a functional vector space with the natural structure of an algebra, in which vector multiplication is ordinary multiplication of wave functions. This algebra is finite-dimensional, with exactly $N!^{d-1}$ generators for $N$ identical particles, bosons or fermions, in $d$ dimensions. The generators are called *shapes*. Each shape is a possible many-body vacuum. Shapes are natural generalizations of the ground-state Slater determinant to more than one dimension. Physical states, including the ground state, are superpositions of shapes with symmetric-function coefficients, for both bosons and fermions. These symmetric functions may be interpreted as bosonic excitations of the shapes. The algebraic structure of Hilbert space described here provides qualitative insights into long-standing issues of many-body physics, including the fermion sign problem and the microscopic origin of bands in the spectra of finite systems.

I. INTRODUCTION

The problem of constructing many-body wave functions of identical particles is almost as old as quantum mechanics itself. Soon after Pauli articulated his famous principle, Heisenberg and Dirac found that it could be mathematically expressed by wave functions in determinantal form, which came to be known as Slater determinants. Given that Slater determinants form a complete basis of Hilbert space, the so-called second-quantized formalism, which made their manipulation technically feasible even for large systems, established them as a secure formal foundation for all microscopic descriptions of many-fermion systems.

While formally universal, the Slater-determinant approach — as implemented most characteristically in the time-dependent perturbation formalism — has a pattern of success indicating that it is better adapted to some problems than others. Broadly speaking, it works when the interacting system can be described in terms of relatively simple excitations of the non-interacting system. Even an infinity of such excitations, creating collective modes and new ground states, is within the purview of the approach, provided that each individual excitation can be expressed as a small departure from the non-interacting ground state. The paradigm for such small departures are the well-known particle-hole excitations of the Fermi sea. Similarly, Cooper pairing is just a resonance in two-particle head-on collisions.

On the other hand there are so-called strongly correlated systems, for which the Slater determinant formulation does not seem to offer advantages by itself. These are characterized by a number of properties which need not all be present, but typically include:

- a finite number of particles;
- localization in space;
- strong short-range or unscreened long-range interactions.

All three characteristics are present in atoms, nuclei, and small molecules. The two-dimensional electron gas, found in the inversion layers of semiconducting heterostructures, has only the third property in the absence of a magnetic field, but acquires the other two when a strong field is turned on. Of course, the number of electrons does not suddenly become finite, rather the localization of trajectories caused by the field means that only a small number of electrons create a strongly correlated wave function, which is then repeated throughout space. This number was three in Laughlin’s original description of the fractional quantum Hall effect (FQHE) at $1/3$ filling, where the strongly correlated motion in question was their rotation as the vertices of a “stiff” equilateral triangle. Some contemporary approaches to strongly correlated materials share the same pattern: the local part of the problem is treated by dynamical mean-field theory (DMFT), while the extension in space is treated by density-functional theory (DFT), i.e., by Slater determinants. A significant difference between the latter two cases is that all electrons need to be antisymmetrized in the FQHE, while in crystals the electrons localized within a unit cell need not be antisymmetrized with those in the other cells. The separation between the local and the itinerant degrees of freedom in such cases is an important issue beyond the scope of the present review.

Here, the first tentative steps of a new approach are described, which shows some promise to be “native” for few-particle strongly correlated cases, much as the Slater determinants natively describe long-wavelength excitations of extended systems. The present review places this approach in its natural mathematical context and addresses
various physical ramifications in a qualitative way. Proofs of the main results have appeared elsewhere. The primary ambition, unfulfilled at present, is to obtain realistic wave functions of few-body systems, without necessarily improving on existing numerical methods either in terms of speed or accuracy in the calculation of binding energies. In this sense the philosophy is converse to that of DFT, which consciously sacrifices realism of the wave functions in favor of precise calculation of energies.

II. MATHEMATICAL BACKGROUND

The mathematics invoked in the present work has a long and distinguished lineage. Combinatorics and the theory of invariants were first brought into modern form by Leonhard Euler and David Hilbert, respectively. The purpose of the present section is only to introduce as much background as necessary to understand the subsequent physical development. The level is chosen to make the material accessible to any physics student. If the mathematical training of physicists were devoted half as much to abstract algebra as it is to complex analysis, the whole section would be unnecessary. The style is informal, with mathematical rigor left to the references. Although every statement is true of physicists were devoted half as much to abstract algebra as it is to complex analysis, the whole section would be unnecessary. The style is informal, with mathematical rigor left to the references. Although every statement is true

A. Euler and generating functions

Euler invented generating functions in 1741, ostensibly to answer a question from a “most insightful” correspondent: in how many ways can the number 50 be written as a sum of 7 distinct natural numbers? Of course, permutations of the same sum are not counted, so the question may be rephrased, “... sum of 7 strictly increasing natural numbers.” Euler realized that if he could compute the sum

$$\sum_{1 \leq n_1 < n_2 < n_3 < n_4 < n_5 < n_6 < n_7 < \infty} q^{n_1+n_2+n_3+n_4+n_5+n_6+n_7},$$  \hspace{1cm} (1)

the solution would appear as the coefficient of $q^{50}$. In terms of contemporary physics, his task was to compute the degeneracy of the level with energy $50 \hbar \omega$ of a one-dimensional harmonic oscillator well, filled with 7 fermions, and spectrum given by $\varepsilon_n = n \hbar \omega$, $n \geq 1$, and $q = \exp(-\beta \hbar \omega)$. (The answer is 522.)

The sum (1) is simple enough to be computed directly. By some clever tricks with indices, one can find that

$$\sum_{0 \leq n_1 \leq \cdots \leq n_N < \infty} q^{n_1+\cdots+n_N} = q^{N(N-1)/2} \sum_{d=0}^{N} \frac{1}{1-q^{-d}} = \frac{1}{1-q^{-1}} \sum_{d=0}^{N} q^{-d} = q^{N(N-1)/2} E,$$ \hspace{1cm} (2)

where the origin of the $n_i$ is shifted to zero for later convenience (the original sum yields the prefactor $q^{N(N+1)/2}$). Interestingly, if one changes the restrictions on the indices to $\leq$ instead of $<$, which means replacing fermions with bosons, only the prefactor changes to reflect the different boson ground-state energy. Fermions and bosons are not really different in one dimension, an observation whose proper generalization to $d > 1$ will become apparent below.

Euler did not compute the sum directly. Instead he presented the result (2) constructively, as just one particular manipulation of the simpler generating functions, appearing as terms in the product. He inaugurated the theory of partitions by extending such manipulations to prove his famous “pentagonal number theorem,” a development which need not concern us here. We shall however need another of his observations: upon expanding and multiplying the geometric series in the product

$$\frac{1}{1-e_1} \frac{1}{1-e_2} \cdots \frac{1}{1-e_N},$$  \hspace{1cm} (3)

each distinct monomial $e_1^{n_1} e_2^{n_2} \cdots e_N^{n_N}$ appears exactly once. While the observation itself may appear obvious enough, it marks a historical shift towards an abstract use of mathematical symbols, in which “letters” are not considered as place-holders for numbers, but as mathematical objects in their own right. The observation makes sense to one who is prepared to use a mathematical expression like (3) as a sort of symbolic machine to generate other expressions, namely the said monomials. The statement (3) is then a precise prescription to manipulate symbols, not any numerical value. Here it will be used as a working part of a bigger symbolic machine, to generate expressions for the shape wave functions.
B. Hilbert and invariants

While a particular date may be assigned to the invention of generating functions, invariants have been present in mathematical thought since the earliest times. As soon as they were discovered in the 4th century BC, conic sections were classified according to how the plane cutting the cone was tilted: too little (ellipse), just enough (parabola), or too much (hyperbola). The invariant nature of this classification is intuitively obvious to anyone looking at the intersection from the outside. A significant step forward was to realize that a small bug living in the plane could also distinguish the three cases, by fitting the curve to the equation \( Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0 \) and computing the discriminant \( B^2 - 4AC \). This program can be carried out in two ways. One is to study a small neighborhood of a point on a curve, leading eventually to differential geometry. The discriminant is then just the Hessian of the quadratic form, describing the local curvature of the conic.

An alternative to the differential-geometric is the algebraic point of view, which notes that the fitting needs to evaluate the curve only at a finite number of points. The coefficients are now obtained by an investigation limited in a different sense: instead of being continuous in an infinitesimal neighborhood, it is discrete in a finitely extended neighborhood. The polynomial is nothing but its list of coefficients, which are numbers in a certain relationship. The relationship is best presented by keeping the old notation for a polynomial, but now the variables \( x \) and \( y \) are just letters, or notational tags, to keep track of the roles played by the coefficients, e.g. when calculating the discriminant. Relabeling the tags by a Euclidean transformation of the pair \( (x, y) \) changes the coefficients without changing the discriminant: it is said to be an invariant of the quadratic form under action of the Euclidean group in the plane. In this “classical” program, usually associated with Cayley, the main concern was how to find all the invariants of a particular group action in any given case.

If Euler had opened the study of generating functions, Hilbert was widely credited with closing the classical study of invariants, by proving a structural result which relegated the computation of particular invariants to applications. His attitude can be introduced in a succession of steps. First, there is a mapping between the coefficients and roots of invariants, by proving a structural result which relegated the computation of particular invariants to applications.

Symmetric functions, the new variables, one parametrizes all the polynomials at once. Instead of the old dummy variables \( x, y \) being used as handles for group action in the geometric “outer” space over which the polynomials were defined, attention shifts to the abstract “inner” space of the polynomials themselves, as parametrized by their roots. This crucial change of focus is almost imperceptible in the notation, because of course the roots may be visualized as points in the very same geometric space in which the original polynomial was being evaluated. In the mathematical literature, it is not uncommon to treat the \( e_i \) themselves as free parameters, given that they parametrize the polynomials equally well. As will appear below, in physics the difference between the two must remain marked, because roots are related to coefficients like one-body to many-body wave functions.

Taking the discriminant of a quadratic \( x^2 - e_1 x + e_2 \) as an example,

\[
e_1 = t_1 + \ldots + t_N = \sum_i t_i,
\]

\[
e_2 = t_1 t_2 + t_1 t_3 + \ldots + t_{N-1} t_N = \sum_{i<j} t_i t_j,
\]

\[
\vdots
\]

\[
e_N = t_1 t_2 \cdots t_N.
\]

These are just the Viète formulas, first encountered in high-school algebra. All functions of the coefficients, including the invariants such as the discriminant, are thus necessarily symmetric functions of the roots. Taking the roots as the new variables, one parametrizes all the polynomials at once. Instead of the old dummy variables \( x, y \) being used as handles for group action in the geometric “outer” space over which the polynomials were defined, attention shifts to the abstract “inner” space of the polynomials themselves, as parametrized by their roots. This crucial change of focus is almost imperceptible in the notation, because of course the roots may be visualized as points in the very same geometric space in which the original polynomial was being evaluated. In the mathematical literature, it is not uncommon to treat the \( e_i \) themselves as free parameters, given that they parametrize the polynomials equally well. As will appear below, in physics the difference between the two must remain marked, because roots are related to coefficients like one-body to many-body wave functions.

Taking the discriminant of a quadratic \( x^2 - e_1 x + e_2 \) as an example,

\[
e_1^2 - 4e_2 = (t_1 - t_2)^2,
\]

one sees immediately that it is an invariant of the Euclidean group, which by definition preserves distances. In fact the discriminant may in general be defined as the square of the Vandermonde determinant, \( \Delta \),

\[
\Delta(t_1, \ldots, t_N) \equiv \begin{vmatrix} t_1^{N-1} & \cdots & t_1^{N-1} \\ \vdots & \ddots & \vdots \\ t_1 & \cdots & t_1 \\ 1 & \cdots & 1 \end{vmatrix} = \prod_{1 \leq i < j \leq N} (t_i - t_j).
\]

One immediate consequence of this point of view is that one has generated a great many rather obvious invariants: because all functions of the coefficients are symmetric in the roots, they are all invariant under the full group of
permutations of the $N$ roots, the symmetric group $S_N$. These may be understood as invariants with respect to renaming the roots. They can all be generated by Euler’s expression \[ e_i \]. To be explicit, the monomials generated by \( e_i \) are a basis in the space of invariants: any invariant of the symmetric group can be expressed as a linear combination of these monomials, i.e. a polynomial in the $e_i$, $i = 1, \ldots, N$.

In the next step, obtaining “interesting” invariants becomes a program of reduction of the complete monomial basis obtained above. This program cannot miss any invariants, because any finite group operating on the $N$ points $t_i$ can be understood as a subgroup of the permutation group, a result due to Cayley. For example, some invariants under root reflection $t_i \rightarrow -t_i$ are generated from the coefficients of even index $e_{2i}$, and others from squares of coefficients of odd index, $e_{2i+1}^2$. The corresponding reduced generating expression \[ e_i \] is obtained simply by squaring all the $e_i$, with odd indices appearing in the denominators. However, this expression misses “mixed” reflection-symmetric terms, such as $e_1 e_3$. A moment’s thought suffices to realize that the generating function of all invariants of (say) cubic polynomials $x^3 - e_1 x^2 + e_2 x - e_3$ under root reflection is just

\[
\frac{1}{2} \left( \frac{1}{1 - e_1} \frac{1}{1 - e_2} \frac{1}{1 - e_3} + \frac{1}{1 + e_1} \frac{1}{1 - e_2} \frac{1}{1 + e_3} \right) = \frac{1 + e_1 e_3}{(1 - e_1^2)(1 - e_2)(1 - e_3)^2}, \tag{7}
\]

because it lists all and only monomials which are unchanged by the change of sign. In other words, any invariant under root reflection takes the form

\[
R(e_1, e_2, e_3) = P(e_1^2, e_2, e_3) \cdot 1 + Q(e_1^2, e_2, e_3^2) \cdot e_1 e_3, \tag{8}
\]

where $P$ and $Q$ are arbitrary polynomials in three variables.

An expression like \[ e_i \] or \[ e_i \] is the most general answer one can give to a problem of finding invariants. Hilbert’s conclusive contribution was to realize not only that such expressions were always possible, but in addition that the numerator in Eq. \[ 7 \], or the sum in Eq. \[ 8 \], will be finite, i.e. not an infinite series, for a very large class of symmetry groups\(^\text{15}\) so large that physicists need not be concerned with the exceptions.

C. The algebra of invariants

The structure of Hilbert’s insight is visible in Eq. \[ 3 \]: in some sense, there are only two interesting invariants in the problem, namely the set \( \{1, e_1 e_3\} \), listed in the numerator of Eq. \[ 7 \]. By contrast, $P$ and $Q$ are arbitrary, once one has identified their allowed variables. This separation follows the natural reasoning above, which quickly identified $e_{2i}$ and $e_{2i+1}$ as obvious invariants under root reflection, but was hesitant how to include $e_1 e_3$ properly. Terminologically, the monomials appearing in the geometric series (or in $P$ and $Q$) are called primary, while those appearing in the polynomial in the numerator of Eq. \[ 7 \] are called secondary invariants\(^\text{15}\).

The form of the expression \[ 8 \] indicates that the secondary invariants act as a basis, spanning the whole space of invariants. This insight is formalized by noting that polynomials are a vector space over the real (or complex) numbers, so that ordinary multiplication of polynomials is vector multiplication in that space, therefore polynomials naturally form an algebra. The basis vectors intuited above are just the generators of that algebra. Any invariant $p$ may be written

\[
p = \sum_{i=1}^{D} h_i g_i, \tag{9}
\]

where the $h_i$ are arbitrary polynomials in the primary invariants and $g_i$ are secondary invariants, or generators of the algebra of invariants. The sum is always finite, by Hilbert, for all classical and finite groups acting on polynomials over the complex field\(^\text{15}\). It is said that such an algebra is finitely generated, where $D$ is its dimension (number of its generators, $D = 2$ in the example \[ 3 \]).

An additional structure can be inferred from Eq. \[ 9 \]. Let $g'_i$, $i = 1, \ldots, M$, be some linear combinations of the generators $g_i$. Then polynomials $q$ of the form

\[
q = \sum_{i=1}^{M} h_i g'_i, \tag{10}
\]

with $h_i$ the same as before, form an ideal in the space of invariants $p$ in Eq. \[ 9 \]. This proposition is easily checked from the definition. Ideals are subsets closed under addition, $q + q' = \sum (h_i + h'_i) g'_i$, and absorptive under multiplication, $h'q = \sum (h' h_i) g'_i$. An important question now is whether the $q$’s form a proper subset of the $p$’s. Even if $M < D$, one
cannot be sure that the generators $g_i$ were really the minimal set needed to span the space of $p$’s, because a clever choice of the $g'_i$ could in principle transfer some of the burden to the coefficients $h_i$. In other words, because of the flexibility of polynomial multiplication, the dimension of the algebra of invariants can be difficult to divine in practice, leading to a large body of research devoted to basis-reduction algorithms.\(^\text{15}\) Sometimes, however, one can argue a fortiori that the most efficient representation has been achieved. Such is our running example \(^\text{8}\), noting that the term $e_1e_3$ is even under root reflection but cannot appear in $P$ or $Q$.

D. Grading and Hilbert series

Instead of explicitly generating all polynomial invariants, one may ask how many of a given degree exist. Clearly each elementary symmetric function $e_k$ is of degree $k$. Hence the replacement $e_k \rightarrow q^k$ in the example \(^\text{7}\) gives the answer: the number of independent invariants of degree $m$ is the coefficient of $q^m$ in the expression

$$\frac{1 + q^4}{(1 - q^2)^2(1 - q^8)}. \quad (11)$$

Such a series is called a Hilbert (sometimes \(^\text{16}\) Poincaré) series. The classification of polynomials by degree is a particular example of a grading, which is any decomposition of an algebra (or ring) in a direct sum of subspaces $M_i$, labeled by natural numbers $i$, which has the property $M_iM_j \subseteq M_{i+j}$.

The Hilbert series is an important practical tool for finding invariants, because computing it is in principle much easier than finding a closed invariant-generating function like Eq. \(^\text{7}\). Sometimes it gives sufficient hints of the structure of the space of invariants to enable the design of concrete algorithms for their construction. As we shall see now, that is the case with many-body Hilbert space.

III. MAIN RESULTS

Having established the mathematical language, all the main results concerning many-body Hilbert space can be stated transparently. The proofs appear elsewhere.\(^\text{11}\)

A. Sum over states

The natural grading for wave functions is the number of one-body nodes. In order to make the node-numbers independent in the various coordinates, only bases separable in Cartesian coordinates are considered. Then the most efficient way to represent one-body wave functions is as pure powers of some formal variables, with the exponent denoting the grade, e.g., $t^iu^mv^n$ in three dimensions. In one dimension, the ground-state Slater determinant then becomes just the Vandermonde determinant \(^\text{4}\). Any $N$-body wave function can be readily recovered from this representation:

$$t^iu^mv^n \rightarrow H_1(x_i)e^{-x_i^2/2}H_m(y_j)e^{-y_j^2/2}H_n(z_k)e^{-z_k^2/2} \quad (12)$$

for the 3D harmonic oscillator, say, with $i, j, k = 1, \ldots, N$. In this mapping, the one-body functions must not be individually normalized. Only the final superpositions are normalized before concrete calculations.

The Hilbert series for this grading is just the physical partition function of the harmonic oscillator, because the energy is linear in the number of nodes in that case. Thus all oscillator counting results become completely general. The price to pay is, of course, that wave functions classified by grade are not necessarily the eigenfunctions of any Hamiltonian, as soon as one invokes some other one-body realization than the oscillator one, say $\cos mx$ in place of $H_m(x)e^{-x^2/2}$ above. However, that is a very small price, because one does not hope anyway that the initial choice of basis will solve any non-trivial problem. Replacing $e^{-\beta\hbar\omega}$ by the letter $q$, the Hilbert series for $N$ identical particles in $d$ dimensions reads:

$$Z_d(N, q) = Z_E(N, q)^dP_d(N, q), \quad Z_E = \prod_{k=1}^N \frac{1}{1 - q^k}, \quad (13)$$

where $P_d(N, q)$ is a polynomial in $q$ which satisfies Svertan’s recursion

$$NP_d(N, q) = \sum_{k=1}^N (\pm 1)^{k+1}[C^N_k(q)]^dP_d(N - k, q), \quad (14)$$
with the upper sign for bosons, and the lower for fermions. Here
\[
C_d^N(q) = \frac{(1 - q^N) \cdots (1 - q^{N-k+1})}{(1 - q^d)}
\]  
(15)
is a polynomial, and \(P_d(0,q) = P_d(1,q) = 1\).

The Hilbert series \([13]\) already reveals a lot about the structure of \(N\)-body Hilbert space. In particular, the polynomial \(P_d(N,q)\) counts the \(d\)-dimensional states which cannot be induced from the one-dimensional ones by simple combinatorial tricks, such as
\[
\Psi_a(x_1, \ldots, x_N) \to \Psi_a(x_1, \ldots, x_N)\Phi_b(y_1, \ldots, y_N)\Psi_c(z_1, \ldots, z_N).
\]  
(16)
Namely, these trivial extensions of 1D states are counted by the other factor, \(Z_d^E\). Furthermore, comparing Eqs. \([7]\) and \([13]\) shows that \(P_d(N,q)\) is the numerator in these expressions, hence it counts the secondary invariants. Thus the form of Eq. \([13]\) identifies \(N\)-body Hilbert space as a finitely generated graded algebra. Because the number of generators of each grade [coefficient of a power of \(q\) in \(P_d(N,q)\)] must be a nonnegative integer, inserting \(q = 1\) into the recursion \([14]\) gives the total dimension of the algebra, \(P_d(N,1) = N!^{d-1}\). For example, in the case of three-fermion wave functions in two dimensions, \(P_2(3, q) = 1 + 4q + q^2\) and \(P_2(3, 1) = 6 = 3!^1\).

### B. Wave functions

The generators of the Hilbert-space algebra are called shapes. Any state in Hilbert space has a wave function of the form
\[
\Psi = \sum_{i=1}^{N!^{d-1}} \Phi_i \Psi_i,
\]  
(17)
where \(\Psi_i\), are the shapes, while the \(\Phi_i\) are polynomials in the primary invariants. These polynomials are trivially extended from the 1D case along the lines of Eq. \([16]\). Explicitly, let \(t_m\) denote one-node single-particle wave functions along the \(x\)-axis, e.g. \(t_m = e^{2i\pi x_m/L}\) with \(0 < x < L\) for \(N\) particles in a box, \(m = 1, \ldots, N\). Then all the primary invariants in the \(x\)-direction are generated by Euler’s expression \([19]\), in other words they are all unrestricted polynomials in the elementary symmetric functions \(e_k\) \([14]\). Replacing \(t\) by \(u\) for the \(y\)-direction, and so on, the independent primary invariants are just all the monomials generated by multiplying together \(d\) copies of Eq. \([6]\), one for each direction in space. The functions \(\Phi_i\) above are arbitrary polynomials in these monomials, with complex coefficients. [It is most convenient, although not necessary, to interpret powers of the \(e_k\) in these monomials without cross terms, e.g. \(e_1^2(t_1, t_2) \to t_1^2 + t_2^2\).]

In this context the \(e_k\) are called Euler bosons. They are the same for bosons and for fermions. Thus the shapes \(\Psi_i\) alone encode both the space dimension and the distinction between bosons and fermions. Euler bosons have no zero-point energy, because it is contained in the shapes, which play the role of vacua to Euler-boson excitations.

The insights above, based on the Hilbert series \([13]\), are restrictive enough to obtain the wave functions of the shapes explicitly \([18]\). The construction is recursive and exhaustive. For each grade, one first constructs all states based on shapes of lower grade, using the formula \([17]\) with all possible \(\Phi_i \neq 1\). The shapes are then obtained as the orthogonal complement in the Hilbert space of that grade, which is independently generated by Slater determinants \([28]\) in the standard way. This algorithm makes it immediately obvious that the dimension of the Hilbert-space algebra is indeed \(N!^{d-1}\), i.e. the number of shapes cannot be further reduced. Namely, no shape at a given grade can be expressed in the form \([17]\) with \(\Phi_i \neq 1\), because all the states which can be so expressed are constructed explicitly before taking their orthogonal complement. Of course, the orthogonal-complement procedure defines the shapes of a given grade only up to linear basis transformations among themselves. That freedom is trivial theoretically, but may be important in applications.

Unfortunately the above general algorithm is quite inefficient in practice, because it requires the computation of the complete Hilbert spaces of a given grade, which are much larger than the number of shapes. There is a much more efficient algorithm, which is however only applicable to fermions in odd dimensions \([18]\).

### IV. DISCUSSION

The developments reviewed above are quite recent, so that the present discussion is necessarily more prospective than retrospective. There seems to be more work than any one person or group can do to explore all possible ramifications of the shape paradigm. Here only three which come to mind immediately are briefly mentioned.
A. Slater determinants in finite systems

While Slater determinants still appear as an auxiliary tool in the algorithm which constructs shapes, one feels that they have become redundant in physical descriptions, at least of finite systems. There is a mathematical way to express this feeling. Specialize to one dimension, where the only shape is the ground-state Slater determinant $\Psi_0$. One may ask, what is $\Phi$ in the expression $\Psi = \Phi \Psi_0$, if $\Psi$ is an excited-state Slater determinant? We have seen above that the most convenient way to write $\Phi$ is in terms of Euler bosons, but then $\Psi$ is not a Slater determinant, in general. If it is, then the ratio $\Psi/\Psi_0$ is called a Schur function, which is the generating function of non-standard Young tableaux. The physical meaning of such an object is quite obscure, and so is, by extension, the physical meaning of a generic Slater determinant. By contrast, the elementary symmetric functions (Euler bosons) have simple physical connotations in general. Thus $e_1$ in Eq. (1) is a sum of one-body wave functions, which is physically a liquid, while $e_N$ is their product, physically a gas.

While the lowest-graded shapes are always just the Slater determinants of the (possibly degenerate) ground state, for $d > 1$ shapes are generally superpositions of Slater determinants with roughly equal amplitudes. With complexity increasing by grade, they are the natural choices for strongly correlated trial wave functions. Conversely, if the DFT approach gives realistic one-body wave functions, the shape paradigm reduces to the Slater-determinant one, at least for the ground state. Even in that case, shapes may increase the scope of calculations of excited states and related radiation transitions, which are an independent indicator of how realistic the wave function is.

B. Bands in spectra

A spectrum is organized into bands when states of the same band are easily connected by excitations, while states of different bands are not, i.e. they behave as if they were of qualitatively different kinds. The lowest state in each band is called a bandhead. There is a natural physical picture behind this scheme: bandheads correspond to different configurations of particles in laboratory space. Some of these may be easy to excite by vibration, others by rotation, while it is difficult to change a configuration from one prone to vibration to another, prone to rotation.

The abstract structure of ideals of many-body Hilbert space, described in Eq. (10), matches the above physical pattern. The band may be understood mathematically as the ideal generated by the bandhead. The ideal is closed under wave-function superposition, and excitations within it can be described by multiplying the bandhead with Euler bosons. Physically, this multiplication corresponds to bosonic excitations of the bandhead. In this way one can distinguish theoretically between excitations within a band, which are bosons, and excitations from one band to another, which involve reconfigurations of the bandhead. The latter cannot be obtained multiplicatively, because shapes are like prime numbers, $\Psi \neq \Phi \Psi'$ for any two distinct shapes $\Psi$ and $\Psi'$: one is not divisible by the other.

In order for such a mathematical interpretation to have physical meaning, the interaction matrix elements between the shapes should be small. This proposition has been checked in small numerical examples in $d = 2$ and $d = 3$ with the Coulomb interaction $V_C$, for a harmonic oscillator potential (spin-polarized electrons in a quantum dot). It has been found that $\langle \Psi_i | V_C | \Psi_j \rangle \ll \langle S_i | V_C | S_j \rangle$, typically by about two orders of magnitude, between any two shapes $\Psi_{i,j}$ and any two Slater determinants $S_{i,j}$ of the same grade. This result is of course just a sanity check, as the opposite outcome would have doomed the interpretation immediately.

The ideal structure explains why the original idea of Bloch to represent excitations of fermionic systems as density waves was generically successful only in one dimension. Bosonisation corresponds to multiplying the ground state by a symmetric function. It can describe all excitations in one dimension, where there is only one shape, the ground-state Slater determinant, or all within one band for $d > 1$. In general, however, excitations may also involve a reconfiguration of the ground state, which is an additive correction as explained above, e.g. $\Psi \rightarrow \Psi + \Phi \Psi'$, where $\Psi$ and $\Psi'$ are “relatively prime.” Thus the difficulty in representing excitations of fermionic systems by bosons appears as just another case of the incompatibility between addition and multiplication, ubiquitous throughout mathematics, of which, say, translation and rotation are a particularly well-known example.

C. The fermion sign problem

The fermion sign problem appears in simulations of fermionic many-body systems in real space. It is most easily understood in a sum-over-histories formulation. When a transition matrix element is formed as a sum over trajectories in fermion many-body space, one has to distinguish contributions which interfere destructively for physical reasons, from those which should interfere constructively but have opposite signs because a phase convention for the many-body wave function has not been implemented consistently across many incremental updates of different trajectories.
The sign problem appears only because there is more than one shape. In one dimension, where there is only one shape $\Psi_0$, the factorization $\Psi = \Phi \Psi_0$ immediately translates the fermionic problem into a bosonic one involving the symmetric functions $\Phi$. Physically, in one dimension it is possible to fix a phase convention simply by forbidding particles to skip over each other in a simulation. If they never exchange places, the difference between bosons and fermions cannot manifest itself either, so the orbital solution is actually a symmetric function for both fermions and bosons, the difference between the two cases being in the fixed factor $\Psi_0$.

The representation (17) provides a generalization of this insight to $d > 1$. Instead of writing the wave function as in (17), one can list the coefficients $\Phi_i$ as a vector-like object,

$$(\Phi_1, \Phi_2, \ldots, \Phi_{N!d-1}).$$

When the $\Phi_i$ are symmetric polynomials, such a structure is called a free module (as distinct from a vector space, where the $\Phi_i$ would be just numbers). It carries the idea that the shapes are a basis to its natural conclusion, proposing to calculate in the space (15) of “coordinates” $\Phi_i$ instead of directly in the space (17) of wave functions $\Psi$. Calculations in the free module have no sign problem a priori, because the $\Phi_i$ are symmetric functions. It remains to be seen whether they will be practical. At least, there is a chance to manage complexity, because one can imagine truncating the list (15) to limit the calculation to one ideal, or band of excitations. Such an approach is similar in spirit to a fixed-node approximation in usual simulations.

The proposal to use the free module in order to avoid the sign problem can be placed in the more general setting of constraint elimination. In some design problems constraints can be encoded as requirements that certain polynomials $g_i$ simultaneously evaluate to zero, leading to the expression of allowed solutions in the form (9). Eliminating constraints means mapping the original space of the problem to some reduced space in which they are satisfied automatically. The whole geometric locus of zeros in the original space (kernel of this mapping) maps to a single point, zero, in the reduced space. This is the case when wave functions are mapped to the free module: $\Psi = 0$ in Eq. (17) corresponds to $(0, 0, \ldots, 0)$ in Eq. (15).

Hilbert’s Nullstellensatz (“zeroplacesclaim”) is an either/or proposition about constraint elimination: either the constraints $g_i = 0$, $i = 1, \ldots, D$, are incompatible, or every solution $f$ of the problem can be written as an algebraic root of the expression (9), $f^m = p$ with an integer $m \geq 1$. The many-body problem is an interesting variation of this general framework. Normally the simultaneous solutions of a set of polynomial equations are a discrete set of points, called an algebraic variety. Each shape vanishes according to the Pauli principle when $r_i = r_j$ with $i \neq j$ for any two particles, $i, j = 1, \ldots, N$. These points of coincidence are the simultaneous zeros of the shapes, corresponding to the algebraic variety of the problem. However, as noticed long ago in the many-body context when $d > 1$ the algebraic variety is a subset of a larger object, the nodal surface of the total wave function $\Psi$. The nodal surface is a (possibly multiply-connected) differentiable manifold defined by $\Psi = 0$, on which each individual shape need not vanish. It appears only because the Pauli principle is triggered by an equality of vector variables, a weaker condition for zeros than explicitly envisaged by Hilbert. The nodal surface is the reason for the practical difficulty in defining the wave-function phase consistently in simulations, because it is not known in advance. Thus it is of considerable interest to understand its relation to the algebraic variety. Of course, a polynomial like (9) will in general have more zeros than there are common zeros of the $g_i$. However, for $d = 1$ the extra zeros are discrete and separate from the algebraic variety. The specific feature of the problem for $d > 1$ is that the algebraic variety naturally generates a whole differential-geometric “zero object,” the nodal surface, which contains it.

The free module (15) is a structured implementation of Heisenberg’s matrix mechanics, which refines Dirac’s vector-space interpretation. Heisenberg’s algebraic approach eschews wave-function arguments — real-space coordinates — in favor of wave-function values, as encoded by the matrix elements. The textbook harmonic oscillator is a one-body realization of this program, where replacing $x \pm d/dx$ by the creation and destruction operators faithfully maps laboratory space onto wave-function space, so that one never needs to revert to the variable $x$ for concrete calculation. In close analogy, the $\Phi_i$ are polynomials in the elementary symmetric functions (1), which are themselves expressed directly in terms of the values of the one-body wave functions. Changing powers of the $\epsilon_i$ in this formalism corresponds to harmonic-oscillator ladder operations. The representation (15) of the free module thus opens the possibility of practically implementing Heisenberg’s approach in a general many-body setting. This program has a much larger scope than the motivating fermion sign problem.

V. CONCLUSIONS

The general algebraic structure of many-body Hilbert space described in this review provides a firm mathematical foundation to study the physics of finite systems in a pleasantly intuitive language, with suggestive correspondences between mathematical structures and observations. Physical vacua appear mathematically as generators of ideals in the algebra of many-body invariants, while these ideals physically correspond to bands in the excitation spectra.
Although the required mathematics far exceeds contemporary training of physics students in abstract algebra, such is remarkably not the case with students of engineering. Industrial design optimization uses engineering constraints as generators of allowed solutions in much the same way as shapes are used here. Such a large body of practical knowledge gives rise to optimism for the proposed physical applications.

At the same time, specifics of the physical many-body problem should not be overlooked. In particular, the arrangement of $Nd$ variables in $N$ columns (vectors) of $d$ rows, however natural when describing particles, does not seem to have been pursued in the mathematical literature on invariants. Monographs and textbooks typically treat all variables on an equal footing, corresponding to the many-body problem in one dimension. Due to this additional structure in the variables when $d > 1$, the shape invariants described here appear to be new to mathematics as well, although the author cannot claim so with authority.

Perhaps the most interesting insight based on the shape paradigm at present is the reinterpretation of matrix mechanics in terms of a free module rather than a vector space. It is tantalizing to speculate how far the young Heisenberg would have pursued his algebraic approach if Schrödinger’s analytic work had never appeared, or if Hilbert or Noether had been the one to search for their common ground. Hopefully the present brief review will encourage readers to explore shapes from the point of view of their own expertise.

Acknowledgements

I thank D. Svrtan for his help and interest. This work was supported by the Croatian Ministry of Science grant 119-1191488-0512 and by the University of Zagreb grant 202759.

* Electronic address: dks@phy.hr

1. W. Pauli, Zeitschrift für Physik 31, 765 (1925).
2. W. Heisenberg, Zeitschrift für Physik 38, 411 (1926).
3. P. A. M. Dirac, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 112, 661 (1926).
4. J. C. Slater, Phys. Rev. 34, 1293 (1929).
5. A. A. Abrikosov, L. P. Gorkov, and I. E. Dzaloshinskii, Methods of Quantum Field Theory in Statistical Physics (Dover, 1975).
6. G. D. Mahan, Many-Particle Physics, second edition (Plenum, New York, 1990).
7. R. B. Laughlin, Phys. Rev. B 27, 3383 (1983).
8. H. Park, A. J. Millis, and C. A. Marianetti, Phys. Rev. B 90, 235103 (2014).
9. A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
10. W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
11. D. K. Sunko, Phys. Rev. A 93, 062109 (2016).
12. L. Euler, Comm. Acad. Petrop. 13, 64 (1741–43, 1751), see p. 80, or arxiv:0711.3656 (transl. by J. Bell), p. 15.
13. G. E. Andrews, The Theory of Partitions (Addison-Wesley, New York, 1976).
14. A. C. Aitken, Determinants and Matrices (Oliver and Boyd, Edinburgh and London, 1939).
15. H. Derksen and G. Kemper, Computational Invariant Theory (Springer Berlin Heidelberg, 2002).
16. R. P. Stanley, Advances in Mathematics 28, 57 (1978).
17. Slater determinants are replaced by permanents (lose the alternating sign) for identical bosons.
18. D. K. Sunko, Journal of Superconductivity and Novel Magnetism (2016), 10.1007/s10948-016-3799-1.
19. R. P. Stanley, Enumerative Combinatorics, Vol. 2 (Cambridge University Press, Cambridge, 1999).
20. F. Bloch, Helv. Phys. Acta 5, 385 (1934).
21. S. Tomonaga, Progress of Theoretical Physics 5, 544 (1950).
22. E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B 41, 9301 (1990).
23. V. I. Iglovikov, E. Khatami, and R. T. Scalettar, Phys. Rev. B 92, 045110 (2015).
24. D. Ceperley, Journal of Statistical Physics 63, 1237 (1991).
25. V. Filinov, High Temperature 52, 615 (2014).
26. D. Bressanini, Phys. Rev. B 86, 115120 (2012).
27. Jinpeng Lv, Scalable formal verification of finite field arithmetic circuits using computer algebra techniques, Ph.D. thesis, University of Utah (2012).
28. Slater determinants are replaced by permanents (lose the alternating sign) for identical bosons.