Group theoretical approaches to many-body problems in chemistry and physics

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Abstract. Group theory finds many applications in chemistry and physics. Here we discuss specifically applications of non-compact Lie groups to problems that involve many identical particles in a harmonic oscillator potential such as in thermodynamic partition functions, modeling quantum dots etc. Powerful methods based upon the theory of symmetric functions play a key role.

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1. Introduction

The concept of symmetry is fundamental to much of chemistry and physics and group theory is the natural mathematical tool for implementing symmetry concepts. A large variety of groups are used in chemistry and physics. The 32 point groups and the 230 space groups find wide applications in crystallographic problems ranging from crystal field theory to the study of the magnetic properties of crystallographic lattices. These are examples of finite groups. Here my emphasis will be on Lie groups and more particularly on non-compact Lie groups. Whereas the finite groups are characterised by finite numbers of unitary representations the Lie groups possess infinite numbers of unitary representations. The unitary representations of the compact Lie groups are all of finite dimension whereas those of the non-compact Lie groups are all (apart from the trivial representations) of infinite dimension. This creates new possibilities for systems characterized by infinite sets of quantum states such as arise in many-body systems and indeed even in relatively simple systems like the hydrogen atom or the isotropic harmonic oscillator. Applications of non-compact Lie groups occur in a wide range of physical problems in areas such as quantum optics, quantum dots, nuclei, many-electron atoms and molecules.

Here we shall review our current knowledge of the properties of non-compact Lie groups and their present and future applications. The emphasis will be on outlining results without going into deep technical details. For those details we list some of the relevant references. In the following we first briefly discuss some of the properties of the non-compact group $U(2,2)$ and its relevance to the hydrogen atom and many-electron atoms. We then consider the non-compact groups $Mp(2n)$ and $Sp(2n,\Re)$ and their relevance to many-body sytems involving isotropic harmonic oscillator potentials. This work is then applied to consideration of thermodynamic partition functions for many bosonic and fermionic systems. Finally we remark upon the modelling of quantum dot systems.

2. The non-compact group $U(2,2)$

Bohr, in his very first paper[1], on what has become known as “The Bohr-model” of the hydrogen atom, made the surprising discovery that the energy levels could be succinctly expressed (in appropriate units) as

$$E_n = -\frac{1}{n^2} \qquad \text{with} \quad n = 1, 2, \ldots$$

It was not apparent in such a simple equation was hidden the remarkable $2(n)^2$ degeneracy of each energy level. The factor of 2 came from the subsequent discovery of electron spin and the factor of (n) from Pauli’s observation[2] that in a purely Coulombic central field there was the additional constant of the motion associated with the Runge-Lenz vector and from that the realization that the observed degeneracies were precisely the dimensions of certain of the irreducible representations of the *compact*

Lie group $SO(4) \sim SU(2) \times SU(2)$, in particular those commonly designated as $[n-1,0] \sim \{n-1\} \times \{n-1\}$.

Much later, Barut and Kleinert[3] observed that all the states of the discrete levels of a H-atom spanned a single infinite-dimensional irreducible representation (which we will designate as $H_0 = \{1(\bar{0};0)\}$) of the *non-compact* Lie group $SO(4,2) \sim SU(2,2)$ with the group being referred to as the *dynamical group* of the H-atom[3,4]. The Runge-Lenz vector ceases to be a constant of the motion for two or more electrons in a central Coulomb field[4,5] and $SO(4)$ symmetry is broken. Nevertheless, it can be useful to consider the $n-$electron states starting with the single irreducible representation H_0 of $SU(2,2)$, or more simply $U(2,2)$, and then forming symmetrized $n-$fold tensor products. This is a far from trivial problem but some significant progress has been made[6] which I now sketch. Much of the background information can be found in the references[7–9]. Whereas for compact Lie groups the irreducible representations are all of finite dimension and hence all Kronecker products and symmetrized powers involve a finite number of irreducible representations, for non-compact Lie groups the non-trivial irreducible representations are all of infinite dimension and consequently Kronecker products and symmetrized powers involve infinite numbers of infinite dimensional irreducible representations.

A considerable amount is known about computing Kronecker products and symmetrized powers (or plethysms[10,11]) for compact Lie groups[7] drawing heavily upon the theory of symmetric functions[12,13]. Compact expressions in terms of series of Schur symmetric functions ($S-$functions) exist which are readily amenable to computer evaluation. Corresponding expressions can be developed for the unitary irreducible representations of relevant non-compact Lie groups using knowledge of their maximal compact Lie subgroups[8,9,14–17]. As a result it has been possible to give a complete result for the set of $U(2,2)$ irreducible representations contained in the symmetric and antisymmetric parts of the Kronecker square of the fundamental irreducible representation H_0. The symmetric part describes the spin ($S = 0$) singlets while the antisymmetric part describes the spin ($S = 1$) triplets. The groundstate $1s^2(^1S)$ is the first level of an infinite tower of states associated with the $\{2(\bar{0};0)\}$ irreducible representation while the lowest ^3SP level is the first level of an infinite tower associated with the $\{2(\bar{1};1)\}$ irreducible representation. A complete account of the two-electron hydrogen-like states remains to be considered but knowing the relevant $U(2,2)$ irreducible representations is a significant first step.

3. Symplectic models of $n-$particle systems

Symplectic models of many-particle systems have had extensive applications in nuclear physics[18,19]. Less well known are applications to mesoscopic systems such as quantum dots[20–22] and to diatomic molecules[23]. Here we also consider applications of symplectic models to thermodynamic partition functions associated with harmonic oscillators involving identical fermions or bosons.

The symplectic group $Sp(6, \Re)$ is well known as the dynamical group for a single particle in an isotropic three-dimensional harmonic oscillator potential[4]. For $N-$non-interacting particles in d dimensions the dynamical group is the non-compact metaplectic group $Mp(2Nd)$. this group has a rich subgroup structure with various compact and non-compact subgroups[22]. Here I want to keep things relatively simple, starting with a single fermion or boson in a isotropic d-dimensional harmonic oscillator to establish a basis and then discuss the case of various approaches to the problem of N identical noninteracting bosons or fermions. We will assume that the spin of the single particle is s_b (or s_f) for the boson (or the fermion).

4. Single-particle states for a isotropic d-dimensional harmonic oscillator

We introduce three schemes for describing a single particle (fermion or boson) in a isotropic d-dimensional harmonic oscillator.

4.1. A non-compact scheme

The infinite set of spatial states span the basic infinite dimensional unitary harmonic series irreducible representation $\tilde{\Delta}$ and we may classify the states under the scheme

$$SU(2) \times (Mp(2d) \supset Sp(2d, \Re) \supset U(d) \supset O(d) \supset \ldots U(1)) \tag{1}$$

Note that we have a direct product with $SU(2)$ being the group describing the spin part of our wavefunction and the $Mp(2d)$ group and its subgroups the spatial part. Under $Mp(2d) \supset Sp(2d, \Re)$

$$\tilde{\Delta} \rightarrow \Delta_+ + \Delta_- \tag{2}$$

while under $Sp(2d, \Re) \supset U(d)$

$$\Delta_+ \rightarrow M_+ \tag{3a}$$

$$\Delta_- \rightarrow M_- \tag{3b}$$

with

$$M_+ = \sum_{m=0}^{\infty} \{2m\} \tag{4a}$$

$$M_- = \sum_{m=0}^{\infty} \{2m+1\} \tag{4b}$$

$$M \;= M_+ + M_- = \sum_{m=0}^{\infty} \{m\} \tag{4c}$$

Under $U(d) \supset O(d)$ we have the general result[7,24]

$$\{\lambda\} \rightarrow [\lambda/D] \tag{5}$$

where D is the infinite $S-$function series

$$D = \sum_{\delta}^{\infty} \{\delta\} \tag{6}$$

and the summation is over all partitions (δ) whose parts are all *even*.

4.2. The $SU(2) \times U(d)$ scheme

In this scheme the spin s belongs to the group $SU(2)$ and spans the $SU(2)$ irreducible representation $\{2s\}$ while the spatial parts span the infinite set of irreducible representations of $U(d)$ labelled by one-part partitions $\{m\}$ so we can symbolically designate the $SU(2) \times U(d)$ single particle states by

$$\{2s\} \times M = \sum_{m=0}^{\infty} \{2s\} \times \{m\} \tag{7}$$

the distinction between bosons and fermions being made at the $SU(2)$ level. The *even* parity states are associated with the *even* values of m and the *odd* parity states with the *odd* values of m.

4.3. The $U(1) \times U(d)$ scheme

In this scheme we work at the spin projection level where the different m_s states span one-dimensional irreducible representations of the Abelian group $U(1)$ which we will choose to label as $\{m_s\}$ and remember that for $U(1)$ the Kronecker products are such that

$$\{p\} \times \{q\} = \{p+q\} \tag{8a}$$

while for symmetrized powers (or plethysms)

$$\{p\} \otimes \{\lambda\} = \begin{cases} 0 & \text{if } \ell(\lambda) > 1 \\ p \times \lambda_1 & \text{if } \ell(\lambda) = 1 \end{cases} \tag{8b}$$

the complete set of single particle states will span the reducible representation

$$\sum_{m_s=-s}^{m_s=s} \{m_s\} \times M \tag{9}$$

5. $N-$noninteracting particles in a isotropic d-dimensional harmonic oscillator

The distinction between bosons and fermions becomes crucial when we consider more than one particle. Throughout we shall assume that the N particles are indistinguishable. The basic ansatz is that for bosons the $N-$particle wavefunctions must be totally *symmetric* with respect to all permutations of the N particles while for fermions the $N-$particle wavefunctions must be totally *antisymmetric* with respect to all permutations of the N particles. In other words boson wavefunctions are permanental while those of fermions are determinantal. If our wavefunction is constructed as products of spin and spatial parts then the symmetrization of the spin and spatial parts need not themselves be symmetric (or antisymmetric) but their product must follow the correct statistics.

5.1. Plethysm for direct products of groups

In many applications we are involved with the direct product of two groups (more than two poses no new difficulties) say, $\mathcal{G}\times\mathcal{G}'$ with irreducible representations $A_{\mathcal{G}}\times B_{\mathcal{G}'}$ and we need to determine the $\mathcal{G}\times\mathcal{G}'$ content of the $N-$fold product of an irreducible representation say $(A\times B)^{\times N}$ (henceforth we drop the subscripts) and extract the part of the product symmetrized according to the permutational symmetry $\{\lambda\}$. In terms of plethysm we have[10,11]

$$(A\times B)\otimes\{\lambda\}=\sum_{\rho}(A\otimes\{\rho\cdot\lambda\})\times(B\otimes\{\rho\}) \tag{10}$$

where $\{\rho\cdot\lambda\}$ signifies a $S-$function inner product which is null unless the partitions (ρ) and (λ) are of the same weight, i.e. $|\rho|=|\lambda|$. Two special cases are of interest

$$\{\rho\}\cdot\{\lambda\}=\begin{cases}\{\rho\} & \text{if } \{\lambda\}=\{N\} \text{ and } |\rho|=|\lambda| \\ \\ \{\rho'\} & \text{if } \{\lambda\}=\{1^N\} \text{ and } |\rho|=|\lambda|\end{cases} \tag{11}$$

where the partition (ρ') is conjugate to (ρ).

By way of example we have

$$\begin{aligned}(A\times B)\otimes\{4\} &= (A\otimes\{4\})\times(B\otimes\{4\})+(A\otimes\{31\})\times(B\otimes\{31\})\\ &+(A\otimes\{2^2\})\times(B\otimes\{2^2\})+(A\otimes\{21^2\})\times(B\otimes\{21^2\})\\ &+(A\otimes\{1^4\})\times(B\otimes\{1^4\})\end{aligned} \tag{12a}$$

$$\begin{aligned}(A\times B)\otimes\{1^4\} &= (A\otimes\{4\})\times(B\otimes\{1^4\})+(A\otimes\{31\})\times(B\otimes\{21^2\})\\ &+(A\otimes\{2^2\})\times(B\otimes\{2^2\})+(A\otimes\{21^2\})\times(B\otimes\{31\})\\ &+(A\otimes\{1^4\})\times(B\otimes\{4\})\end{aligned} \tag{12b}$$

In many cases of interest only some of the terms in the right-hand-side of (12) will be non-null. This is particularly the case when one of the groups is of low rank, e.g, $SU(2)$ or $U(1)$. To be specific, let us henceforth consider bosons of spin $s_b=1$ and fermions of spin $s_f=\frac{1}{2}$. In this case the boson spin spans the $\{2\}$ irreducible representation of $SU(2)$ while the fermion spin spans the $\{1\}$ irreducible representation of $SU(2)$. There is no difficulty in going to higher spin states.

5.2. The $SU(2)\times Mp(2d)$ scheme

In this scheme the single particle spans the representation $\{2s\}\times\tilde{\Delta}$ of $SU(2)\times Mp(2d)$ and for $N-$noninteracting particles we have

$$(\{2\}\times\tilde{\Delta})\otimes\{N\} \; = \sum_{\rho\vdash N}(\{2\}\otimes\{\rho\})\times(\tilde{\Delta}\otimes\{\rho\}) \quad \text{for bosons} \tag{13a}$$

$$(\{1\}\times\tilde{\Delta})\otimes\{1^N\} = \sum_{\rho\vdash N}(\{1\}\otimes\{\rho'\})\times(\tilde{\Delta}\otimes\{\rho\}) \quad \text{for fermions} \tag{13b}$$

Let us consider the evaluation of the $SU(2)$ plethysms, first for fermions and then for bosons.

We have noted earlier that for fermions of spin $s_f = \frac{1}{2}$ that $\{1\}\otimes\{\rho\} = \{\rho\}$ and that the partition (ρ) can involve at most two parts and in $SU(2)$ we have the irreducible representation equivalence

$$\{\rho_1,\rho_2\}\equiv\{\rho_1-\rho_2\} \tag{14}$$

leading to

$$(\{1\}\times\tilde{\Delta})\otimes\{1^N\} = \sum_{S=S_{min}}^{\frac{N}{2}} {}^{2S+1}(\tilde{\Delta}\otimes\{2^{\frac{N}{2}-S}1^{2S}\}) \tag{15}$$

$$S_{min} = \begin{cases} \frac{1}{2} & \text{if } N \text{ is odd} \\ \\ 0 & \text{if } N \text{ is even} \end{cases} \tag{16}$$

Thus for $N=4$ fermions we have

$$(\{1\}\times\tilde{\Delta})\otimes\{1^4\} ={}^5(\tilde{\Delta}\otimes\{1^4\}) +{}^3(\tilde{\Delta}\otimes\{21^2\}) +{}^1(\tilde{\Delta}\otimes\{2^2\}) \tag{17}$$

Recalling the isomorphisms between $SO(3)$ and its covering group $SU(2)$ we have under $SU(2)\sim SO(3)$ $\{2\}\sim[1]$ leading to

$$\{2\}\otimes\{\rho\}\sim[\rho/D] \tag{18}$$

The right-hand-side of (18) gives the spins for each partition (ρ) appearing in (13a). Furthermore, (ρ) can involve at most three non-zero parts and those involving three non-zero parts are equivalent to a partition with two or less parts via

$$\{\rho_1,\rho_2,\rho_3\}\equiv\{\rho_1-\rho_3,\rho_2-\rho_3\} \tag{19}$$

NB If $[\rho/D]$ leads to partitions involving more than one non-zero part then the $SO(3)$ modification rules need to be applied. Assuming (19) has been applied leaving a $SO(3)$ non-standard irreducible representation $[a,b]$ then

$$[a,b]\equiv\begin{cases} 0 & \text{if } b\geq 2 \\ \\ [a] & \text{if } b=1 \end{cases} \tag{20}$$

with the above in mind we can use (13a) to give for four spin 1 bosons

$$(\{2\}\times\tilde{\Delta})\otimes\{4\} =^{(9+5+1)} (\tilde{\Delta}\otimes\{4\}) +^{(7+5+3)} (\tilde{\Delta}\otimes\{31\}) \\ +^{(3)} (\tilde{\Delta}\otimes\{21^2\}) +^{(5+1)} (\tilde{\Delta}\otimes\{2^2\}) \tag{21}$$

Where again the multiplicities $(2S+1)$ are given as left superscripts. To complete the examples of this scheme one should evaluate the various plethysms for the relevant metapletic group and then branch through the various subgroups. We shall not do that at this time.

5.3. The $SU(2)\times U(d)$ scheme

In this scheme one starts with (7) and evaluates the relevant plethysms as in the previous scheme. For the spin part there are no changes. The $U(d)$ irreducible representations are combined as the single infinite dimensional reducible representation M. Thus for N spin $\frac{1}{2}$ fermions we have from noting (15)

$$(\{1\}\times M)\otimes\{1^N\} = \sum_{S=S_{min}}^{\frac{N}{2}} {}^{2S+1}(M\otimes\{2^{\frac{N}{2}-S}1^{2S}\}) \tag{22}$$

and for four fermions

$$(\{1\}\times M)\otimes\{1^4\} =^5 (M\otimes\{1^4\}) +^3 (M\otimes\{21^2\}) +^1 (M\otimes\{2^2\}) \tag{23}$$

For N bosons of spin 1 the result comes from (21) by simply replacing $\tilde{\Delta}$ by M throughout.

5.4. The $U(1)\times U(d)$ scheme

In this scheme we treat spin at the level of its projection m_s. Clearly in each scheme there must be a complete accounting of all the quantum states and respecting symmetrization. In the case of fermions of spin $\frac{1}{2}$ we have for N particles

$$\big((\{\tfrac{1}{2}\}\times M)+(\{-\tfrac{1}{2}\}\times M)\big)\otimes\{1^N\} \\ = \sum_{x=0}^{N}\big((\{\tfrac{1}{2}\}\times M)\otimes\{1^{N-x}\}\big)\times\big((\{-\tfrac{1}{2}\}\times M)\otimes\{1^x\}\big) \tag{24}$$

Noting (8a) and (8b), we can rewrite (24) as

$$\big((\{\tfrac{1}{2}\}\times M)+(\{-\tfrac{1}{2}\}\times M)\big)\otimes\{1^N\} \\ = \sum_{x=0}^{N}\big(\{\tfrac{N-x}{2}\}\times(M\otimes\{1^{N-x}\})\big)\times\big(\{-\tfrac{x}{2}\}\times(M\otimes\{1^x\})\big) \tag{25}$$

Notice that (25) involves the product of two terms, the first term, $\big(\{\frac{N-x}{2}\}\times(M\otimes\{1^{N-x}\})\big)$, involves states with spin projection $M_S = \frac{N-x}{2}$ (spin-up) which are antisymmetric in their spatial part while the second term,

$\left(\{-\frac{x}{2}\} \times (M \otimes \{1^x\})\right)$,involves states with spin projection $M_S = -\frac{x}{2}$ (spin-down) which are again antisymmetric in their spatial part. Equation (25) involves Kronecker products in $U(1)$ and in $U(d)$ and (25) may be rearranged as

$$\begin{aligned}
&\left((\{\tfrac{1}{2}\} \times M) + (\{-\tfrac{1}{2}\} \times M)\right) \otimes \{1^N\} \\
&= \sum_{x=0}^{N} \left(\{\tfrac{N-x}{2}\} \times \{-\tfrac{x}{2}\}\right) \times \left((M \otimes \{1^{N-x}\}) \times (M \otimes \{1^x\})\right)
\end{aligned} \tag{26}$$

The first Kronecker product can be evaluated using (8a) to give

$$\left(\{\tfrac{N-x}{2}\} \times \{-\tfrac{x}{2}\}\right) = \{\tfrac{N}{2} - x\} \tag{27}$$

and the second using the plethysm property

$$(A \otimes \{\lambda\}) \times (A \otimes \{\mu\}) = A \otimes (\{\lambda\} \times \{\mu\}) \tag{28}$$

leading to

$$\left((M \otimes \{1^{N-x}\}) \times (M \otimes \{1^x\})\right) = M \otimes (\{1^{N-x}\} \cdot \{1^x\}) \tag{29}$$

with the $\cdot$ implying ordinary $S-$function multiplication. Combining (27) and (29) in (26) finally gives

$$\left((\{\tfrac{1}{2}\} \times M) + (\{-\tfrac{1}{2}\} \times M)\right) \otimes \{1^N\} = \sum_{x=0}^{N} \{\tfrac{N}{2} - x\} \times \left(M \otimes (\{1^{N-x}\} \cdot \{1^x\})\right) \tag{30}$$

For four fermions of spin $\frac{1}{2}$ we obtain

$$\begin{aligned}
&\left((\{\tfrac{1}{2}\} \times M) + (\{-\tfrac{1}{2}\} \times M)\right) \otimes \{1^4\} \\
&= \{2\} \times (M \otimes (\{1^4\} \cdot \{0\})) + \{1\} \times (M \otimes (\{1^3\} \cdot \{1\})) \\
&+ \{0\} \times (M \otimes (\{1^2\} \cdot \{1^2\})) + \{-1\} \times (M \otimes (\{1\} \cdot \{1^3\})) \\
&+ \{-2\} \times (M \otimes (\{0\} \cdot \{1^4\})) && \text{(31a)} \\
&= (\{2\} + \{-2\}) \times (M \otimes \{1^4\}) + (\{1\} + \{-1\}) \times (M \otimes (\{1^3\} \cdot \{1\})) \\
&+ \{0\} \times (M \otimes (\{1^2\} \cdot \{1^2\})) && \text{(31b)} \\
&= (\{2\} + \{-2\}) \times (M \otimes \{1^4\}) + (\{1\} + \{-1\}) \times (M \otimes (\{1^4\} + \{21^2\})) \\
&+ \{0\} \times (M \otimes (\{1^4\} + \{21^2\} + \{2^2\})) && \text{(31c)}
\end{aligned}$$

Comparison with (17) and (23) shows, as should be, that the same number of quantum states are obtained in each scheme. We note that the above scheme was first used by Shudeman[25] to determine the states arising from configurations of equivalent electrons ℓ^N though without using group theory. It was then used by Judd[26] to recast atomic shell theory, Judd giving a group formulation to the scheme and naming it $LL-$coupling. I have given further details[27].

Let us return to the spin 1 bosons. Each boson has three spin states ($M_S = 0, \pm 1$) that can be described by the $U(1)$ irreducible representations $\{1\}$, $\{0\}$, $\{-1\}$. For $N-$noninteracting bosons we have from plethysm

$$(\{1\} \times M + \{0\} \times M + \{-1\} \times M) \otimes \{N\}$$

$$= \sum_{x=0}^{N} \sum_{y=0}^{x} [((\{1\} \times M) \otimes \{N-x\}) \times ((\{0\} \times M) \otimes \{x-y\}) \times ((\{-1\} \times M) \otimes \{y\})] \tag{32a}$$

$$= \sum_{x=0}^{N} \sum_{y=0}^{x} [(\{N-x\} \times (M \otimes \{N-x\})) \times (\{0\} \times (M \otimes \{x-y\})) \times (\{-y\} \times (M \otimes \{y\}))] \tag{32b}$$

$$= \sum_{x=0}^{N} \sum_{y=0}^{x} [\{N-x-y\} \times (M \otimes (\{N-x\} \cdot \{x-y\} \cdot \{y\})] \tag{32c}$$

where in (32c) the spin projection quantum number, M_S is

$$M_S = N - x - y \tag{33}$$

For brevity, let us define

$$M_S^{\uparrow\downarrow}(S) = \begin{cases} \{S\} + \{-S\} & \text{if } S > 0 \\ \{0\} & \text{if } S = 0 \end{cases} \tag{34}$$

For four spin 1 bosons we have from (32c)

$$\begin{aligned} &(\{1\} \times M + \{0\} \times M + \{-1\} \times M) \otimes \{4\} \\ &= M_S^{\uparrow\downarrow}(4)(M \otimes \{4\}) + M_S^{\uparrow\downarrow}(3)(M \otimes \{3\} \cdot \{1\}) \\ &+ M_S^{\uparrow\downarrow}(2)(M \otimes (\{3\} \cdot \{1\} + \{2\} \cdot \{2\}) \\ &+ M_S^{\uparrow\downarrow}(1)(M \otimes (\{2\} \cdot \{1\} \cdot \{1\} + \{3\} \cdot \{1\}) \\ &+ M_S^{\uparrow\downarrow}(0)(M \otimes (\{4\} + \{2\} \cdot \{2\} + \{2\} \cdot \{1\} \cdot \{1\}) \end{aligned} \tag{35a}$$

$$\begin{aligned} &= M_S^{\uparrow\downarrow}(4)(M \otimes \{4\}) + M_S^{\uparrow\downarrow}(3)(M \otimes (\{4\} + \{31\})) \\ &+ M_S^{\uparrow\downarrow}(2)(M \otimes (2\{4\} + 2\{31\} + \{2^2\})) \\ &+ M_S^{\uparrow\downarrow}(1)(M \otimes (2\{4\} + 3\{31\} + \{2^2\} + \{21^2\})) \\ &+ M_S^{\uparrow\downarrow}(0)(M \otimes (3\{4\} + 3\{31\} + 2\{2^2\} + \{21^2\})) \end{aligned} \tag{35b}$$

which is consistent with the M_S projection of the spins found in (21).

6. Applications

The proper enumeration of the states of a few-body system in some particular basis is an essential first step in making applications. For many-body systems one is eventually led to statistical problems[28].

6.1. Thermodynamic partition functions for bosons and fermions

With the development of traps that confine a finite number of ultracold atoms in essentially a harmonic potential there has been considerable interest in developing thermodynamic partition functions for a finite number N of non-interacting bosons or fermions[29−32]. The canonical partition function of statistical physics is defined as

$$\mathcal{Z}_N(\beta) = \mathcal{T}r\left(e^{-\beta\mathcal{H}}\right) \tag{36}$$

where $\beta = (k_B T)^{-1}$ and

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_i \tag{37}$$

is the Hamiltonian, the sum of N identical single particle Hamiltonians, with a spectrum of energy eigenvalues $\mathcal{E}_1, \mathcal{E}_2, \ldots$ (with possible degeneracies). For a single particle, boson or fermion,

$$\mathcal{Z}_1(\beta) = \sum_{i=1} e^{(-\beta\mathcal{E}_i)} \tag{38}$$

Introduce a set of variables, $(x) = (x_1, x_2, \ldots)$, not necessarily finite in number, with $x_i = e^{(-\beta\mathcal{E}_i)}$. Note that in terms of symmetric functions[12] $\mathcal{Z}_1(\beta) = s_1(x) = e_1(x) = h_1(x) = p_1(x)$ in such variables. For N-noninteracting particles we are interested in symmetrising N copies of the single particle function in the variables (x) which is an $N-$fold plethysm of the appropriate symmetric functions. Recall $p_1(x) \otimes p_r(x) = p_r(x) = \sum x^r = \mathcal{Z}_1(r\beta)$ (for bosons or fermions). Furthermore, $s_1(x) \otimes \{\lambda\} = \{\lambda\}(x) = p_1(x) \otimes \{\lambda\}$. But,

$$s_\lambda = \sum_\sigma z_\sigma^{-1} \chi_\sigma^\lambda p_\sigma$$

where for any partition (σ)

$$z_\sigma = \prod_{i\geq 1} i^{m_i} m_i!$$

with $m_i = m_i(\sigma)$ is the number of parts of σ equal to i. The term χ_σ^λ is a characteristic of the symmetric group $S_{|\sigma|}$. For N fermions we choose $\{\lambda\} = \{1^N\}$ while for bosons $\{\lambda\} = \{N\}$ and are immediately led to

$$\mathcal{Z}_N(\beta)^{\pm} = \sum_{|\sigma|=N} \varepsilon_\sigma^{\pm} z_\sigma^{-1} \mathcal{Z}_1(\sigma\beta) \tag{39}$$

where $\varepsilon^+ = 1,\ \varepsilon^- = (-1)^{|\sigma|-\ell(\sigma)}$ and

$$\mathcal{Z}_1(\sigma\beta) = \prod_{i=1}^{\ell(\sigma)} \mathcal{Z}_1(\sigma_i\beta) \tag{40}$$

Thus the canonical partition function for N-noninteracting bosons or fermions is completely determined by the single particle partition function. The coefficients sum to unity for bosons (+) and to zero for fermions (−). For example:-

$$\mathcal{Z}_5(\beta)^{\pm} = \frac{1}{120}\left(24\mathcal{Z}_1(5\beta) \pm 30\mathcal{Z}_1(4\beta)\mathcal{Z}_1(\beta) \pm 20\mathcal{Z}_1(3\beta)\mathcal{Z}_1(2\beta)\right.$$

$$\left. +20\mathcal{Z}_1(3\beta)\mathcal{Z}_1(\beta)^2 + 15\mathcal{Z}_1(2\beta)^2\mathcal{Z}_1(\beta) \pm 10\mathcal{Z}_1(2\beta)\mathcal{Z}_1(\beta)^3 + \mathcal{Z}_1(\beta)^5\right) \quad (41)$$

However, (41) assumes a single spin state. For fermions of spin $s = \frac{1}{2}$ (41) is the partition function appropriate to five such fermions with maximal spin projection $M_S = \frac{5}{2}$. The complete partition function $\mathcal{Z}_5^T$ covering the complete set of spin states can be constructed analogously to (31) to give

$$\begin{aligned}\mathcal{Z}_5^T &= \mathcal{Z}_5^{\uparrow}(\beta) + \mathcal{Z}_4^{\uparrow}(\beta)\mathcal{Z}_1^{\downarrow}(\beta) + \mathcal{Z}_3^{\uparrow}(\beta)\mathcal{Z}_2^{\downarrow}(\beta) \\ &+ \mathcal{Z}_2^{\uparrow}(\beta)\mathcal{Z}_3^{\downarrow}(\beta) + \mathcal{Z}_1^{\uparrow}(\beta)\mathcal{Z}_4^{\downarrow}(\beta) + \mathcal{Z}_5^{\downarrow}(\beta)\end{aligned} \quad (42)$$

where the $Z_n^{\uparrow}(\beta)$ indicates that the spin projection is $M_S = \frac{n}{2}$ and $Z_n^{\downarrow}(\beta)$ a spin projection $M_S = -\frac{n}{2}$. Analogous results can be constructed for other spin states of both fermions and bosons. We note the close correspondence with the LL−coupling of atomic physics[26].

6.2. Non-compact group modeling of quantum dots

Quantum dots form another example of identical particles in an approximate harmonic oscillator potential. Here we sketch only the basic ideas.

Experimentally the electrons of a quantum dot are contained in a parabolic potential and hence we expect a close relationship with a many-electron system subject to a harmonic oscillator potential. The interaction potential $V(r_i, r_j)$ between particles i and j moving in a two-dimensional confining potential in the $x-y$ plane is taken to saturate at small particle separations and to decrease quadratically with increasing separation. In free space we would expect the interaction between two electrons to vary as $|r_i - r_j|^{-1}$. In a quantum dot the form of $V(r_i, r_j)$ is modified by the presence of image charges. The wavefunctions of the electrons confined in the quantum dots have a small but finite extent in the z−direction perpendicular to the $x-y$ plane. This results in a smearing of the electron charges along the z−direction. As a result the interparticle repulsion tends to saturate at small distances. This suggests choosing the interaction as

$$V(r_i, r_j) = 2V_0 - \frac{1}{2}m^*\Omega^2|r_i - r_j|^2 \quad (43)$$

where m^* is the electron effective mass and V_0 and Ω are positive parameters.

Consider an N−electron quantum dot each with a charge $-e$, a g−factor g^*, spatial coordinates r_i and spin components $s_{z,i}$ along the z−axis. Suppose there is a magnetic field B along the z−axis. The spatial part of the Hamiltonian can be written as

$$H_{space} = \frac{1}{2m^*}\sum_i \left[p_i + \frac{eA_i}{c}\right]^2 + \frac{1}{2}m^*\omega_0^2\sum_i |r_i|^2 + \sum_{i<j} V(r_i, r_j) \quad (44)$$

and the spin part as

$$H_{spin} = -g^* \mu_B B \sum_i s_{z,i} \tag{45}$$

where the momentum and vector potential associated with the $i-th$ electron are given by

$$p_i = (p_{x,i}, p_{y,i}) \qquad A_i = (A_{x,i}, A_{y,i}) \tag{46}$$

and μ_B is the Bohr magneton.

The eigenstates of H will involve the product of the spatial and spin eigenstates obtained from $H_{spatial}$ and H_{spin}. The total spin projection $S_Z = \sum_i s_{z,i}$ will be a good quantum number. Choosing a circular gauge $A_i = B(-y_i/2, x_i/2, 0)$ Eqn. (44) becomes

$$\begin{aligned} H_{space} = \frac{1}{2m^*}\sum_i p_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |r_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|r_i, r_j|^2\right] \\ + \frac{\omega_c}{2}\sum_i L_{z,i} \end{aligned} \tag{47}$$

where $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$ and $\omega_c = eB/m^*c$.

The dynamical algebra of our mesoscopic $N-$electron system in d dimensions (usually $d = 1, 2$) is that of the non-compact Lie group $Sp(2Nd, \Re)$. We can construct subalgebras of $Sp(2Nd, \Re)$ by forming subsets of the defining generators that close under commutation. So that contracting on the particle or space indices we can obtain further Lie subalgebras such as

$$\begin{aligned} Sp(2Nd, \Re) &\supset Sp(2, \Re) \times O(Nd) \supset Sp(2, \Re) \times O(N) \times O(d) \\ &\supset U(1) \times O(N) \times O(d) \end{aligned} \tag{48a}$$

$$\begin{aligned} Sp(2Nd, \Re) &\supset Sp(2N, \Re) \times O(d) \supset U(N) \times O(d) \\ &\supset U(1) \times O(N) \times O(d) \end{aligned} \tag{48b}$$

$$\begin{aligned} Sp(2Nd, \Re) &\supset Sp(2d, \Re) \times U(N) \supset U(d) \times O(N) \\ &\supset U(1) \times O(N) \times O(d) \end{aligned} \tag{48c}$$

$$Sp(2Nd, \Re) \supset U(Nd) \supset U(N) \times U(d) \supset U(1) \times O(N) \times O(d) \tag{48d}$$

Note the separation of the spatial $O(d)$ and particle $O(N)$ dependencies.

The Hamiltonian (47) can eventually be written in terms of the generators of $Sp(2, \Re)$, $O(d)$ and $Sp(2N, \Re)$. Practical calculation then involves the evaluation of matrix elements of the group generators in a harmonic oscillator basis.

7. Concluding remarks

The past few years have seen substantial progress in understanding the properties of non-compact groups. Now the time is ripe for practical applications to many-body problems in chemistry and physics.

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Appendix: Degeneracy, Pascal's triangle and $N-$dimensional H-atoms and harmonic oscillators

The non-relativistic $H-$atom and the isotropic harmonic oscillator in three dimensions are well-known to all students of quantum physics. The degeneracy groups for the corresponding $N-$dimensional problems are $SO(N+1)$ for the $H-$atom and $SU(N)$ for the isotropic harmonic oscillator[4]. In the former case the degenerate orbital states span the $[n]$ irreducible representaions of $SO(N+1)$ and are of dimension

$$D_{N+1}([n]) = (N+2n-1)\frac{(N+n-2)!}{n!(N-1)!} \tag{A1}$$

while in the latter case they span the $\{n\}$ irreducible representation of $SU(N)$ and are of dimension

$$D_N(\{n\}) = \frac{(N+n-1)!}{n!(N-1)!} \tag{A2}$$

Both cases may be nicely displayed using Pascal's triangle for the harmonic oscillator and the asymmetric Pascal triangle[33] as shown in Fig. 1 and 2 below. The degeneracy groups are shown on the left diagonal and the irreducible representations along the right diagonal.

{0}

SU_1 1

{1}

SU_2 1 1

{2}

SU_3 1 2 1

{3}

SU_4 1 3 3 1

{4}

SU_5 1 4 6 4 1

{5}

SU_6 1 5 10 10 5 1

{6}

SU_7 1 6 15 20 15 6 1

{7}

SU_8 1 7 21 35 35 21 7 1

{8}

SU_9 1 8 28 56 70 56 28 8 1

Fig. 1 Pascal's triangle for the degeneracies of an isotropic $N-$dimensional harmonic oscillator

[0]

SO_2 1

[1]

SO_3 1 2

[2]

SO_4 1 3 2

[3]

SO_5 1 4 5 2

[4]

SO_6 1 5 9 7 2

[5]

SO_7 1 6 14 16 9 2

[6]

SO_8 1 7 20 30 25 11 2

[7]

SO_9 1 8 27 50 55 36 13 2

[8]

SO_{10} 1 9 35 77 105 91 49 15 2

Fig. 2 The Asymmetric Pascal's triangle for the degeneracies of an $N-$dimensional hydrogen atom

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